Density-Fixing: Simple yet Effective Regularization Method based on the Class Prior

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Abstract—Machine learning models suffer from overfitting, which is caused by a lack of labeled data. To tackle this problem, we proposed a framework of regularization methods, called density-fixing, that can be used commonly for supervised and semi-supervised learning. Our proposed regularization method improves the generalization performance by forcing the model to approximate the class’s prior distribution or the frequency of occurrence. This regularization term is naturally derived from the formula of maximum likelihood estimation and is theoretically justified. We further investigated the asymptotic behavior of the proposed method and how the regularization terms behave when assuming a prior distribution of several classes in practice. Experimental results on multiple benchmark datasets are sufficient to support our argument, and we suggest that this simple and effective regularization method is useful in real-world machine learning problems.

I. INTRODUCTION

Machine learning has achieved great success in many areas. However, such machine learning models suffer from an overfitting problem caused by a lack of data [1], [2]. To tackle such problems, research on semi-supervised learning [3], [4] or regularization [5], [6] has been very active. The main idea of semi-supervised learning is to solve supervised learning problems with few labels by utilizing unlabeled data. In real-world machine learning problems, labeled data is often scarce, but unlabeled data is abundant. Therefore, semi-supervised learning methods that make good use of unlabeled data are essential.

We focus on leveraging the class density of the entire dataset as prior knowledge about labeled and unlabeled data. This means that we assume that the density of each class is obtained as prior knowledge. This assumption is a natural one in many actual machine learning problems. Based on this idea, we propose a framework of regularization methods, called density-fixing, both supervised and semi-supervised settings can commonly use that. Our proposed density-fixing regularization improves the generalization performance by forcing the model to approximate the class’s prior distribution or the frequency of occurrence. This regularization term of density-fixing is naturally derived from the formula for maximum likelihood estimation and is theoretically justified. We further investigated the asymptotic behavior of the density-fixing and how the regularization terms behave when assuming a prior distribution of several classes in practice. Experimental results on multiple benchmark datasets are sufficient to support our argument, and we suggest that this simple and effective regularization method is useful in real-world problems.

Contribution: We propose the density-fixing regularization, which has the following properties:

• simplicity: density-fixing is very simple to implement and has almost no computational overhead.
• naturalness: density-fixing is derived naturally from the formula for maximum likelihood estimation and has a theoretical guarantee.
• versatility: density-fixing is generally applicable to many problem settings.

In a nutshell, density-fixing forcing the balance of class density:

\[ L_\theta(x, y) = \ell(x, y) + \gamma \cdot D_{KL}(p_\theta(y)||q(y)), \]

where \( \ell(x, y) \) is the some loss function (e.g. cross-entropy loss), and \( \gamma \geq 0 \) is the parameter of the regularization term. For the true distribution \( q(y) \) of a class, we can use it if it is given as prior knowledge, otherwise we can average the frequency of occurrence of the labels in the training sample and use it as an estimator \( \hat{q}(y) \):

\[ \hat{q}(y) = \{y^1, \ldots, y^K\}, \quad y^j = \frac{1}{N} \sum_{i=1}^N \mathbb{1}_{\{c(x_i) = i\}}. \]

The sample mean provides the unbiased and consistent estimator of the frequency of class occurrence, so it is sufficient to use it.

The source-code necessary to replicate our CIFAR-10 experiments is available at GitHub [1].

II. RELATED WORKS

In this section, we introduce some related works that are relevant to our work.

A. Over-fitting and Regularization

Machine learning models suffer from an over-fitting problem caused by a lack of data. In order to avoid overfitting, various regularization methods have been proposed. For example, Dropout [6] is a powerful regularization method that introduces ensemble learning-like behavior by randomly removing connections between neurons of the Deep Neural Network. Another recently proposed simple regularization

https://github.com/nocotan/density_fixing
method is mixup and its variants \[5\], \[7\], \[8\], which takes a linear regularization method of training data as a new input. There are many regularization methods for some specific models (e.g., for Generative Adversarial Networks \[9\], \[10\]).

B. Semi-Supervised Learning

There are many studies on semi-supervised learning. The method of assigning pseudo-labels to unlabeled data as new training data is very popular \[11\]. Another approach to semi-supervised learning is the use of Generative Adversarial Networks, which are famous for their expressive power \[12\].

III. NOTATONS AND PROBLEM FORMULATION

Let \( \mathcal{X} \) be the input space, \( \mathcal{Y} = \{1, \ldots, K\} \) be the output space, \( K \) be the number of classes and \( \mathcal{C} \) be a set of concepts we may wish to learn. We assume that each input vector \( x \in \mathbb{R}^d \) is of dimension \( d \). We also assume that examples are independently and identically distributed (i.i.d) according to some fixed but unknown distribution \( \mathcal{D} \).

Then, the learning problem formulated as follows: we consider a set of possible concepts \( \mathcal{H} \), called hypothesis set. We receive a sample \( \mathcal{B} = (x_1, \ldots, x_N) \) drawn i.i.d. according to \( \mathcal{D} \) as well as the labels \( (c(x_1), \ldots, c(x_N)) \), which are based on a specific target concept \( c \in \mathcal{C} : \mathcal{X} \rightarrow \mathcal{Y} \). In the semi-supervised learning problem, we additionally have access to unlabeled sample \( \mathcal{B}^U = (x_1', \ldots, x_{N'}') \) drawn i.i.d. according to \( \mathcal{D} \). Our task is to use the labeled sample \( \mathcal{B} \) and unlabeled sample \( \mathcal{B}^U \) to find a hypothesis \( h^* \in \mathcal{H} \) that has a small generalization error for the concept \( c \). The generalization error \( \mathcal{R} \) is defined as follows.

**Definition 1. (Generalization error)** Given a hypothesis \( h \in \mathcal{H} \), a target concept \( c \in \mathcal{C} \), and unknown distribution \( \mathcal{D} \), the generalization error of \( h \) is defined by

\[
\mathcal{R}(h) = \mathbb{E}_{x \sim \mathcal{D}} \left[ \mathbb{I}_{h(x) \neq c(x)} \right],
\]

where \( \mathbb{I}_\omega \) is the indicator function of the event \( \omega \).

The generalization error of a hypothesis \( h \) is not directly accessible since both the underlying distribution \( \mathcal{D} \) and the target concept \( c \) are unknown. Then, we have to measure the empirical error of hypothesis \( h \) on the observable labeled sample \( \mathcal{B} \). The empirical error \( \mathcal{R}(h) \) is defined as follows.

**Definition 2. (Empirical error)** Given a hypothesis \( h \in \mathcal{H} \), a target concept \( c \in \mathcal{C} \), and a sample \( \mathcal{B} = (x_1, \ldots, x_N) \), the empirical error of \( h \) is defined by

\[
\hat{R}(h) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}_{h(x_i) \neq c(x_i)}.
\]

In learning problems, we are interested in how much difference there is between empirical and generalization errors. Therefore, in general, we consider the relative generalization error \( \mathcal{R}(h) - \hat{R}(h) \).

IV. DENSITY-FIXING REGULARIZATION

In this paper, we assume that \( \mathcal{H}_p \) is a class of functions mapping input vectors to the class densities:

\[
h(x) = \left\{ x \mapsto p(y|x) \right\},
\]

Therefore, we can replace the learning problem with a problem that approximates the true distribution \( q(y|x) \) with the estimated distribution \( p(y|x) \).

We assume that the class-conditional probability for labeled data \( p(x|y) \) and that for unlabeled data (or test data) \( q(x|y) \) are the same:

\[
p(x|y) = q(x|y).
\]

Then, our goal is to estimate \( q(y|x) \) from labeled data \( \{x_i, y_i\}_{i=1}^N \) drawn i.i.d from \( p(x, y) \) and unlabeled data \( \{x'_i\}_{i=1}^{N'} \).

**Theorem 1.** Let \( p_\theta(y|x) \) be the estimated distribution parameterized by \( \theta \), and \( q(y|x) \) be the true distribution. Then, we can write the sum of log-likelihood function as follows:

\[
\sum \log L(\theta) = \sum \log p_\theta(y|x) - D_{KL}[p_\theta(y) || q(y)].
\]

where \( D_{KL}[P||Q] \) is the Kullback-Leibler divergence \[13\] from \( Q \) to \( P \):

\[
D_{KL}[P||Q] = \sum p(x) \log \frac{P(x)}{Q(x)} \tag{8}
\]

\[
= - \sum p(x) \log \frac{Q(x)}{P(x)} \tag{9}
\]

This means that when we consider maximum likelihood estimation, we can decompose the objective function into two terms: the term depending on \( x \) and the term depending only on \( y \).

**Proof.** From Bayes’ theorem, we can obtain

\[
p(x|y) = \frac{p(y|x)p(x)}{p(y)},
\]

\[
q(x|y) = \frac{q(y|x)q(x)}{q(y)}. \tag{11}
\]

Then, combining Eq \(6\), \(10\) and \(11\),

\[
p(y|x)p(x) = \frac{q(y|x)p(x)}{q(y)}
\]

\[
q(y|x) = \frac{q(y)p(x)}{p(y)q(x)p(y|x)} \tag{12}
\]

Considering maximum likelihood estimation, we can have the log-likelihood function \( \log L(\theta) \) as follows:

\[
\log L(\theta) = \log \left\{ \frac{q(y)}{p_\theta(y)} p_\theta(y|x) \right\}
\]

\[
= \log p_\theta(y|x) + \log \frac{q(y)}{p_\theta(y)}. \tag{13}
\]
Finally, we compute the sum of log-likelihood function,
\[
\sum \log L(\theta) \approx \sum \log p_\theta(y|x) + E \left[ \log \frac{q(y)}{p_\theta(y)} \right]
\]
and then, we have Eq (7).

Considering that we maximize Eq (7), it is clear that \( D_{KL}[p_\theta(y)||q(y)] \) should be closer to 0. The Kullback-Leibler divergence is defined only if \( \forall y, q(y) = 0 \) implies \( p_\theta(y) = 0 \), and this property is so called absolute continuity.

From the above theorem, if the probability of class occurrence is known in advance, it can be used to perform regularization. We call this term density-fixing regularization. Regularization is performed so that the density of each class in the inference result for the unlabeled sample \( p_\theta(y) \) approximates the \( q(y) \). In addition, the KL-divergence has the following property: the best approximation \( p_\theta \) satisfies
\[
\hat{p}_\theta(y) = 0,
\]
for \( y \) at which \( q(y) = 0 \). This property is called zero-forcing, and we can see that our regularization behave as if the probabilities of classes we do not know remain 0.

**V. ASYMPTOTIC NORMALITY**

In this section, we discuss how the density-fixing regularization behaves asymptotically.

**Theorem 2.** Let \( \ell(\theta) = \log L(\theta) \). The asymptotic variance of the maximum likelihood estimator applying the density-fixing regularization is given by \( \frac{1}{\eta(\theta)} \). Here, \( \eta(\theta) \) is a function that always takes a positive value, parameterized by \( \theta \).

**Proof.** In the maximum likelihood estimator \( \hat{\theta}_N \) for the number of samples \( N \), we can obtain the following by Taylor expansion of \( \ell(\theta) \) around \( \theta_0 \):
\[
\begin{align*}
0 & = \frac{\partial \ell(\theta_0)}{\partial \theta} + \frac{\partial^2 \ell(\theta_0)}{\partial \theta^2} (\hat{\theta}_N - \theta_0) + \frac{\partial^3 \ell(\theta_0)}{\partial \theta^3} (\hat{\theta}_N - \theta_0)^2, \\
\hat{\theta}_N - \theta_0 & = -\frac{\partial^2 \ell(\theta_0)}{\partial \theta^2} (\hat{\theta}_N - \theta_0) - \frac{\partial^3 \ell(\theta_0)}{\partial \theta^3} (\hat{\theta}_N - \theta_0)^2 + \frac{2\partial^4 \ell(\theta_0)}{\partial \theta^4} (\hat{\theta}_N - \theta_0)^3
\end{align*}
\]
and central limit theorem, we can obtain
\[
\sqrt{N}(\hat{\theta}_N - \theta_0) \sim N\left(0, \frac{1}{I(\theta)} \right),
\]
when \( N \) is sufficiently large. Here, \( I(\theta) \) is the Fisher information matrix:
\[
I(\theta) = -E\left[ \frac{\partial^2}{\partial \theta^2} \ell(\theta) \right].
\]

Then, let \( \log p_\theta(y|x) = f(\theta) \) as the original likelihood function, we can obtain
\[
\begin{align*}
\frac{\partial^2}{\partial \theta^2} \left[ \log f(\theta) + E \left[ \log \frac{q(y)}{p_\theta(y)} \right] \right] & = \frac{\partial^2}{\partial \theta^2} f(\theta) + E \left[ \log \frac{q(y)}{p_\theta(y)} \right] + \frac{\partial^2}{\partial \theta^2} f(\theta) - \frac{\partial^2}{\partial \theta^2} \left[ \log p_\theta(y) \right],
\end{align*}
\]
and
\[
\begin{align*}
0 & = \frac{\partial^2}{\partial \theta^2} f(\theta) + \frac{\partial^2}{\partial \theta^2} f(\theta) - \frac{\partial^2}{\partial \theta^2} \left[ \log p_\theta(y) \right],
\end{align*}
\]
Therefore, the maximum likelihood estimator applying the density-fixing regularization $\hat{\theta}_N$ satisfies the following:

$$\sqrt{N}(\hat{\theta}_N - \theta_0) \sim N\left(0, \frac{1}{I(\theta) + \frac{\partial^2}{\partial \theta^2} E[\log p_0(y)]}\right).$$  \quad (23)

Since the logarithmic function is a monotonic increasing function, the second derivative is always positive. Therefore, we can obtain the proof of Theorem 2 with $\eta = \frac{1}{\frac{\partial^2}{\partial \theta^2} E[\log p_0(y)]}$.

This theorem implies that the convergence rate of the asymptotic variance of the maximum likelihood estimator becomes faster by $\eta(\theta)$ by applying the density-fixing regularization. Figure 4 illustrates the asymptotic behavior of the estimator by our regularization.

VI. SOME EXAMPLES

In this section, we investigate the behavior of our proposed method by assuming some class distributions as examples. To summarize our results:

- For discrete uniform distribution, the effect of regularization becomes weaker as the number of classes increases.
- For Bernoulli distribution, our regularization behaves to give strong regularization when there is a class imbalance.

Figure 2 shows the behavior of the regularization terms under each distribution.

A. Discrete Uniform Distribution

We assume that the probability density function of classes $p(y)$ is as follows:

$$p(y) = \begin{cases} \xi & y = 1 \\ (1 - \xi) & y = 0 \end{cases},$$  \quad (26)

here $\xi \in [0, 1]$ and this is the Bernoulli distribution. Then, our regularization term is

$$\frac{\partial^2}{\partial \xi^2} \left\{ E[\log p(y)] \right\} = E\left[ \frac{\partial^2}{\partial \xi^2} \log p(y) \right] = I(\xi) = \frac{1}{\xi (1 - \xi)}. \quad (27)

Thus, we can see that regularization is stronger when $\xi$ is away from 1/2. This means that in a binary classification, it behaves to give strong regularization when there is a class imbalance.

VII. EXPERIMENTAL RESULTS

In this section, we introduce our experimental results. We implement the density-fixing regularization as follows:

$$L(x, y) = L_{CE}(x, y) + \gamma D_{KL}[p_\theta(y)||p(y)],$$  \quad (28)

where $L_{CE}(x, y)$ is the cross-entropy loss and $\gamma$ is the weight parameter for the regularization term. The implementation of density-fixing regularization is straightforward, Figure 6 shows the few lines of code necessary to implement density-fixing regularization in PyTorch [14].

The datasets we use are CIFAR-10 [15], CIFAR-100 [15], STL-10 [16] and SVHN [17]. We determined the prior distribution of classes based on the number of data accounted for in each class of the data set, and we used ResNet-18 [18] as the baseline model.

A. Supervised Classification

In this experiment, we assumed a discrete uniform distribution for the class distribution.

Figure 3 shows the experimental results for CIFAR-10 with density-fixing regularization. As seen in the left of this figure, baseline model and density-fixing converge at a similar speed to their best test errors. At around 100 epoch, a second loss reduction, Deep Double Descent [19], can be observed, but this phenomenon is not disturbed by density-fixing. From the right, we can see that by increasing the parameter $\gamma$, we can reduce the generalization gap.

Also, Table 1 shows the contribution of density-fixing to the reduction of test errors.

B. Semi-Supervised Classification

In our experiments, we assumed a discrete uniform distribution for the class distribution and treated 1/5 of the training data as labeled and 4/5 of the training data as unlabeled.

Figure 4 shows test loss and train-test differences for each $\gamma$ in the semi-supervised setting. We can see that by increasing the parameter $\gamma$, it reduce the generalization gap. In addition,
CIFAR-10 and CIFAR-100, which consist of images from the same domain, have 10 and 100 classes, respectively, but the experimental results show that CIFAR-10 has a more significant regularization effect than CIFAR-100. This result supports our example in Eq (25).

Table II shows a comparison of classification error for each γ. These experimental results show that our regularization leads to improving error on the test data.

C. Stabilization of Generative Adversarial Networks

Generative Adversarial Networks (GANs) [20] is one of the powerful generative model paradigms that are currently successful in various tasks. However, GANs have the problem that their learning is very unstable. We suggest that regularization by density-fixing contributes to improving the stability of GANs. The density-fixing formulation of GANs is:

$$\max_{G}\min_{D} \mathbb{E}_{x \sim p_{data}}[\ell(D(x), 1)] + \mathbb{E}_{z \sim p_{z}}[\ell(D(G(z)), 0)] + D_{KL}(p_{D}(y)||q(y)),$$

where $D$ is the discriminator, $G$ is the generator, $\ell$ is the binary cross entropy and $q(y) = \text{Ber}(0.5)$.

Figure 5 illustrates the stabilizing effect of density-fixing the training of GAN when modeling a toy dataset (blue samples). The neural networks in these experiments are fully-connected and have three hidden layers of 512 ReLU units. We can see that density-fixing contributes to the stabilization of the training of GANs.
Fig. 4. Test loss and train-test differences for each $\gamma$ in the semi-supervised setting. We can see that by increasing the parameter $\gamma$, we can reduce the generalization gap. We can see that the generalization gap tends to be smaller as we increase the value of $\gamma$.

Fig. 5. Effect of density-fixing on stabilizing GAN training with $\gamma = 1$.

Fig. 6. Few lines of code necessary to implement density-fixing regularization in PyTorch.