Learning from Aggregate Observations

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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 probabilistic framework that is applicable to a variety of aggregate observations, e.g., pairwise similarity for classification and mean/difference/rank observation for regression. We propose a simple yet effective method based on the maximum likelihood principle, which can be simply implemented for various differentiable models such as deep neural networks and gradient boosting machines. Experiments on three novel 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 [Jordan and Mitchell, 2015]. However, in many real-world problems, it is either impossible to observe individual labels directly or prohibited to release individual information to the public, while we can obtain some forms of supervision for sets of instances. This issue arises in many scenarios:

1. Individual annotations are intrinsically unavailable. E.g., in the drug activity prediction problem [Dietterich et al., 1997], we want to predict a binary value indicating if a molecule binds to a target binding site, but we can only observe the existence/maximum/average of the drug activity of alternative conformations (possible shapes) of a molecule.

2. Individual information cannot be released to the public due to privacy concerns [Horvitz and Mulligan, 2015]. Making some forms of data public, such as opinion polls, census, medical and public health data, may pose potential threats to privacy-sensitive information. One way to anonymize data is to use differential privacy techniques and inject noise into the data [Dwork et al., 2014]; another possible way is to only release some summary statistics of small groups to the public so that individual information can be protected.

3. Exact and accurate labels are expensive [Zhou, 2017]. In some applications, it is time-consuming or infeasible to collect a large amount of precisely labeled data. E.g., it is laborious and costly to annotate images or segment videos, because images may contain multiple objects and videos may contain multiple events [Wu et al., 2015, Lai et al., 2014].
The simplest way to use such data is to use the features only and totally ignore the labels, i.e., *unsupervised learning*. However, a large amount of information is discarded and not exploited, although it can be highly useful. Alternatively, we can also settle for *set-level prediction* by treating a set of instances as a whole and applying usual supervised learning methods. In this way, almost all supervised learning algorithms can find their set-level counterparts, although they may suffer from combinatorial explosion due to the exponential growth of the number of possible sets. Nevertheless, such set-level prediction methods are not applicable if the goal is to conduct instance-level prediction. Therefore, the purpose of this paper is to develop a method that has high flexibility in terms of both the kinds of aggregate information and the choice of models.

**Related work.** A few aggregate observation problems have been considered in the literature. A notable example is *multiple instance learning* (MIL) [Zhou, 2004], where training instances are arranged in sets and supervision is provided for entire sets. MIL has found applications in drug activity prediction [Dietterich et al., 1997], computer-aided diagnosis [Kandemir and Hamprecht, 2015], and many other areas [Yang, 2005, Carbonneau et al., 2018]. However, most earlier studies as well as recent work focus on binary classification and the type of aggregation is limited. The standard MIL only considers the existence of positive instances in a set as the type of aggregate observation. *Learning from label proportions* (LLP) [Kück and de Freitas, 2005, Quadrianto et al., 2009, Yu et al., 2013, Patrini et al., 2014] is another example of aggregate observation problems, where the proportion of positive instances in each set is observed. The label proportion used in LLP is more informative than the existence used in MIL, while the anonymity of data is still preserved. Nevertheless, the majority of prior research is limited to binary classification. Recently, *learning from pairwise similarities* [Bao et al., 2018, Hsu et al., 2019] for classification has been studied, where we can obtain a binary value indicating whether two instances belong to the same category or not. Hsu et al. [2019] demonstrated the possibility of using pairwise comparison data for multiclass classification.

In contrast to classification, regression from aggregate observations has been assessed to only a limited extent. An example is *multiple instance regression* [Ray and Page, 2001, Amar et al., 2001], 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 work is *uncoupled regression from pairwise comparison* [Xu et al., 2019], where it is required to have uncoupled data in addition to pairwise comparison data. Our work extends existing work to a variety of aggregate observations such as the mean, the difference, and the rank of multiple real-valued targets.

From the method perspective, the maximum likelihood method has been explored for instance-level weak supervisions such as classification from noisy labels, complementary labels, and coarse-grained labels [Patrini et al., 2017, Yu et al., 2018, Zhang et al., 2019]. In learning from aggregate observations, we are only aware of the work by Hsu et al. [2019], which is a special case of our framework when we consider classification from pairwise similarity observations.

**Our contributions.** We formulate the problem of *learning from aggregate observations*, where supervision signals are given to sets of instances, while the goal is still to predict labels of unseen individuals (Section 2). We propose a simple yet effective solution to this class of problems (Section 3). We also provide several examples of not only classification but also regression tasks that can be solved by the proposed method (Section 4). We develop the concept of *consistency up to an equivalence relation* to analyze the characteristics of our estimator (Section 5). Finally, we show
Figure 1: Graphical representation of the data generating process. Here, $X$ 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 $g : Z^K \to Y$, 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 observations of $(X_{1:K}, Y)$-pairs so that we can predict the true target $Z$ from a single feature vector $X$.

Table 1: Examples of Learning from Aggregate Observations

| Task                  | Learning from . . . | Aggregate Observation $Y = g(Z_{1:K})$ |
|-----------------------|---------------------|----------------------------------------|
| Classification (Section 4.1) | similarity/dissimilarity | if $Z_i$ and $Z_j$ are the same or not |
|                       | triplet comparisons  | if $d(Z_a, Z_p)$ is smaller than $d(Z_a, Z_n)$, where $d(\cdot, \cdot)$ is some kind of “distance” between classes |
| Regression (Section 4.2) | mean/sum            | the arithmetic mean or the sum of $Z_{1:K}$ |
|                       | difference/rank      | the difference $Z_i - Z_j$, or the relative order $Z_i > Z_j$ |
| Ranking (Section 4.3)  | rank                | (pairwise) if $Z_i = Z_j$ |
|                       |                     | (listwise) if $Z_1 > Z_2 > \cdots > Z_K$ |

the effectiveness of the proposed method through experiments on three novel problem settings — classification via triplet comparison (Section 6.1), regression via mean observation, and regression via rank observation (Section 6.2).

2 Problem

In this section, we clarify the notation and assumptions, and provide a taxonomy of the problem of learning from aggregate observations.

2.1 Notation

Let $X \in \mathcal{X}$ be the feature vector, and $Z \in \mathcal{Z}$ be the true target (direct observation) 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 $Z$ as long as we can model the conditional probability $p(Z|X)$. If $Z$ is a finite set, e.g., $\{1, \ldots, N\}$,
the task is $N$-class classification; and if $Z$ 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 several instances. Concretely, let $Y \in \mathcal{Y}$ be an aggregate observation of a set of $Z$ of cardinality $K$, $Z_{1:K}$, which can be determined via an aggregate function $g : \mathcal{Z}^K \mapsto \mathcal{Y}$, i.e., $Y = g(Z_{1:K})$. Figure 1 illustrates the graphical representation of the data generating process.

In this work, uppercase letters $X, Y, Z$ are random variables, lowercase letters $x, y, z$ are instances of random variables, and calligraphic letters $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$ are their support spaces. The subscript such as $Z_{1:K}$ is an abbreviation for the set $\{Z_1, Z_2, \ldots, Z_K\}$. 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.

2.2 Assumptions

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

**Assumption 1** (aggregate observation assumption).

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

(1)

This means that $Y$ and $X_{1:K}$ are conditionally independent given $Z_{1:K}$. This assumption is common in existing studies [Carbonneau et al., 2018, Hsu et al., 2019, Xu et al., 2019, Cui et al., 2019]. It can be implied in the data collection process, e.g., when we first collect $(X, Z)$-pairs but only some summary statistics of $Z_{1:K}$ can be used 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 via the aggregate function $g$ by $Y = g(Z_{1:K})$, the conditional probability becomes $p(Y|Z_{1:K}) = \delta_{g(Z_{1:K})}(Y)$, where $\delta(\cdot)$ denotes the Dirac delta function.

**Assumption 2** (independent observations assumption).

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

(2)

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 [Carbonneau et al., 2018]. We leave the problem without the independent observations assumption to future work.

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

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

(3)

2.3 Aggregate Function

The aggregate function $g : \mathcal{Z}^K \mapsto \mathcal{Y}$ characterizes different problems within our framework. It induces an equivalence relation $\sim$ over the set $\mathcal{Z}^K$ as $z_{1:K}^{(i)} \sim z_{1:K}^{(j)} \iff g(z_{1:K}^{(i)}) = g(z_{1:K}^{(j)})$. The
coarseness of \( \sim \) influences how hard the problem is. Since \( \sim \) is usually much coarser than the equality equivalence relation on \( Z^K \), 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 5 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 Method

In this section, we describe the 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 (3), 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 \( Z_{1:K} \):

\[
p(Y|X_{1:K}) = \int_{Z^K} \delta_{g(Z_{1:K})}(Y) \prod_{i=1}^{K} p(z_i|X_i) \, dz_{1:K}
\]

\[
= \mathbb{E}_{Z_i \sim p(Z_i|X_i)} \left[ \delta_{g(Z_{1:K})}(Y) \right],
\]

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 \( \theta \). Note that we do not restrict the family of \( f \). It can be a deep neural network [LeCun et al., 2015] or a gradient boosting machine [Friedman, 2001], 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

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

To approximate \( \ell(W) \) based on i.i.d. samples of \( (X_{1:K}, Y) \)-pair of size \( n \), \( \left\{ x^{(i)}_{1:K}, y^{(i)} \right\}_{i=1}^{n} \overset{i.i.d.}{\sim} p(X_{1:K}, Y) \), the log-likelihood is defined as

\[
\ell_n(W) = \frac{1}{n} \sum_{i=1}^{n} \log p(y^{(i)}|x^{(i)}_{1:K};W),
\]

which converges to \( \ell(W) \) almost surely as \( n \rightarrow \infty \) [Van der Vaart, 2000]. Then, the maximum likelihood estimator (MLE) of \( W \) given aggregate observations is defined as

\[
\hat{W}_n = \arg \max_{W} \ell_n(W).
\]

Although MLE exists for all kinds of aggregate observations in theory, the question now is in what problems we can obtain it efficiently in practice. The likelihood can be hard to calculate because of the integral involved in Equation (4).
4 Examples

Next, we illustrate several problems in which 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.

In this section, 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.

4.1 Classification via Comparison

In classification problems, the true target is categorical: $Z \in \{1, \ldots, N\}$, where $N$ is the number of classes. We model it using a categorical distribution $Z \sim \text{Categorical}(p_{1:N})$, with probability parameters $p_i > 0$, $\sum_{i=1}^{N} p_i = 1$.

Because $|Z^K| = N^K$ is always finite in classification, the integration in Equation (4) becomes a summation and the log-likelihood is always analytically calculable.

Pairwise similarity observation 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,

$$ Y = g_{\text{sim}}(Z_i, Z_j) = [Z_i = Z_j], \quad (8a) $$

$$ p(Y = 1) = \sum_{k=1}^{N} p(Z_i = k)p(Z_j = k), \quad (8b) $$

where $[\cdot]$ denotes the Iverson bracket.\(^1\) This problem is also considered to be semi-supervised clustering in the literature [Xing et al., 2003, Basu et al., 2004, Bilenko et al., 2004, Davis et al., 2007]. Recently, Hsu et al. [2019] 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.

Triplet comparison observation is related to pairwise similarity observation, where we can obtain information of the form “$A$ (anchor) is more similar to $P$ (positive) than $N$ (negative).” Here $K = 3$. Assuming that $d : Z \times Z \mapsto \mathbb{R}$ is some kind of “distance” that captures similarities between classes, we have

$$ Y = g_{\text{tri}}(Z_a, Z_p, Z_n) = [d(Z_a, Z_p) < d(Z_a, Z_n)], \quad (9a) $$

$$ p(Y = 1) = \sum_{d(i,j) < d(i,k)} p(Z_a = i)p(Z_p = j)p(Z_n = k). \quad (9b) $$

Based on Equation (7), the loss functions for both pairwise similarity and triplet comparison are in the form of binary cross entropy

$$ L(W) = -\frac{1}{n} \sum_{i=1}^{n} [y^{(i)} = 1] \log p(y^{(i)} = 1|z_{1:K}; W) $$

$$ -\frac{1}{n} \sum_{i=1}^{n} [y^{(i)} = 0] \log p(y^{(i)} = 0|z_{1:K}; W). $$

\(^1\) Iverson bracket $[\cdot]$: for any logic expression $P$, $[P] = 1$ if $P$ is true, otherwise 0.
Although triplet comparison data has been used for metric learning and representation learning [Sohn, 2016, Schroff et al., 2015], studies on classification based on triplet comparison remain limited. Recently, Cui et al. [2019] 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. Based on our framework, we show that a multiclass classifier is learnable from triplet comparison data. We also compare the performance of learning from pairwise similarity and triplet comparison observations experimentally in Section 6.1.

Note that parameters of the model given only the pairwise similarity or the triplet comparison are not identifiable, thus corresponding MLE cannot be consistent. However, we can show that it is learnable up to a permutation of classes. Then if we can obtain a validation dataset, we can solve an assignment problem to obtain an estimation of $p(Z|X)$. This issue is addressed in Hsu et al. [2019] in a similar way. More analyses on the consistency issue are provided in Section 5.

4.2 Regression via Aggregation

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. We recapitulate this fact in Appendix A. 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. Hence, we can model several aggregate observations, e.g., the mean observation and the difference observation and obtain an analytical expression of the log-likelihood, as discussed below.

**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:

$$Y = g_{\text{mean}}(Z_{1:K}) = \frac{1}{K} \sum_{i=1}^{K} Z_i,$$

$$Y \sim \mathcal{N}\left(\frac{1}{K} \sum_{i=1}^{K} \mu_i, \frac{1}{K^2} \sum_{i=1}^{K} \sigma_i^2\right).$$

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

$$L(W) = \frac{1}{n} \sum_{i=1}^{n} \left( y^{(i)} - \frac{1}{K} \sum_{j=1}^{K} f(x_j^{(i)}; W) \right)^2.$$

In Section 6.2, we demonstrate that it is feasible to learn from mean observations using our method and achieve MSE that is comparable with learning from direct observations.

**Difference observation** is the difference of two real-valued targets $Z_1$ and $Z_2$, which is also normally distributed:

$$Y = g_{\text{diff}}(Z_1, Z_2) = Z_1 - Z_2,$$

$$Y \sim \mathcal{N}(\mu_1 - \mu_2, \sigma_1^2 + \sigma_2^2).$$
Similarly, the loss function is defined as
\[ L(W) = \frac{1}{n} \sum_{i=1}^{n} \left( y^{(i)} - \left( f(x_1^{(i)}; W) - f(x_2^{(i)}; W) \right) \right)^2. \]

**Rank observation** is highly related to the difference observation in the sense that we only know if the difference is positive or not. The likelihood can be derived from the cumulative distribution function of a Gaussian distribution
\[ Y = g_{\text{rank}}(Z_1, Z_2) = [Z_1 > Z_2], \quad (12a) \]
\[ p(Z_1 > Z_2) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{\mu_1 - \mu_2}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) \right], \quad (12b) \]
where \( \text{erf}(\cdot) \) is the error function. Even though \( \text{erf}(\cdot) \) is a special function, its value can be approximated and its gradient is analytically calculable.\(^2\) Thus the gradient-based optimization is still applicable.

Without loss of generality, we assume \( z_1^{(i)} > z_2^{(i)} \) in the dataset. The loss function derived from Equation (12) is
\[ L(W) = -\frac{1}{n} \sum_{i=1}^{n} \log \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{f(x_1^{(i)}; W) - f(x_2^{(i)}; W)}{2\sigma} \right) \right]. \]
The rank observation, or called **pairwise comparison** in the context of regression, has been studied recently in Xu et al. [2019] to solve an uncoupled regression problem. We show that it is possible to learn from rank observations only, and the prediction and the true target differ by only a constant under mild conditions, which is analyzed in Section 5 and supported by experiments in Section 6.2. Then, if we know the mean or can obtain a few direct observations, precise prediction becomes possible.

### 4.3 Ranking via Scoring

**Learning to rank** [Liu, 2011] is widely used in preference learning and information retrieval. In ranking problems, we assume that each item is related to a latent score \( Z \in \mathbb{Z} \) that is partially ordered. The most common choice for \( Z \) is the set of real numbers \( \mathbb{R} \) with the usual “greater than” (>) relation. In this way, it is closely related to regression via rank observation in Section 4.2. The difference is that the output of a regression function is compared to the ground-truth, while the value of the latent score in ranking is not important as long as the relative order is preserved.

As the focus of this paper is not on designing a novel ranking method, here we provide new insights into popular methods in learning to rank, such as RankNet [Burges et al., 2005] and ListNet [Cao et al., 2007] based on our probabilistic framework. Consequently, we point out that some ranking algorithms cannot be used naively for regression via rank observation problems, which is validated in Section 6.2.

We summarize the result in the following propositions:

**Proposition 3.** Assume that the latent score follows a Gumbel distribution, the maximum likelihood for regression via pairwise rank observation leads to the loss function of RankNet [Burges et al., 2005].

\[^2\] \( \text{erf}(x) = \frac{1}{\sqrt{\pi}} \int_{-x}^{x} e^{-t^2} \, dt, \quad \frac{d}{dx} \text{erf}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}. \)
Table 2: Classification via pairwise similarity and triplet comparison on MNIST-like datasets. 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       |
| MNIST      | 52.30        | 85.82               | 98.45              | 98.84      |
|            | (1.15)       | (24.86)             | (0.11)             | (0.10)     |
| Kuzushiji  | 40.22        | 61.30               | 89.65              | 93.45      |
|            | (0.01)       | (17.41)             | (0.19)             | (0.32)     |
| Fashion    | 50.94        | 62.86               | 88.49              | 90.59      |
|            | (3.28)       | (17.97)             | (0.28)             | (0.26)     |
|            |              |                     |                    |            |
|            |              | Tuplet              | Triplet            | Ours       |
| MNIST      | 18.42        | 22.77               | 94.94              | 99.04      |
|            | (1.08)       | (9.38)              | (3.68)             | (0.08)     |
| Kuzushiji  | 16.00        | 20.39               | 81.94              | 94.47      |
|            | (0.27)       | (2.03)              | (4.59)             | (0.21)     |
| Fashion    | 21.98        | 27.27               | 81.49              | 91.97      |
|            | (0.72)       | (12.82)             | (0.94)             | (0.24)     |

Proposition 4. ListNet [Cao et al., 2007] is equivalent to regression via listwise rank observation based on Gumbel distributed latent scores.

We defer their proofs to Appendix C. More details on the relationship between learning to rank and our framework can be found in Appendix B.

Note that Burges et al. [2005] and Cao et al. [2007] only focused on the surface form of these loss functions, but not the underlying probabilistic models. With the probabilistic interpretation of these losses, we can further analyze the asymptotic behavior of the model, when we can use these methods, and more importantly, their limitations.

An important question that naturally arises is which loss we should use. A rule of thumb is that the model hypothesis should match the data distribution. It is well-known that the Gaussian distribution is the limit distribution of the mean of random variables under mild conditions (the central limit theorem), while the normalized maximum of random variables may converge to a Gumbel distribution (the extreme value theorem, a.k.a. the Fisher-Tippett-Gnedenko theorem [De Haan and Ferreira, 2007]). Therefore, if the true target is a real value that is determined by the average of some random factors, the Gaussian distribution assumption is more reasonable; if the true target is a "score" that represents the maximum or the existence of some random factors, we should prefer the Gumbel distribution assumption. We validate this finding through experiments in Section 6.2.

5 Analyses

In this section, we show that although the estimator may not converge to the true parameter, it can still capture some important information about the true parameter.

Assume that the parameter $W$ is in a metric space $W$ with a metric $d$, and denote the true parameter by $W_0$. An estimator $\hat{W}_n$ based on $n$ sample points is said to be consistent if $\hat{W}_n \xrightarrow{p} W_0$ as $n \to \infty$, where $\xrightarrow{p}$ means convergence in probability. The MLE is consistent under mild conditions [Van der Vaart, 2000], 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 5** (equivalence). An *equivalence relation* ~ on W induced by the likelihood is defined according to

\[ W \sim W' \text{ if and only if } \ell(W) = \ell(W'). \]

The equivalence class of W is denoted by \([W]\). Let \(d(W, [W_0]) = \inf_{W' \in [W_0]} d(W, W'_0)\). Then, consistency up to an equivalence relation is defined as

**Definition 6** (consistency up to ~). An estimator \(\hat{W}_n\) is said to be consistent up to an equivalence relation ~, if \(d(\hat{W}_n, [W_0])\to 0\) as \(n \to \infty\).

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 [1949] and Van der Vaart [2000], we can confirm that the MLE given aggregate observations has the desired behavior:

**Theorem 7.** The MLE \(\hat{W}_n\) based on Equation (6) is consistent up to ~ if the following conditions hold:

1. The parameter space \(W\) is compact;
2. For every \(W \in W\), the log-likelihood \(\ell(W|X_{1:K}, y) = \log p(x_{1:K}, y; W)\) is upper-semicontinuous for almost all \((x_{1:K}, y)\);
3. For every sufficiently small ball \(U \subset W\), the function \(\ell^U(W|X_{1:K}, y) = \sup_{W \in U} \ell(W|X_{1:K}, y)\) is measurable and satisfies \(E[\ell^U(W|X_{1:K}, Y)] < \infty\);
4. \(\ell_n(\hat{W}_n) \geq \ell_n(W'_0) - \delta_n\) for some \(W'_0 \in [W_0]\), where \(\delta_n\) is a sequence of random variables such that \(\delta_n \to 0\).

Further, we study the structure of \([W_0]\) for the mean observation and the rank observation. Concretely, following Section 4.2, let the true target be \(Z_i = f(X_i; W_0) + \varepsilon_i\) for \(i = 1, \ldots, K\), where \(\varepsilon_i \sim i.i.d. \mathcal{N}(0, \sigma^2)\). Then, we obtain the following two propositions:

**Proposition 8** (regression via mean observation is consistent). For the mean observations obtained by Equation (10),

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

**Proposition 9** (regression via rank observation is consistent up to an additive constant). For the rank observations obtained by Equation (12),

\[ [W_0] = \{W \in W : \exists C \in \mathbb{R},\]

\[ f(X; W) - f(X; W_0) = C \text{ a.e.}\}. \]

We defer their proofs to Appendix C.

This provides us three ways to use aggregate observations. (1) If we do not have any other information, we can analyze the aggregate function \(g\) and find the characteristics of the solution, as in Proposition 8 and Proposition 9; (2) if a small number of direct observations are available, we can naturally combine them with aggregate observations in a “semi-weakly-supervised” fashion; (3) if we can obtain two kinds of aggregate observations, we can also combine them to maximize the performance. Note that it is easy to combine different weak supervisions and also strong supervisions within our framework because they are handled based on the same maximum likelihood principle.
6 Experiments

In this section, we present the empirical results of the proposed method. All experiment details can be found in Appendix D. Additional experiments on 20 regression datasets and 30 classification datasets are provided in Appendix E. 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 Observation

We demonstrate that a multiclass classifier is learnable using only triplet comparison data introduced in Section 4.1. We evaluate our method on three image classification datasets, namely MNIST, Fashion-MNIST, and Kuzushiji-MNIST, which consist of $28 \times 28$ grayscale images in 10 classes.

As for the distance $d$, we follow Cui et al. [2019] and simply use $d = |Z_i \neq Z_j|$ as the distance between classes. We also compared learning from pairwise similarity data, which is studied in Hsu et al. [2019]. Both pairwise similarity and triplet comparison observations are 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, we follow Hsu et al. [2019] and evaluate the performance by modified accuracy that allows any permutation of classes, which is obtained by solving a linear sum assignment problem [Kuhn, 1955].

**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 Siamese network [Koch et al., 2015] and contrastive loss [Hadsell et al., 2006] for pairwise similarity, (2+1)-tuplet loss [Sohn, 2016] and tirplet loss [Schroff et al., 2015] 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, 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 if the data is i.i.d. drawn from the distribution.

6.2 Regression via Mean/Rank Observation

We compare regression via direct/mean/rank observations introduced in Section 4.2. We present results on synthetic data for illustrative purposes and 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 [Burges et al., 2005] for regression (Equation 23) to compare different distribution hypotheses.

**Synthetic data.** In Figure 2 we showed an example where both the feature $X$ and the target $Z$ are one-dimensional. We can confirm that learning from mean observations is consistent (Proposition 8), while it is only learnable up to an additive constant from rank observations.

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3 MNIST handwritten digit database [LeCun et al., 1998]
http://yann.lecun.com/exdb/mnist/

4 Fashion-MNIST fashion product database [Xiao et al., 2017]
https://github.com/zalandoresearch/fashion-mnist

5 Kuzushiji-MNIST Kuzushiji database [Clanuwat et al., 2018]
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 |                     |                     | Supervised |
|--------------|------------------|----------------------|----------------------|------------|
|              | Baseline         | Ours                 | RankNet, Gumbel      | Ours, Gaussian |            |
|              | LR   GBM         | LR   GBM             | LR   GBM             | LR   GBM   |
| abalone      | 7.91 (0.4)       | 5.27 (0.4)           | 5.81 (0.4)           | 5.30 (0.5) |
| airfoil      | 38.57 (2.0)      | 23.59 (1.8)          | 37.15 (1.8)          | 27.95 (1.1) |
| auto-mpg     | 41.59 (5.7)      | 14.61 (3.2)          | 27.26 (4.0)          | 17.34 (2.0) |
| concrete     | 198.51 (12.8)    | 115.06 (10.1)        | 244.06 (17.1)        | 233.93 (20.0) |
| housing      | 67.40 (20.8)     | 27.54 (6.8)          | 52.51 (10.8)         | 44.40 (13.4) |
| power-plant  | 172.64 (7.1)     | 20.73 (0.8)          | 163.64 (4.8)         | 44.82 (6.1) |

(Proposition 9). As for the baseline, the prediction of mean observation baseline tends to be more smooth and the prediction of RankNet tends to be extreme. This provides evidence suggesting that some ranking algorithms cannot be used naively due to the mismatch between the underlying probabilistic model and the actual data distribution. This finding is also showed empirically in Xu et al. [2019].

Real-world dataset. We also conducted experiments on 6 UCI benchmark datasets 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 measure 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,

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

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 with 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.

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6 UCI Machine Learning Repository [Dua and Graff, 2017]

https://archive.ics.uci.edu
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.
**Acknowledgments**

We thank Zhenghang Cui, Takuya Shimada, Liyuan Xu, and Zijian Xu for helpful discussion. NC was supported by MEXT scholarship. MS was supported by JST CREST Grant Number JPMJCR18A2.

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Appendix

A Preliminary: Mean Squared Error and Gaussian Distribution

In this section, we provide preliminaries related to Section 4.2.

A.1 Mean Squared Error

It is well known that the mean squared error (MSE) loss function can be derived from the maximum likelihood estimation under an additive homoscedastic Gaussian noise model [see also Bishop, 2006, p. 140]. Concretely, let the target $Z$ be given by a deterministic function $f(X; W)$ with additive Gaussian noise $\varepsilon$ with zero mean and fixed variance:

$$Z = f(X; W) + \varepsilon,$$

where $\varepsilon \sim N(0, \sigma^2)$. (13)

Or equivalently,

$$Z \sim N(\mu, \sigma^2),$$

where $\mu = f(X; W)$. (14)

Here we assume the noise is homoscedastic so the variance of the noise $\sigma^2$ is a fixed value, i.e., the noise is independent on the values of features $X$. Thus the parameter is only the mean, $\theta = \{\mu\}$. This assumption may be inappropriate for some applications when the noise is heteroscedastic. In such case, we can let the deterministic function $f$ predict both the mean $\mu$ and the variance $\sigma^2$, i.e., $\theta = \{\mu, \sigma^2\}$.

The log-likelihood derived from Equation (14) is

$$
\log p(\{x^{(i)}, z^{(i)}\}_{i=1}^n; W) = -\frac{1}{n} \sum_{i=1}^n \left[ \frac{(z^{(i)} - f(x^{(i)}; W))^2}{2\sigma^2} \right] - \frac{1}{2} \log(2\pi\sigma^2). \tag{15}
$$

To maximize the log-likelihood w.r.t. $W$, the loss function can be defined by

$$L(W) = \frac{1}{n} \sum_{i=1}^n \left( z^{(i)} - f(x^{(i)}; W) \right)^2, \tag{16}
$$

which is the mean squared error (MSE). Denote the maximum likelihood estimator of $W$ by $\hat{W}_{ML} = \arg\min_W L(W)$.

Note that the variance $\sigma^2$ is not used in the loss function in Equation (16). To estimate the variance, we can again maximize the likelihood of Equation (15) and obtain the maximum likelihood estimation of $\sigma^2$: $\hat{\sigma^2}_{ML} = L(\hat{W}_{ML})$.

A.2 Gaussian Distribution

Gaussian distributions have desired properties, including

(A) stability: the family of Gaussian distributions is closed under affine transformations:

$$aZ + b \sim N(\alpha\mu + b, a^2\sigma^2); \tag{17}$$

$$\begin{align*}
\text{(A)} & \quad \text{stability: the family of Gaussian distributions is closed under affine transformations:} \\
& \quad aZ + b \sim N(\alpha\mu + b, a^2\sigma^2); \\
& \quad \text{where } a, b, \mu, \sigma \text{ are real numbers.}
\end{align*}$$
(B) *decomposability:* the sum of independent Gaussian random variables is still Gaussian:

\[ Z_1 + Z_2 \sim \mathcal{N}(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2). \] (18)

Based on these two properties, any linear combination of independent Gaussian random variables is still Gaussian distributed. Thus, several aggregate observations such as the mean observation and the rank observation can be easily modeled and their log-likelihood has an analytical expression, as discussed in Section 4.2.
B Additional Notes on Rank Observation

B.1 Related Tasks

Regression via rank observation problem is different from learning to rank problem in terms of the type of training data and test data. As discussed in Section 4.3, the exact value of the latent score in learning to rank is not important as long as the relative order is preserved, but the output of a regression function is compared to the ground-truth so that not only the order but also the scale need to be predicted. Another related task is ordinal regression [Gutierrez et al., 2015], where the target is usually discrete and ordered, but only the relative order between different values is important. The type of training and test data of several supervised learning tasks is listed in Table 4, and examples of the type of measurements are given in Table 5.

Table 4: The type of training and test data of supervised learning tasks

| Task                   | Training data | Test data |
|------------------------|---------------|-----------|
| Classification         | categorical   | categorical |
| Ordinal Regression     | ordinal       | ordinal   |
| Regression             | continuous    | continuous |
| Regression via Rank     | rank          | continuous |
| Learning to Rank       | continuous/rank | rank      |

Table 5: Examples of the type of measurements

| Measurement | Properties         | Operators | Example                  |
|-------------|--------------------|-----------|--------------------------|
| categorical | discrete, unordered| =, ≠      | dog, cat, bear, otter, ...|
| ordinal     | discrete, ordered  | >, <      | excellent, great, good, fair, bad |
|              | (binary)           |           | (high, low)              |
| continuous  | continuous         | +, −      | −2.71, 0, 3.14, ...      |

B.2 Pairwise Rank Observation

In Section 4.2, we discussed a probabilistic model based on the Gaussian distribution for regression via rank observation. In this part, we provide other possible probabilistic models based on distributions other than the Gaussian distribution. We can also obtain an analytical expression of the log-likelihood for these distributions. Here, \( f_Z \) and \( F_Z \) denote the probability density function (PDF)
and the cumulative distribution function (CDF) of a real-valued random variable $Z$, respectively.

**Gumbel distribution.** Gumbel distributed latent scores are used implicitly in RankNet [Burges et al., 2005] and ListNet [Cao et al., 2007], as described in Proposition 3 and Proposition 4.

Concretely, let $Z \sim \text{Gumbel}(\alpha, \beta) \in \mathbb{R}$ with location parameter $\alpha \in \mathbb{R}$ and scale parameter $\beta \in (0, \infty)$. Its PDF and CDF are defined by

$$f_Z(z) = \frac{1}{\beta} e^{-\left(\frac{z - \alpha}{\beta}\right)}, \text{ where } z' = \frac{z - \alpha}{\beta}, \quad (19a)$$

$$F_Z(z) = e^{-e^{-z'}}. \quad (19b)$$

Then, if two Gumbel distributed random variable $Z_1$ and $Z_2$ have the same scale $\beta$, we can derive that the difference of two Gumbel distributed random variables follows a logistic distribution:

$$Z_1 - Z_2 \sim \text{Logistic}(m = \alpha_1 - \alpha_2, b = \beta), \quad (20)$$

where

$$f_{Z_1 - Z_2}(d) = \frac{e^{-d'}}{\beta(1 + e^{-d'})^2}, \text{ where } d' = \frac{d - m}{b}, \quad (21a)$$

$$F_{Z_1 - Z_2}(d) = \frac{1}{1 + e^{-d'}}. \quad (21b)$$

Similarly to Equation (12), we can derive that

$$p(Z_1 > Z_2) = 1 - F_{Z_1 - Z_2}(0) = \frac{1}{1 + e^{-\frac{1}{\beta}(\alpha_1 - \alpha_2)}}. \quad (22)$$

Let $\alpha = s$ be the output of the function $f(X; W)$ and fix the scale $\beta = 1$, we can get the probability of the rank

$$p(Z_1 > Z_2) = \frac{1}{1 + e^{-(s_1 - s_2)}} = \frac{e^{s_1}}{e^{s_1} + e^{s_2}}. \quad (23)$$

The negative log-likelihood is used as the loss function of RankNet [Burges et al., 2005], as described in Proposition 3.

Note that the probability is in the form of the logistic function. The scales $\beta$ should be the same for different Gumbel random variables in order to have an analytical expression of the likelihood of the difference.

**Exponential distribution.** In addition to the interpretation of Gumbel distributed latent scores in Proposition 3 and Proposition 4, we provide another probabilistic model based on the exponential distribution that leads to the same learning objective.

Let $Z \sim \text{Exp}(\lambda) \in [0, \infty)$ with inverse scale parameter $\lambda \in (0, \infty)$, where

$$f_Z(z) = \lambda e^{-\lambda z}, \quad (24a)$$

$$F_Z(z) = 1 - e^{-\lambda z}. \quad (24b)$$
Then, we can derive that the difference of two exponential distributed random variables follows an asymmetric Laplace distribution:

\[ Z_1 - Z_2 \sim \text{AsymmetricLaplace}\left(m = 0, \lambda = \sqrt{\lambda_1 \lambda_2}, \kappa = \sqrt{\lambda_1 / \lambda_2}\right), \]  

(25)

where

\[
\begin{align*}
    f_{Z_1-Z_2}(d) &= \frac{\lambda_1 \lambda_2}{\lambda_1 + \lambda_2} \begin{cases} 
        e^{\lambda_2 d} & d < 0 \\
        e^{-\lambda_1 d} & d \geq 0
    \end{cases}, \\
    F_{Z_1-Z_2}(d) &= \begin{cases} 
        \frac{\lambda_1}{\lambda_1 + \lambda_2} e^{\lambda_2 d} & d < 0 \\
        1 - \frac{\lambda_2}{\lambda_1 + \lambda_2} e^{-\lambda_1 d} & d \geq 0
    \end{cases}.
\end{align*}
\]

(26a, 26b)

Similarly to Equation 12, we can obtain the probability of the rank

\[ p(Z_1 > Z_2) = 1 - F_{Z_1-Z_2}(0) = \frac{\lambda_2}{\lambda_1 + \lambda_2}. \]

(27)

Let \( \lambda = e^{-s} \) and let \( s \) be the output of the function \( f(X; W) \), then

\[ p(Z_1 > Z_2) = \frac{1}{1 + e^{-(s_1-s_2)}} = \frac{e^{s_1}}{e^{s_1} + e^{s_2}}. \]

(28)

Note that \(- \log(Z) \sim \text{Gumbel}(- \log \lambda, 1)\), which relates to the interpretation of Gumbel distributed latent scores.

If we use other positive function instead of \( e^{-s} \) that maps the output of function \( f(X; W) \) to the inverse scale parameter \( \lambda \), we can derive different learning objectives. The extension is left for future work.

**Cauchy distribution.** Similarly to the Gaussian distribution, any distribution in the stable distribution family has the property that the difference of two independent random variables follows the same distribution up to location and scale parameters. Among the stable distribution family, the Cauchy distribution is studied for the robust regression problem in Liu and Tao [2014], called Cauchy regression. Since the Cauchy distribution is stable, the difference is still Cauchy distributed and we can obtain an analytical expression of the log-likelihood.

Concretely, let \( Z \sim \text{Cauchy}(a, b) \in \mathbb{R} \) with location parameter \( a \in \mathbb{R} \) and scale parameter \( b \in (0, \infty) \), where

\[
\begin{align*}
    f_Z(z) &= \frac{1}{\pi b(1 + z'^2)}, \text{ where } z' = \frac{z - a}{b}, \\
    F_Z(z) &= \frac{1}{\pi} \arctan(z') + \frac{1}{2}. \tag{29a, 29b}
\end{align*}
\]

Then then the difference is again Cauchy distributed:

\[ Z_1 - Z_2 \sim \text{Cauchy}(a = a_1 - a_2, b = b_1 + b_2), \]

(30)
while the probability of the rank is

\[
p(Z_1 > Z_2) = 1 - F_{Z_1 - Z_2}(0) = \frac{1}{\pi} \arctan \left( \frac{a_1 - a_2}{b_1 + b_2} \right) + \frac{1}{2}.
\]

(31)

In conclusion, different distribution assumptions correspond to different sigmoid functions in regression via rank observation and learning to rank problems. Gumbel distributions correspond to the logistic function (the hyperbolic tangent), Gaussian distributions correspond to the error function, and Cauchy distributions correspond to the arctangent function. Figure 3 illustrates their densities.

For regression via rank observation, the distribution assumption should match the data distribution, especially when we assume that the noise is homoscedastic so the variance is a fixed value. For learning to rank, the Gumbel distribution allows for modeling the maximum of a set of scores explicitly, which is discussed as below. On the other hand, it is more flexible to model the uncertainty of scores using two-parameter Gaussian distribution or Cauchy distribution if we assume that the noise is heteroscedastic. Because of the fat tails of the Cauchy distribution, it allows for values far from the expected value so that learning could be more robust.

![Figure 3: Example of the densities of the Gumbel distribution, the Gaussian distribution and the Cauchy distribution.](image)

**B.3 Listwise Rank Observation**

In some applications, rank observations are in the form of the permutation of a list instead of pairwise comparisons, e.g., \( Z_1 > Z_2 > \cdots > Z_K \). A naive way to utilize such data is to decompose it to pairwise comparisons. However, the size of all possible pairs is \( \binom{K}{2} = \frac{K(K-1)}{2} \), which could be too large if \( K \) is large.

On the other hand, for the Gumbel random variables, we could simplify the calculation based on some properties of the Gumbel distribution, including

(A) **max-stability**: the maximum of a set of independent Gumbel random variables is still Gumbel distributed:
Let $\overline{Z} = \max\{Z_1, \ldots, Z_K\}$, then

$$Z \sim \text{Gumbel}(\overline{\alpha}, \beta), \quad \text{where} \quad \overline{\alpha} = \beta \log \sum_{i=1}^{K} \exp \frac{\alpha_i}{\beta}. \quad (32)$$

Therefore,

$$p(Z_1 > \max\{Z_{2:K}\}) = \frac{1}{1 + \sum_{i=2}^{K} e^{-(s_1-s_i)}} = \frac{e^{s_1}}{\sum_{i=1}^{K} e^{s_i}}; \quad (33)$$

(B) $p(Z_1 > \max\{Z_2, Z_3\}) = p(Z_1 > Z_2 | Z_2 > Z_3) = p(Z_1 > Z_3 | Z_3 > Z_2)$:

Proof.

$$p(Z_1 > \max\{Z_2, Z_3\}) = \frac{1}{1 + e^{-\beta}(\alpha_1 - \beta \log(e^{\alpha_2} + e^{\alpha_3}))} = \frac{e^{\alpha_1}}{e^{\alpha_1} + e^{\alpha_2} + e^{\alpha_3}}. \quad (34)$$

$$p(Z_1 > Z_2 > Z_3) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{Z_1}(z_1) f_{Z_2}(z_2) f_{Z_3}(z_3) \, dz_3 \, dz_2 \, dz_1$$

$$= \frac{e^{\alpha_1}}{e^{\alpha_1} + e^{\alpha_2} + e^{\alpha_3}} \frac{e^{\alpha_2}}{e^{\alpha_2} + e^{\alpha_3}} \frac{e^{\alpha_3}}{e^{\alpha_3}}$$

$$= p(Z_1 > \max\{Z_2, Z_3\})p(Z_2 > Z_3). \quad (35)$$

Therefore $p(Z_1 > Z_2 | Z_2 > Z_3) = \frac{p(Z_1 > Z_2 > Z_3)}{p(Z_2 > Z_3)} = p(Z_1 > \max\{Z_2, Z_3\})$.

We can prove the second equation in a similar way.

Based on these two properties, it is trivial to generalize it and prove that for Gumbel random variables following property holds:

$$p(Z_1 > Z_2 > \cdots > Z_K) = \prod_{i=1}^{K-1} p(Z_i > \max\{Z_{i+1:K}\}), \quad (36)$$

which is used in the loss function of ListNet [Cao et al., 2007], as described in Proposition 4.

However, other distributions such as the Gaussian distribution and the Cauchy distribution do not have these properties, so it is hard to extend pairwise rank observation to listwise rank observation in this way for these distributions. Note that some special cases of our framework for rank observations are studied in psychometrics and econometrics, including Bradley-Terry model (pairwise, Gumbel) [Bradley and Terry, 1952], Plackett-Luce model (listwise, Gumbel) [Plackett, 1975], and Thurstone-Mosteller model (pairwise, Gaussian) [Thurstone, 1927], which inspired algorithms such as RankNet [Burgess et al., 2005] and ListNet [Cao et al., 2007]. However, the focus is not on the underlying probabilistic model, e.g., the property shown in Equation 33 is treated as an axiom called Luce’s choice axiom (LCA) [Luce, 1959] in economics rather than the property of the Gumbel distribution. Our work clarifies the assumptions and the underlying probabilistic model and extends existing work to a variety of aggregate observations.
C Proofs

In this section, we provide missing proofs in Section 4 and Section 5.

C.1 Proof of Proposition 3 and Proposition 4

See Gumbel distribution parts in Appendix B.

C.2 Proof of Proposition 8

Proof. Given $X_{1:K}, Y = \frac{1}{K} \sum_{i=1}^{K} Z_i \sim \mathcal{N}\left( \frac{1}{K} \sum_{i=1}^{K} f(X_i; W_0), \frac{\sigma^2}{K} \right)$. Denote $\mu(X_{1:K}, W) = \frac{1}{K} \sum_{i=1}^{K} f(X_i; W)$.

We have

$$\ell(W) = \mathbb{E}[\mathbb{E}[\log p(Y|X_{1:K}; W)|X_{1:K}]] = - \frac{K}{2\sigma^2} \mathbb{E}[\mathbb{E}[(Y - \mu(X_{1:K}, W))^2|X_{1:K}]] + C,$$

where $C$ is a constant.

Noting that

$$\mathbb{E}[(Y - \mu(X_{1:K}, W))^2|X_{1:K}] = \mathbb{E}[(Y - \mu(X_{1:K}, W_0) + \mu(X_{1:K}, W_0) - \mu(X_{1:K}, W))^2|X_{1:K}]
\quad = \mathbb{E}[(Y - \mu(X_{1:K}, W_0))^2|X_{1:K} + \mathbb{E}[(\mu(X_{1:K}, W_0) - \mu(X_{1:K}, W))^2|X_{1:K}]
\quad + 2 \mathbb{E}[(Y - \mu(X_{1:K}, W_0))(\mu(X_{1:K}, W_0) - \mu(X_{1:K}, W))|X_{1:K}]
\quad = \mathbb{E}[(Y - \mu(X_{1:K}, W_0))^2|X_{1:K} + (\mu(X_{1:K}, W_0) - \mu(X_{1:K}, W))^2
\quad + 2(\mu(X_{1:K}, W_0) - \mu(X_{1:K}, W)) \mathbb{E}[Y - \mu(X_{1:K}, W_0)|X_{1:K}]
\quad = \mathbb{E}[(Y - \mu(X_{1:K}, W_0))^2|X_{1:K} + (\mu(X_{1:K}, W_0) - \mu(X_{1:K}, W))^2, (37)

$$

$$\ell(W) = \ell(W_0)$$ implies that

$$\mathbb{E} \left[ \left( \sum_{i=1}^{K} f(X_i; W) - \sum_{i=1}^{K} f(X_i; W_0) \right)^2 \right] = 0. (39)$$

Denote $f(X_i; W) - f(X_i; W_0)$ as $\Delta(X; W)$. Equation (39) can be expanded as follows

$$0 = \mathbb{E} \left[ \sum_{i=1}^{K} \Delta(X_i, W)^2 \right]
\quad = \sum_{i=1}^{K} \mathbb{E}[\Delta^2(X_i, W)] + 2 \sum_{1 \leq i < j \leq K} \mathbb{E}[\Delta(X_i, W)\Delta(X_j, W)]
\quad = \sum_{i=1}^{K} \mathbb{E}[\Delta^2(X_i, W)] + 2 \sum_{1 \leq i < j \leq K} \mathbb{E}[\Delta(X_i, W)]\mathbb{E}[\Delta(X_j, W)]
\quad = \sum_{i=1}^{K} \mathbb{E}[\Delta^2(X_i, W)] + 2 \sum_{1 \leq i < j \leq K} (\mathbb{E}[\Delta(X_i, W)])^2. (40)$$

Thus, $\mathbb{E}[\Delta^2(X_i, W)] = \mathbb{E}[\Delta(X_i, W)] = 0$. We have $\Delta(X_i, W) = 0$, a.e., therefore $f(X, W) = f(X, W_0)$, a.e.
C.3 Proof of Proposition 9

Proof. Denote \( X' = (X_1, X_2) \) and denote \( p(Y = i|X_1, X_2; W) \) as \( p_i(X', W), i = 0, 1 \).

Following simple algebra,

\[
\ell(W) = \mathbb{E}[\mathbb{E}[\log p(Y|X', W)|X']] = \mathbb{E}\left[ \sum_{i=0}^{1} p_i(X', W_0) \log p_i(X', W) \right]. \tag{41}
\]

So, the difference of \( \ell(W) \) and \( \ell(W_0) \) satisfies

\[
\ell(W) - \ell(W_0) = \mathbb{E}\left[ \sum_{i=0}^{1} p_i(X', W_0) \log \frac{p_i(X', W)}{p_i(X', W_0)} \right] \\
\leq \mathbb{E}\left[ \sum_{i=0}^{1} p_i(X', W_0) \left( \frac{p_i(X', W)}{p_i(X', W_0)} - 1 \right) \right] \tag{42} \\
= \mathbb{E}\left[ \sum_{i=0}^{1} p_i(X', W) - \sum_{i=0}^{1} p_i(X', W_0) \right] \\
= 0.
\]

The inequality holds because \( \log x \leq x - 1 \) for \( x > 0 \), where “=” holds if and only if \( x = 1 \).

Hence \( \ell(W) = \ell(W_0) \), which implies that \( p_i(X', W) = p_i(X', W_0) \), a.e. for \( i = 0, 1 \). Together with Equation (12), we have

\[
\text{erf}\left( \frac{1}{2\sigma} (f(X_1, W) - f(X_2, W)) \right) = \text{erf}\left( \frac{1}{2\sigma} (f(X_1, W_0) - f(X_2, W_0)) \right). \tag{43}
\]

Hence, \( f(X_1, W) - f(X_2, W) = f(X_1, W_0) - f(X_2, W_0) \), a.e.
D Experiment Details

In this section, we provide missing experiment details in Section 6.

D.1 Classification via Triplet Comparison (Section 6.1)

Data. We used MNIST [LeCun et al., 1998], Fashion-MNIST [Xiao et al., 2017] and Kuzushiji-MNIST [Clanuwat et al., 2018] datasets without any data augmentation. They all contain 28 × 28 grayscale images in 10 classes. The size of the original training dataset is 60000 and the size of the original test dataset is 10000.

Data preprocessing. For both pairwise similarity and triplet comparison data, pairs and triplets of data were sampled randomly with replacement from the original training dataset according to our assumptions in Section 2.2. The size of generated datasets for direct, pairwise, and triplet observations are 60000, 120000, and 180000, respectively.

Model. We used a sequential convolutional neural network as the model $f(X; W)$: Conv2d(#channel = 32), ReLU, Conv2d(#channel = 64), MaxPool2d(size = 2), Dropout(p = 0.25), Linear(#dim = 128), ReLU, Dropout(p = 0.5), Linear(#dim = 10). The kernel size of convolutional layers is 3, and the kernel size of max pooling layer is 2.

Optimization. We used the Adam optimizer with decoupled weight decay regularization [Loshchilov and Hutter, 2019] to train the model. The learning rate is $1 \times 10^{-3}$, the batch size is 128, and the model is trained for 10 epochs.

D.2 Regression via Mean/Rank Observation on Synthetic Data (Section 6.2)

Data. We used $f(x) = \cos(x) + 0.5x$ as the true function and added a Gaussian noise with standard deviation of 0.5. We generated 200 sample points uniformly for $x \in [-6, 6]$. 

Figure 4: Learning from mean observations and rank observations on synthetic data. (4a) The expectation of the mean observation $Y = \frac{1}{2} (Z_i + Z_j)$; (4b) The probability of the rank observation $Y = [Z_i > Z_j]$ being positive. Mean observations and rank labels are also plotted in the horizontal planes in 4a and 4b, respectively.
Data preprocessing. We used batch learning and the batch size is set to be 64. Mean and rank observations are generated in each batch according to our assumptions in Section 2.2. The expectation of the mean observation and the probability of the rank observation being positive are plotted in Figure 4.

Model. We used a fully connected neural network with two hidden layers and ReLU activation as the model $f(X; W)$, i.e., the dimensions are $1 - 64 - 64 - 1$.

Optimization. We used the Adam optimizer Kingma and Ba [2015] to train the model. The learning rate is $1 \times 10^{-3}$, and $\beta_1 = 0.9$ and $\beta_2 = 0.999$. The batch size is 64, and the model is trained for 500 epochs.

D.3 Regression via Mean/Rank Observation on UCI Datasets (Section 6.2)

Data. We used 6 benchmark regression datasets from the UCI machine learning repository [Dua and Graff, 2017]. Table 7 shows the statistic of these datasets.

Table 6: Statistic of 6 UCI Benchmark Datasets.

| Dataset  | Dimension | Number of data |
|----------|-----------|----------------|
| abalone  | 10        | 353            |
| airfoil  | 5         | 1202           |
| auto-mpg | 7         | 313            |
| concrete | 8         | 824            |
| housing  | 13        | 404            |
| power-plant | 4        | 7654           |

Data preprocessing. We split the original datasets into training, validation, and test sets randomly by 60%, 20%, and 20% for each trial. Only training sets are used for generating the mean and the rank observations. The feature vectors $X$ are standardized to have 0 mean and 1 standard deviation and the targets $Z$ are normalized to have 0 mean using statistics of training sets. For mean observations, the number of sets is the same as the the number of original datasets and each set contains four instances. For rank observations, ten times of data are generated.

Model. We used linear model and gradient boosting machine as the model $f(X; W)$. We used LightGBM [Ke et al., 2017] to implement the gradient boosting machine as the model $f(X; W)$.

Optimization. For the linear model, we used stochastic gradient descent (SGD) with no momentum to train the model. The learning rate is 0.1, the batch size is 256, and the model is trained for 20 epochs. For the gradient boosting machines, the boosting type is gradient boosting decision trees (GBDT), the number of boost rounds is 100, and the number of early stopping rounds is 20.
E Additional Experiments

In this section, we provide additional experimental results on the datasets different from Section 6. The experiment setup is identical to that of the experiment in Section 6. For the classification task, we used 20 binary classification datasets and 10 multiclass classification datasets. For the regression task, we used additional 20 regression datasets.

E.1 Classification

We conduct additional experiments on classification via pairwise similarity and triplet comparison in both binary and multiclass classification settings.

E.1.1 Binary Classification

Table 7 shows the statistic of the additional binary classification datasets. The datasets are obtained from OpenML [Vanschoren et al., 2013], the UCI machine learning repository [Dua and Graff, 2017] and LIBSVM [Chang and Lin, 2011]. Table 8 shows the experimental results. For the pairwise similarity case, we can see that contrastive learning and our method can perform comparably to the supervised method in many datasets when we have only two classes. For the triplet comparison, our method clearly outperformed other methods in most cases. Interestingly, Tuplet baseline performs relatively well and arguably better than the Triplet baseline in the binary case. As we will see in the multiclass case, the performance of Tuplet drops miserably compared with other methods.

Table 7: Statistic of 20 Additional Binary Classification Datasets.

| Dataset   | Dimension | Positive | Negative | Number of data |
|-----------|-----------|----------|----------|----------------|
| adult     | 104       | 7508     | 22652    | 30160          |
| ayi       | 100       | 1385     | 1362     | 2747           |
| banana    | 2         | 2376     | 2923     | 5299           |
| codrna    | 8         | 162855   | 325709   | 488564         |
| custrev   | 100       | 2405     | 1365     | 3770           |
| ijcnn     | 22        | 18418    | 173262   | 191680         |
| image     | 18        | 1187     | 898      | 2085           |
| magic     | 10        | 12330    | 6687     | 19017          |
| mpqa      | 100       | 3311     | 7291     | 10602          |
| mushroom  | 98        | 3487     | 2155     | 5642           |
| phishing  | 30        | 6157     | 4896     | 11053          |
| phoneme   | 5         | 3817     | 1586     | 5403           |
| ringnorm  | 20        | 3663     | 3736     | 7399           |
| rt-polarity| 100      | 5331     | 5330     | 10661          |
| spambase  | 57        | 1811     | 2788     | 4599           |
| splice    | 60        | 1344     | 1646     | 2990           |
| subj      | 100       | 5000     | 4999     | 9999           |
| susy      | 18        | 45974    | 54024    | 99998          |
| twonorm   | 20        | 3703     | 3696     | 7399           |
| w8a       | 300       | 1933     | 62766    | 64699          |
Table 8: Classification via pairwise similarity and triplet comparison. Means and standard deviations of accuracy in percentage for 10 trials are reported.

| Dataset    | Unsupervised | Pairwise Similarity | Triplet Comparison | Supervised |
|------------|--------------|---------------------|--------------------|------------|
|            |              | Siamese | Contrastive | Ours | Tuplet | Triplet | Ours |            |            |
| adult      | 71.38        | 69.91    | 81.86      | **84.15** | 73.73 | 57.89   | **75.49** | 85.08       |            |
|            | (0.29)       | (11.11)  | (3.57)     | (0.43)   | (0.59) | (7.07)  | (0.63) | (0.29)       |            |
| ayi        | 53.25        | 66.93    | **76.67**  | **77.65** | 52.16 | **54.22** | **54.51** | 78.47       |            |
|            | (1.58)       | (10.90)  | (1.20)     | (1.68)   | (2.09) | (1.40)  | (3.28) | (1.40)       |            |
| banana     | 56.16        | 70.22    | **89.80**  | **89.47** | 53.26 | **56.75** | **57.53** | 88.42       |            |
|            | (0.94)       | (16.99)  | (1.20)     | (0.79)   | (2.50) | (6.25)  | (5.36) | (1.11)       |            |
| codrna     | 55.58        | 59.23    | 96.38      | **96.57** | 61.06 | 59.28   | **66.72** | 96.47       |            |
|            | (0.10)       | (12.33)  | (0.08)     | (0.11)   | (2.43) | (8.68)  | (0.18) | (0.07)       |            |
| custrev    | 51.70        | 60.76    | 70.84      | **74.56** | 53.24 | 52.33   | **60.92** | 75.32       |            |
|            | (1.26)       | (9.07)   | (1.27)     | (1.10)   | (1.67) | (2.13)  | (4.67) | (2.13)       |            |
| icnm       | 58.39        | 58.48    | **99.13**  | 98.98    | 74.02 | 52.88   | **92.15** | 99.08       |            |
|            | (1.65)       | (13.02)  | (0.04)     | (0.19)   | (10.74)| (4.34)  | (0.56) | (0.05)       |            |
| image      | 60.94        | 75.44    | **94.10**  | **93.81** | 54.51 | **56.09** | **59.02** | 89.76       |            |
|            | (1.44)       | (18.45)  | (0.84)     | (1.16)   | (3.15) | (3.31)  | (7.21) | (0.99)       |            |
| magic      | 54.55        | 77.18    | 86.44      | **86.93** | 67.49 | 58.79   | 65.94   | 86.31       |            |
|            | (0.81)       | (12.22)  | (0.59)     | (0.52)   | (2.50) | (5.27)  | (1.08) | (0.41)       |            |
| mpqa       | 62.56        | 59.38    | **84.76**  | **84.60** | 53.33 | 53.18   | **73.06** | 85.89       |            |
|            | (0.86)       | (13.56)  | (0.68)     | (0.87)   | (2.73) | (1.24)  | (1.41) | (0.67)       |            |
| mushroom   | 85.14        | 82.17    | **99.98**  | **99.96** | 61.37 | 56.47   | **88.46** | 99.97       |            |
|            | (0.75)       | (21.95)  | (0.04)     | (0.08)   | (4.28) | (6.04)  | (8.43) | (0.08)       |            |
| phishing   | 54.80        | 77.65    | **96.07**  | **96.43** | 55.64 | 57.08   | **73.28** | 95.25       |            |
|            | (0.82)       | (21.31)  | (0.37)     | (0.56)   | (3.02) | (4.82)  | (2.44) | (0.35)       |            |
| phoneme    | 68.24        | 60.64    | 80.82      | **83.59** | 59.16 | 62.16   | **71.39** | 81.06       |            |
|            | (0.51)       | (9.46)   | (1.00)     | (1.27)   | (8.19) | (8.20)  | (0.72) | (0.75)       |            |
| ringnorm   | 76.05        | 82.95    | 97.20      | **98.07** | 72.54 | 58.82   | **67.92** | 97.97       |            |
|            | (1.05)       | (20.56)  | (0.39)     | (0.22)   | (4.11) | (8.26)  | (9.70) | (0.31)       |            |
| rt-polarity| 51.99        | 57.44    | 69.73      | **71.04** | 52.26 | 52.82   | **54.20** | 72.37       |            |
|            | (0.82)       | (8.92)   | (0.71)     | (0.53)   | (1.64) | (2.27)  | (2.53) | (1.01)       |            |
| spambase   | 60.04        | 81.70    | 93.61      | **94.23** | 57.66 | 60.00   | **71.85** | 93.73       |            |
|            | (1.17)       | (18.05)  | (0.44)     | (0.48)   | (1.50) | (6.13)  | (7.39) | (0.88)       |            |
| splice     | 66.69        | 70.15    | 87.79      | **90.95** | 53.16 | 54.23   | **59.05** | 89.48       |            |
|            | (1.25)       | (19.07)  | (1.16)     | (1.23)   | (1.59) | (2.78)  | (7.63) | (1.11)       |            |
| subj       | 82.28        | 74.99    | 87.48      | **88.79** | 53.12 | 54.79   | **64.36** | 89.18       |            |
|            | (0.86)       | (16.71)  | (0.56)     | (0.53)   | (2.42) | (3.60)  | (6.80) | (0.85)       |            |
| susy       | 67.19        | 66.07    | 79.48      | **79.78** | 58.68 | 53.67   | 54.65   | 79.87       |            |
|            | (0.27)       | (12.93)  | (0.37)     | (0.20)   | (2.84) | (2.93)  | (4.60) | (0.26)       |            |
| twonorm    | 97.66        | 84.36    | **97.64**  | **97.64** | 60.60 | **58.16** | **63.47** | 97.65       |            |
|            | (0.36)       | (20.17)  | (0.37)     | (0.42)   | **8.76** | (2.99)  | (9.13) | (0.37)       |            |
| w8a        | 96.38        | 61.49    | **98.00**  | **98.26** | 96.97 | 57.98   | **97.78** | 99.05       |            |
|            | (1.79)       | (12.33)  | (0.59)     | (1.00)   | (0.15) | (2.36)  | (0.15) | (0.04)       |            |
E.1.2 Multiclass Classification

Table 9 shows the statistic of the additional multiclass classification datasets. The datasets are obtained from OpenML [Vanschoren et al., 2013]. In Table 10, our methods nicely outperformed representation learning based methods in all cases for triplet comparison. For pairwise similarity, contrastive learning outperformed our method in cardiotocography and isolet datasets, while our method clearly outperformed other methods on artificial-character, coverty, gas-drift, and satimage.

Table 9: Statistic of 10 Additional Multiclass Datasets.

| Dataset          | Dimension | Number of classes | Number of data |
|------------------|-----------|-------------------|----------------|
| artificial-character | 7         | 10                | 10217          |
| cardiotocography  | 35        | 10                | 2125           |
| coverty          | 54        | 7                 | 581011         |
| gas-drift        | 128       | 6                 | 13909          |
| isolet           | 617       | 26                | 7796           |
| japanevovowels   | 14        | 9                 | 9960           |
| letter           | 16        | 26                | 19999          |
| pendigits        | 16        | 10                | 10991          |
| satimage         | 36        | 6                 | 6429           |
| vehicle          | 18        | 4                 | 845            |
Table 10: **Classification via pairwise similarity and triplet comparison.** Means and standard deviations of accuracy in percentage for 10 trials are reported.

| Dataset        | Unsupervised | Pairwise Similarity | Triplet Comparison | Supervised |
|----------------|--------------|---------------------|--------------------|------------|
|                |              | Siamese             | Contrastive        | Ours       | Tuplet   | Triplet | Ours    |
| artificial-character | 22.05        | 34.93               | 46.31              | **50.29**  | 22.18    | 23.04   | **47.71** | 57.71 |
|                 | (0.75)       | (2.76)              | (0.78)             | **(1.19)** | (1.97)   | (1.90)  | **(1.56)** | (1.00) |
| cardiocography  | 88.14        | 85.88               | **99.88**          | 95.39      | 36.89    | 37.27   | **94.35** | 99.95 |
|                 | (6.57)       | (15.75)             | **(0.24)**         | (1.73)     | (2.90)   | (4.52)  | **(6.76)** | (0.09) |
| coverype        | 36.24        | 47.81               | 54.17              | **81.15**  | 36.14    | 25.17   | **64.85** | 84.69 |
|                 | (3.97)       | (6.17)              | (4.03)             | **(1.09)** | (3.80)   | (2.89)  | **(7.37)** | (0.35) |
| gas-drift       | 37.29        | 61.32               | 90.40              | **98.40**  | 26.32    | 38.71   | **82.60** | 98.56 |
|                 | (0.78)       | (15.06)             | (7.57)             | **(0.59)** | (1.58)   | (4.86)  | **(5.55)** | (0.33) |
| isoleat         | 55.69        | 73.04               | **86.24**          | 78.79      | 17.32    | 22.38   | **57.73** | 96.12 |
|                 | (2.38)       | (1.88)              | **(2.27)**         | (3.44)     | (1.02)   | (2.90)  | **(3.14)** | (0.57) |
| japanesevowels  | 38.42        | 73.29               | **96.25**          | **96.61**  | 27.80    | 31.69   | **94.66** | 96.55 |
|                 | (1.00)       | (12.45)             | **(0.37)**         | **(0.55)** | (2.68)   | (3.49)  | **(0.75)** | (0.38) |
| letter          | 29.06        | 48.43               | **73.59**          | **73.86**  | 21.08    | 23.12   | **64.56** | 89.41 |
|                 | (1.74)       | (5.10)              | **(1.65)**         | **(2.14)** | (1.46)   | (1.95)  | **(1.57)** | (0.57) |
| pendigits       | 68.22        | 83.17               | **99.03**          | **99.02**  | 43.01    | 41.01   | **97.24** | 98.68 |
|                 | (2.74)       | (8.09)              | **(0.18)**         | **(0.22)** | (3.68)   | (3.08)  | **(2.12)** | (0.20) |
| satimage        | 64.32        | 65.41               | 83.52              | **88.23**  | 44.28    | 47.30   | **84.33** | 87.82 |
|                 | (6.01)       | (4.21)              | (1.87)             | **(0.52)** | (4.03)   | (6.11)  | **(0.84)** | (0.84) |
| vehicle         | 38.40        | 46.21               | **69.35**          | **68.34**  | 35.92    | 41.60   | **57.10** | 69.23 |
|                 | (1.70)       | (7.79)              | **(5.35)**         | **(4.90)** | (3.39)   | (5.63)  | **(7.28)** | (2.66) |
E.2 Regression

Table 11 shows the statistic of the additional regression datasets. The datasets are obtained from OpenML [Vanschoren et al., 2013] and the UCI machine learning repository [Dua and Graff, 2017]. Table 12 shows the mean squared error results for each method. For the regression via mean observation, our method based on linear regression outperformed the linear regression baseline consistently in all cases, similarly for the gradient boosting machine case. Sometimes they are comparable to the supervised method. For the regression via rank observation, it is interesting to see that our method based on a Gaussian distribution failed in house-16h and house-8l datasets. We hypothesize that it is because the target distribution is heavy-tailed in these datasets.

Table 11: **Statistic of 20 Additional Regression Datasets.**

| Dataset         | Dimension | Min     | Max     | Number of data |
|-----------------|-----------|---------|---------|----------------|
| 2d-planes       | 10        | -12.6943| 12.2026 | 40767          |
| bank-32nh       | 32        | 0       | 82      | 8191           |
| bank-8fm        | 8         | 0       | 80.2263 | 8191           |
| bike-sharing    | 33        | 0.022   | 8.71    | 730            |
| cpu-act         | 21        | 0       | 99      | 8191           |
| diabetes        | 10        | 25      | 346     | 441            |
| elevator        | 6         | -15     | 15.1    | 9516           |
| fried           | 10        | -1.228  | 30.522  | 40767          |
| house-16h       | 16        | 0       | 50      | 22783          |
| house-8l        | 8         | 0       | 50      | 22783          |
| insurance-charge| 11        | 1.12    | 63.8    | 1336           |
| kin-8nm         | 8         | 4.016538| 145.8521| 8191           |
| puma-8nh        | 8         | -12.4153| 11.87619| 8191           |
| real-estate     | 6         | 7.6     | 117.5   | 413            |
| rmftsa-ladata   | 10        | 4.15    | 30.43   | 507            |
| space-ga100     | 6         | -305.704| 10.00835| 3106           |
| stock           | 9         | 34      | 62      | 949            |
| wine-quality    | 11        | 3       | 9       | 6496           |
| wine-red        | 11        | 3       | 8       | 1598           |
| wine-white      | 11        | 3       | 9       | 4897           |
Table 12: **Regression via mean observation and rank observation.** Means and standard deviations of error variance (rank observations) or MSE (otherwise) for 10 trials are reported.

| Dataset       | Mean Observation | Rank Observation | Supervised |
|---------------|------------------|------------------|------------|
|               | Baseline         | Ours             | RankNet, Gambel | Ours, Gaussian | GM | GM | GM | GM |
| 2d-planes     | 13.49 (11.40)    | 5.70 (1.01)      | 8.86 (19.14)   | 5.72 (1.03)    | 5.72 (1.00)  |
|               | (0.20)           | (0.20)           | (0.10)        | (0.10)         | (0.1)       |
| bank-32nh     | 112.42 (111.55)  | 69.30 (70.32)    | 123.63 (142.97) | 71.25 (87.79)  | 70.62 (68.83) |
|               | (5.70)           | (4.00)           | (6.50)        | (3.90)         | (3.1)       |
| bank-8fm      | 134.99 (133.56)  | 15.23 (10.07)    | 86.92 (230.19) | 34.19 (33.17)  | 15.45 (9.21) |
|               | (5.70)           | (4.50)           | (2.60)        | (1.20)         | (0.7)       |
| bike-sharing  | 2.36 (2.40)      | 0.77 (0.63)      | 1.61 (3.79)   | 0.68 (0.57)    | 0.64 (0.45)  |
|               | (0.20)           | (0.20)           | (0.30)        | (0.10)         | (0.1)       |
| cpu-act       | 235.22 (200.64)  | 98.20 (6.10)     | 231.24 (343.39) | 145.88 (150.27) | 102.68 (5.07) |
|               | (23.70)          | (18.40)          | (10.20)       | (0.40)         | (1.7)       |
| diabetes      | 4688.70 (4937.20)| 3355.22 (3746.14)| 5765.28 (5918.11) | 3771.73 (3323.98) | 3462.89 (491.2) |
|               | (541.30)         | (430.40)         | (782.30)      | (440.60)       | (464.6)     |
| elevator      | 18.91 (18.21)    | 13.03 (10.87)    | 17.38 (25.99) | 12.93 (10.65)  | 12.83 (10.57) |
|               | (0.80)           | (0.50)           | (0.40)        | (0.30)         | (0.3)       |
| fried         | 17.15 (14.84)    | 6.92 (1.28)      | 12.04 (25.03) | 6.94 (1.62)    | 7.03 (1.21)  |
|               | (0.20)           | (0.20)           | (0.10)        | (0.30)         | (0.1)       |
| house-16h     | 24.33 (20.21)    | 21.28 (9.69)     | 22.69 (27.26) | 1462200.27 (71.52) | 22.33 (9.88) |
|               | (2.20)           | (1.20)           | (1.50)        | (963977.00) (1.50) | (1.9) (0.8) |
| house-8l      | 23.71 (20.08)    | 17.95 (8.71)     | 21.16 (26.51) | 197143.11 (15.99) | 18.04 (8.80) |
|               | (1.50)           | (1.10)           | (1.40)        | (1.20)         | (1.3)       |
| insurance-charge | 95.74 (91.59)  | 36.46 (25.26)    | 99.42 (143.41) | 68.98 (46.36)  | 40.66 (20.72) |
|               | (8.80)           | (8.40)           | (4.50)        | (7.40)         | (6.2)       |
| kin-8nm       | 566.46 (489.96)  | 406.42 (192.96)  | 660.73 (689.58) | 523.07 (187.33) | 411.87 (169.30) |
|               | (14.40)          | (14.10)          | (18.70)       | (19.60)        | (12.4)      |
| puma-8nm      | 26.68 (22.64)    | 19.60 (10.77)    | 26.31 (31.56) | 19.82 (10.36)  | 19.90 (10.40) |
|               | (0.60)           | (0.40)           | (0.40)        | (0.40)         | (0.6)       |
| real-estate   | 155.19 (118.97)  | 68.82 (64.47)    | 130.77 (191.92) | 128.28 (61.10) | 92.49 (54.94) |
|               | (42.10)          | (34.70)          | (51.70)       | (27.90)        | (37.3)      |
| rmftsa-ladata | 6.93 (5.19)      | 3.77 (4.34)      | 5.59 (8.94)   | 3.89 (5.56)    | 3.99 (4.00)  |
|               | (1.00)           | (1.00)           | (0.90)        | (1.60)         | (1.1)       |
| space-ga100   | 313.80 (301.18)  | 237.95 (127.45)  | 366.00 (384.73) | 300.72 (162.05) | 221.42 (115.54) |
|               | (40.60)          | (40.40)          | (54.70)       | (52.80)        | (47.8)      |
| stock         | 26.02 (24.76)    | 6.50 (1.44)      | 17.35 (43.21) | 13.19 (1.32)   | 5.86 (0.79)  |
|               | (1.90)           | (1.30)           | (1.30)        | (1.40)         | (0.7)       |
| wine-quality  | 0.66 (0.62)      | 0.55 (0.45)      | 0.63 (0.77)   | 0.55 (0.44)    | 0.55 (0.43)  |
|               | (0.00)           | (0.00)           | (0.00)        | (0.00)         | (0.0)       |
| wine-red      | 0.55 (0.53)      | 0.40 (0.40)      | 0.54 (0.64)   | 0.44 (0.37)    | 0.41 (0.36)  |
|               | (0.00)           | (0.00)           | (0.00)        | (0.00)         | (0.0)       |
| wine-white    | 0.69 (0.63)      | 0.56 (0.46)      | 0.61 (0.81)   | 0.57 (0.45)    | 0.58 (0.44)  |
|               | (0.00)           | (0.00)           | (0.00)        | (0.00)         | (0.0)       |