Combating the Instability of Mutual Information-based Losses via Regularization

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Abstract

Notable progress has been made in numerous fields of machine learning based on neural network-driven mutual information (MI) bounds. However, utilizing the conventional MI-based losses is often challenging due to their practical and mathematical limitations. In this work, we first identify the symptoms behind their instability: (1) the neural network not converging even after the loss seemed to converge, and (2) saturating neural network outputs causing the loss to diverge. We mitigate both issues by adding a novel regularization term to the existing losses. We theoretically and experimentally demonstrate that added regularization stabilizes training. Finally, we present a novel benchmark that evaluates MI-based losses on both the MI estimation power and its capability on the downstream tasks, closely following the pre-existing supervised and contrastive learning settings. We evaluate six different MI-based losses and their regularized counterparts on multiple benchmarks to show that our approach is simple yet effective.

1 INTRODUCTION

Identifying a relationship between two variables of interest is one of the key problems in mathematics, statistics, and machine learning [Goodfellow et al., 2014; Ren et al., 2015; He et al., 2016; Vaswani et al., 2017]. One of the fundamental approaches is information theory-based measurement, namely the measure of mutual information (MI). Due to its mathematical soundness and the rise of deep learning, many have designed differentiable MI-based losses for neural networks. Some utilize the MI-based losses to bridge the gap between latent variables and representations in generative adversarial networks [Nowozin et al., 2016; Chen et al., 2018].

Although many have shown computational tractability and usefulness of MI-based losses, others still struggle with their instability during optimization. Contrastive learning literature with MI-based losses such as Chen et al. [2020], He et al. [2020] use huge batch sizes to reduce the variance of losses. Bardes et al. [2021] adds a regularization term to the neural network embeddings to stabilize the training. McAllester and Stratos [2020] and Song and Ermon [2020] further provide theoretical limitations of variational MI estimators, arguing that the limited batch size induces a MI estimation variance too large to handle. We argue that mitigating the variance of MI-based losses is critical for stabilizing training, where it is well known that more stable optimization of neural networks yields better predictive performance on the downstream tasks [Rothfuss et al., 2019; Bear and Cushman, 2020; Chavdarova et al., 2019; Richter et al., 2020; Zeng et al., 2020; Colombo et al., 2021].

In this paper, we concentrate on identifying the cause behind the instability of MI-based losses and propose a simple yet effective regularization method that can be applied to various MI-based losses. We start by analyzing the behaviors of two MI estimators; the MI Neural Estimator (MINE) loss [Belghazi et al., 2018] and Nguyen-Wainwright-Jordan loss (NWJ) loss [Nguyen et al., 2018]. We identify two distinctive behaviors that induce instability during training, drifting and exploding neural network outputs. Based on these observations, we design two novel dual representations of the KL-divergence called Regularized Donsker-Varadhan representation (ReDV) and Regularized NWJ representation (ReNWJ). We show theoretically and experimentally that adding our regularizer term suppresses two behaviors...
of drifting and exploding, avoiding instability during training. Finally, we design a novel benchmark that bridges the gap between variational MI estimators and real-world tasks, whereas previous works either do not directly show the MI estimation performance or evaluate only on toy problems. We reformulate both the supervised and the contrastive learning problem [Chen et al., 2020] He et al., 2020 Kholas et al., 2020] as MI estimation problems and show that our regularization yields better performance on both perspectives, downstream task and MI estimation performance.

2 BACKGROUND & RELATED WORKS

Definition of MI The mutual information between two random variables $X$ and $Y$ is defined as

$$I(X, Y) = D_{KL} (P_{XY} || P_X \otimes P_Y)$$

$$= E_{P_{XY}} \left( \log \frac{dP_{XY}}{dP_X \otimes P_Y} \right)$$

where $P_{XY}$ and $P_X \otimes P_Y$ are the joint distribution and the product of the marginal distributions, respectively. $D_{KL}$ is the Kullback-Leibler (KL) divergence. Without loss of generality, we consider $P_{XY}$ and $P_X \otimes P_Y$ as being distributions on a compact domain $\Omega \subset \mathbb{R}^d$.

MI through dual representation of $D_{KL}$ We first introduce two dual representations of $D_{KL}$, as MI is defined using $D_{KL}$. The most widely known is the Donsker-Varadhan representation $D_{DV}$ [Donsker and Varadhan, 1975]. For given two distribution $P$ and $Q$ on some compact domain $\Omega \subset \mathbb{R}^d$,

$$D_{DV}(X, Y) := \sup_{T: \Omega \to \mathbb{R}} E_P(T) - \log E_Q(e^T)$$

where both the expectations $E_P(T)$ and $E_Q(e^T)$ are finite. If we substitute $P$ and $Q$ into $P_{XY}$ and $P_X \otimes P_Y$, $D_{DV}$ yields the definition of MI. The optimal $T^* = \log \frac{dP}{dQ} + C$, where $C \in \mathbb{R}$ can be any constant.

In contrast to $D_{DV}$, the Nguyen-Wainwright-Jordan representation $D_{NWJ}$ [Nguyen et al., 2010] is induced by the convex conjugate known as Fenchel’s inequality [Hiriart-Urruty and Lemaréchal, 2004]:

$$D_{NWJ}(X, Y) := \sup_{T: \Omega \to \mathbb{R}} E_P(T) - E_Q(e^{-T})$$

The optimal $T^* = \log \frac{dP}{dQ} + 1$ is unique unlike the optimal $T^*$ of $D_{DV}$ due to its self-normalizing property [Belghazi et al., 2018]. However, $D_{DV}$ guarantees tighter lower bounds than $D_{NWJ}$ [Ruderman et al., 2012] Polyanskiy and Wu, 2014]. These two representations provide the theoretical soundness for numerous variational MI bounds.

Variational MI estimation With the increasing success of neural networks, several neural network-driven variational bounds of MI are proposed. They are widely employed, such as contrastive learning [van den Oord et al., 2018] He et al., 2020 Chen et al., 2020] or generative adversarial training [Belghazi et al., 2018] Nowozin et al., 2016]. Variational bounds of MI commonly focus on estimating $T^*$ via a neural network $T_\theta: \Omega \to \mathbb{R}$, called the statistics network [Belghazi et al., 2018], which outputs a single real value given the input sample pairs.

$$I_{MINE} [Belghazi et al., 2018]$$

directly maximize $D_{DV}$ as the objective function by feeding the samples $(x, y)$ of $P_{XY}$ and $P_X \otimes P_Y$ into $T_\theta$:

$$I_{MINE}(X, Y) := E_{P_{XY}(n)}(T_\theta(x, y)) - \log(e^{T_\theta(x, y)})$$

where $P_{XY}$ is the empirical distribution associated to n i.i.d. samples for given distribution $P$. [Belghazi et al., 2018] also utilizes moving averages of mini-batches to reduce the MI estimation variance caused by the limited batch size.

$$I_{InfoNCE} [van den Oord et al., 2018]$$

is also commonly used due to its stability and decent performance:

$$I_{InfoNCE}(X, Y) = \frac{1}{N} \sum_{i=1}^N \log \frac{e^{T_\theta(x_i, y_i)}}{\frac{1}{N} \sum_j e^{T_\theta(x_i, y_j)}}$$

where the $N$ samples $(x_i, y_i)$ are drawn from $P_{XY}$, which becomes equivalent to using the Softmax function with the negative log loss. $I_{InfoNCE}$ is also equivalent to $I_{MINE}$ up to a constant, but upper bounded by $\log N$, hence not able to estimate large MI values [van den Oord et al., 2018].

Poole et al., 2019 introduced $I_{TUBA}$, a unified lower bound, by expanding $D_{NWJ}$ [Barber and Agakov, 2003] Nguyen et al., 2010].

$$I_{NWJ}(X, Y) := E_{P_{XY}(n)}(T_\theta(x, y)) - E_{P_X \otimes P_Y(n)}(e^{T_\theta(x, y)})$$

$$I_{TUBA}(X, Y) := E_{P_{XY}(n)}(T_\theta(x, y))$$

$$- E_{P_X(n)}(e^{T_\theta(x, y)})/a(y) + \log(a(y)) - 1$$

where $a(y)$ is the variational parameter. However, unlike $I_{MINE}$ or $I_{InfoNCE}$, directly using the exponential term often causes numerical instability. Even if $T_\theta$ outputs a moderately sized value, $e^{T_\theta}$ can easily exceed the floating-point range.

To avoid this problem, Poole et al., 2019 introduce $D_{NWJ}$-based lower bound $I_{JS}$ by using a softplus-activated neural network as $T_\theta$:

$$I_{JS}(X, Y) := 1 + E_{P_{XY}(n)}(T_\theta(x, y))$$

$$- E_{P_Y \otimes P_X(n)}(e^{T_\theta(x, y)})$$

(8)
Variance problem of MI estimators  Despite the variety of bounds proposed, many still suffer from the bias-variance trade-off [Poole et al., 2019, McAllester and Stratos [2020] and Song and Ermon [2020] prove that the \( I_{\text{MINE}} \) estimator must have a batch size proportional to the exponential of the true MI to control the variance of the estimation.

Many bounds try to mitigate this problem by reducing the variance of low-biased estimators, such as by interpolating the formal theoretical guarantees [McAllester and Stratos, 2020, Song and Ermon [2020] proposed \( I_{\text{SMILE}} \) to clip the range of \( T_0 \) trained with \( I_{\text{MINE}} \), sacrificing the estimation quality to reduce the variance.

\[
I_{\text{SMILE}}(X,Y) := \mathbb{E}_{p(v)}(T_0(x,y)) - \log(\mathbb{E}_{p(v)}(\text{clip}(e^{T_0(x,y)}, e^{-\tau}, e^{\tau}))),
\]

where \( \text{clip}(v,l,u) = \max(\min(v,u),l) \) for \( v,u,l \in \mathbb{R} \).

Practical usages of MI  MI-based losses are often applied in generative modeling, such as for better mode coverage [Belghazi et al., 2018] or learning disentangled representations without supervision [Chen et al., 2016, Ojha et al., 2020, Li et al., 2021b, Jeon et al., 2021]. Representation learning employs MI-based losses [Tian et al., 2020, Hjelm et al., 2019, Tschannen et al., 2020, Cheng et al., 2020, Wu et al., 2020, Wen et al., 2020, Boudiaf et al., 2020, Tian et al., 2020a, Li et al., 2021a] to yield feature extractors that reflect its downstream tasks well. We emphasize that these approaches can be further utilized to measure the performance of MI estimators.

Comparing between MI estimators  Toy datasets such as correlated multivariate Gaussian distributions has been widely accepted for the evaluation of MI estimation [Belghazi et al., 2018, Poole et al., 2019, Song and Ermon [2020, Cheng et al., 2020, Lin et al., 2019]. However, we emphasize that using synthetic data as a definitive benchmark will end up in a disparity with real-world tasks. There have been some approaches that compared different MI estimators on generative modeling [Belghazi et al., 2018, Hjelm et al., 2019] or representational learning [Tian et al., 2020b]. However, finding the ideal MI for each downstream task is not trivial, making it impossible to directly assess the MI estimation quality. Moreover, Tschannen et al. [2020] and Tian et al. [2020b] showed the gap between MI estimation quality and downstream performance on specific tasks. Hence, it is crucial to evaluate both perspectives. The closest work to our benchmark is the consistency test of Song and Ermon [2020] using CIFAR-10 [Krizhevsky [2009] and MNIST [LeCun et al., 1998]. However, the test only offered to assess the ratio of two separate MI estimations, making it difficult to separately measure the quality of each estimation.

3 INSTABILITY OF MI BOUNDS

To demonstrate and analyze the instability of variational MI bounds, we design a synthetic problem with the One-hot dataset. We then solve the task via \( I_{\text{MINE}} \) and \( I_{\text{NWJ}} \), which are the losses derived from the two most commonly used representations without supervision, \( D_{\mathrm{DV}} \) and \( D_{\mathrm{NWJ}} \), respectively. Both losses consist of two terms, each derived from the statistics of joint distribution \( \mathbb{E}_{p(x,y)} \) and the product of marginal distributions \( \mathbb{E}_{p(x) \otimes p(y)} \). Hence, to observe the behavior of each loss during training, we plot the two terms separately. Also, to observe how each distribution differ by the statistics network outputs \( T_0(x,y) \), we plot each output from \( (x,y) \sim \text{Supp}(p_{XX}) \) and \( (x',y') \sim \text{Supp}(p_X \otimes p_{XX}) \), where we denote the support of \( p \) as \( \text{Supp}(p) \). Support is the set of values that the random variable can take [Taboga [2021]].

One-hot Dataset  We design a one-hot discrete problem with uniform distribution \( X \sim U(1,N) \) to estimating \( I(X,X) = \log N \) for a given integer \( N \). This task is intentionally created to easily discern samples \( (x,x) \sim p_{XX} \) from \( (x,x) \sim p_X \otimes p_X \), so that we can directly observe its network outputs \( T_0(x,x) \).

![MINE Loss Breakdown](image1)

![NWJ Loss Breakdown](image2)
Seemingly Stable Case  We first observe the behaviors of the statistics network \( T_\theta \) when the losses are seemingly stable, producing a successful MI estimate. Fig. [1] shows the MI estimates and the two terms that construct each MI estimate per batch. We observe that the first and second term estimates of \( I_{\text{MINE}} \), unlike \( I_{\text{NWJ}} \), drifting in parallel even after the MI estimate converge. This is due to the free constant term \( C \) in the optimal \( T^* \) of \( D_{\text{DV}} \), where the self-normalizing \( D_{\text{NWJ}} \) avoids this problem. This drifting phenomenon implies that \( T_\theta \) is not stable even after the loss seems to be converged, as shown in Fig. [2]. Also, the plot demonstrates how \( T_\theta \) is trained; it isolates the samples \((x, y) \sim \mathbb{P}_{XY}\) from the samples \((x, y) \sim \mathbb{P}_X \otimes \mathbb{P}_Y\).

Unstable Case  We also demonstrate the behaviors of \( T_\theta \) when the losses get unstable in Fig. [3]. We reduce the batch size to make the optimization unstable, where this behavior is often reported in multiple works [van den Oord et al. 2018 He et al. 2020 Chen et al. 2020]. However, even though the losses seem unstable, \( T_\theta \) successfully discards the samples before the outputs explode. We believe that this is because of how \( T_\theta \) is optimized during training. The statistics network outputs \( T_\theta(x_1, x_2) \) of \((x_1, x_2) \in \text{Supp}(\mathbb{P}_{XX})\) gets increased by the first term but occasionally decreased by the second term. However, \( T_\theta(x'_1, x'_2) \) of \((x'_1, x'_2) \in \text{Supp}(\mathbb{P}_{X \otimes X}) \setminus \text{Supp}(\mathbb{P}_{XX})\) gets decreased whatsoever, as \((x'_1, x'_2)\) is used only for the second term. This makes the second term unstable and motivates us to regularize it for better numerical stability during optimization.

To summarize, we suspect the instability of variational bounds comes from two reasons. Firstly, the statistics network did not converge even after the loss seemingly converged. We argue that this is due to the unnormalized constant term in the optimal \( T^* \) of \( D_{\text{DV}} \), where \( D_{\text{NWJ}} \) successfully avoids via self-normalization. Secondly, the loss gets unstable as \( T_\theta(x'_1, x'_2) \) endlessly decrease due to the second term. This observation is also consistent with the theoretical findings of [Song and Ermon 2020 McAllester and Stratos 2020], where they show that large variance of the second term leads to failed MI estimation. We claim that the outputs have to be regularized in some form to avoid the instability.

4 STABILIZING THE MI BOUNDS

In this section, we introduce two novel regularized representations and its corresponding losses to tackle the instability during optimization. We show both theoretically and experimentally that adding regularization mitigates the unstable behavior of the statistics network \( T_\theta \). We also describe a simple windowing method that can sidestep the batch size limitation problem of the MI estimation problem. We defer all the proofs to the Appendix.

Regularized representations  We stabilize the two existing representations \( D_{\text{DV}} \) and \( D_{\text{NWJ}} \) by regularizing the second term. We introduce two novel representations: Regularized DV (\( D_{\text{RDV}} \)) and Regularized NWJ (\( D_{\text{RNWJ}} \)).

\[
D_{\text{RDV}}(X, Y) := \sup_{T: \Omega \rightarrow \mathbb{R}} \mathbb{E}_P(T) - \log(\mathbb{E}_Q(e^T)) - d(\log(\mathbb{E}_Q(e^T)), C^*),
\]

\[
D_{\text{RNWJ}}(X, Y) := \sup_{T: \Omega \rightarrow \mathbb{R}} \mathbb{E}_P(T) - \mathbb{E}_Q(e^{T-1}) - d(\mathbb{E}_Q(e^{T-1}), 1),
\]

where \( C^* \in \mathbb{R} \) is any constant and \( d(*,*) \) is a distance function on \( \mathbb{R} \).

Theorem 1. \( D_{\text{RDV}} \) and \( D_{\text{RNWJ}} \) is a dual representation for \( D_{KL} \) such that

\[
D_{KL}(P||Q) = D_{\text{RDV}}(X, Y),
\]

\[
D_{KL}(P||Q) = D_{\text{RNWJ}}(X, Y).
\]
We emphasize that both representations are not MI-specific but dual representations of $D_{KL}$, which can be easily extended to numerous variational MI bounds based on $D_{DV}$ and $D_{NWJ}$. Especially, the newly added regularizer grants $D_{RDV}$ the normalizing property, effectively solving the drifting problem of $D_{DV}$.

**Regularizing $I_{MINE}$ and $I_{NWJ}$** Based on $D_{RDV}$ and $D_{RNWJ}$, we propose a novel neural network-driven variational MI bound $I_{MINE}$ and $I_{NWJ}$ by choosing the Euclidean distance $d(x, y) = (x - y)^2$ and the log-Euclidean distance $d(x, y) = (\log x - \log y)^2$, respectively.

$$I_{MINE}(X,Y) := \mathbb{E}_{x \sim P_X}(T_\theta(x, y))$$

$$- \log(\mathbb{E}_{y \sim P_Y}(e^{T_\theta(x,y)}))$$

$$- \lambda(\log(\mathbb{E}_{x \sim P_X}(e^{T_\theta(x,y)})) - C^*)^2,$$

$$I_{NWJ}(X,Y) := \mathbb{E}_{x \sim P_X}(T_\theta(x, y))$$

$$- \mathbb{E}_{y \sim P_Y}(e^{T_\theta(x,y)-1})$$

$$- \lambda(\log(\mathbb{E}_{x \sim P_X}(e^{T_\theta(x,y)-1})))^2,$$

where $C^* \in \mathbb{R}$ is any constant and $\lambda$ is a hyperparameter that controls the degree of regularization. We can also easily regularize other losses such as $I_{BeONCE}$, $I_{SMILE}$, $I_{UBA}$, and $I_S$ in a plug-and-play manner. See Table 1 for more details on its regularized counterparts.

**Solving the drifting problem** Due to the self-regularizing nature of $D_{NWJ}$, we must fix $C^* = 1$ for $I_{RNWJ}$. We also set $C^* = 0$ for $I_{MINE}$ in future experiments, but to demonstrate the ability of the regularizer term to stop the drifting, we experiment with various $C^*$ in Fig. 4. Comparing to $I_{MINE}$ in Fig. 1, we can observe that $I_{MINE}$ successfully solves the drifting problem by regularizing the second term to have a single value.

**Solving the explosion problem** We previously observed the instability of $I_{MINE}$ and $I_{NWJ}$ when using a small batch in Fig. 5. We apply the same setting to $I_{MINE}$ and $I_{RNWJ}$ to observe if the regularizer mitigates the instability problem. Both regularized losses successfully avoid the explosion problem and limit the statistics network outputs $T_\theta(x_1, x_2)$ within a certain boundary. As discussed in Section 3, the second term was the culprit of the variance in MI estimation. The newly added term directly regularizes it to stabilize training, giving the statistics network $T_\theta$ additional hints for the second term to converge to a specific value $C^*$ successfully. Furthermore, we empirically found that our regularization works well with $I_{SMILE}$’s strategy of clipping $T_\theta$. Gradient zeros out for the original $I_{SMILE}$ if $T_\theta(x,y)$ exceeds a certain threshold. This behavior makes $T_\theta$ act as if it were frozen, failing to further optimize during training. However, with the regularizer term, we can clip $T_\theta(x,y)$ only on first and second term, i.e., on the original loss. Now, clipping filters out the noisy gradients while the gradients calculated from the regularizer avoid freezing $T_\theta$ entirely.

**Mathematical properties of $I_{MINE}$ and $I_{RNWJ}$** Following Belghazi et al. [2018], we show the soundness of $I_{MINE}$ and $I_{RNWJ}$ in two perspectives, strong consistency and sample complexity. These properties relate to whether the trained $T_\theta$ can be sufficiently similar to the optimal $T^*$.

**Theorem 2.** $I_{MINE}$ and $I_{RNWJ}$ are strongly consistent.

For the two losses, we also provide the mathematical bound on the number of samples required for the empirical MI estimation at a given accuracy and with high confidence. Similar to Belghazi et al. [2018], let $T_\theta$ satisfy $L$-Lipschitz with respect to the parameter $\theta$ such that $|\theta| < K$ and $d$ is dimension of the parameter space of $T_\theta$.

**Theorem 3.** Assume that $T_\theta$ is bounded above by $M$. Let $k$ be the number of sample means. Given any $\epsilon, \delta$ of the desired accuracy and confidence parameters, we have

$$P(|I_{MINE}(X;Y) - I(X,Y)| \leq \epsilon) \geq 1 - \delta,$$

whenever the number $n$ of samples satisfies

$$n \geq d \log(24KL^2d/\epsilon) + 2dM + \log(2/\delta),$$

**Theorem 4.** Assume that $1 \leq |T_\theta| < M$ and $d(x,1) \leq |x - 1|$. Let $k$ be the number of sample means. Given any $\epsilon, \delta$ of the desired accuracy and confidence parameters, we have

$$P(|I_{NWJ}(X;Y) - I(X,Y)| \leq \epsilon) \geq 1 - \delta,$$

whenever the number $n$ of samples satisfies

$$n \geq \frac{d \log(24KL^2d/\epsilon) + 2dM + \log(2/\delta)}{\epsilon^2 k/(2M^2)}.$$
whenever the number $n$ of samples satisfies

$$n \geq \frac{d \log(24K L \sqrt{d}/\epsilon) + 2d M + \log(2/\delta)}{\epsilon^2 k/(2M^2)}.$$  

(19)

**Drifting may lead to noisy MI estimate** We prove that the variance of the second term on the empirical distributions is affected by the constant term $C^*$.  

**Theorem 5.** Let $Q^{(n)}$ be the empirical distributions of $n$ i.i.d. samples from $Q$. For the optimal $T_1 = \log \frac{dp}{dq} + C_1$ and $T_2 = \log \frac{dp}{dq} + C_2$ where $C_1 \geq C_2$,

$$\text{Var}_Q(\mathbb{E}_{Q^{(n)}}(e^{T_1})) \geq \text{Var}_Q(\mathbb{E}_{Q^{(n)}}(e^{T_2}))$$  

(20)

This implies that unregulated $C^*$ may lead to worse MI estimation quality, as the source of the estimate variance are mainly due to the second term.

**Increasing the effective sample size for MI estimation**

The drifting problem caused by the unnormalized constant term $C^*$ raises more issues when estimating MI. Poole et al. [2019] use a simple macro-averaging technique, i.e., averaging the estimated MI from each batch. We can also consider a slight modification to the technique, where we call it the micro-averaging technique, by saving all the statistics network outputs $T_\theta(x, y)$ for each batch and producing a single estimate based on all the outputs. However, we proved that both averaging techniques yield worst possible estimates for biased estimators like $I_{\text{MINE}}$ [Belghazi et al. 2018], $I_{\text{SMILE}}$ [Song and Ermon 2020], $I_{\text{CLUB}}$ [Cheng et al. 2020], and $I_{\text{InfoNCE}}$ [van den Oord et al. 2018].

**Theorem 6.** (Estimation bias caused by drifting) Both macro- and micro-averaging strategies produce a biased MI estimate when the drifting problem occurs.

To the contrary, self-normalizing or regularized MI estimators have the upper hand in this perspective. By utilizing all the samples from multiple batches, they can effectively sidestep the batch size limitation problem [McAllester and Stratos 2020] Song and Ermon 2020].

5 EXPERIMENTS

5.1 MI ESTIMATION VS. DOWNSTREAM TASK PERFORMANCE

**Benchmark Design** To measure the performance of the MI estimators, one must design the target task to have the ground truth MI. This constraint led previous works to evaluate the estimators only on artificial toy problems [Belghazi et al. 2018] Poole et al. 2019], where its connection to actual problems is fairly limited. We design the two types of MI estimation tasks with de facto image datasets to improve the existing benchmarks to reflect on the real-world tasks. We defer all the proofs to the Appendix.

**Theorem 7.** (Supervised learning) Given a dataset $D = (X, Y)$ where $X$ is an sample, $Y$ is the label for $X$, and $H(Y)$ is the entropy of the label set, $I(X, Y) = H(Y)$.

Similarly, the true MI between images from the same class is also tractable based on the same assumption.

**Theorem 8.** (Contrastive learning) Consider the dataset $D = (X, Y)$. Let $X_1$ be a sample drawn from the dataset and $X_2$ be another sample drawn from the subset with the same label $Y$ to $X_1$. Then, $I(X_1, X_2) = I(X_1, Y) = I(X_2, Y) = H(Y)$.

Note that we assume statistical dependence between the image $X$ and label $Y$ from the point of view of information bottleneck [Tishby and Zaslavsky 2015]. We derive the theorems above based on the assumption, where $Y$ implicitly determines $X$.

Based on the above theorems, we use the two MI estimation problems as benchmarks that evaluate the performance of estimators. We intentionally design Theorem 7 and Theorem 8 to mimic the existing tasks closely, namely, supervised and contrastive learning. For Theorem 7 we can set the statistics network $T_\theta(X, Y) = f_\theta(X) \cdot o(Y)$ where $f_\theta(X)$ is the logs obtained from feeding the image $X$ to the classification neural networks and $o(Y)$ is the one-hot representation of the label $Y$. If we use the InfoNCE estimator, this formulation becomes identical to solving the classification problem using negative log loss with the Softmax function, hence the name being the supervised learning benchmark (SLB). Similarly, for Theorem 8 we can set $T_\theta(X_1, X_2) = f_\theta(X_1) \cdot f_\theta(X_2)$ and use the InfoNCE estimator to yield a commonly used contrastive loss [van den Oord et al. 2018] Chen et al. 2020].

Due to the strict assumption of statistical dependence, the theorems above cannot be used on standard datasets like ImageNet dataset [Deng et al. 2009], as its samples often violate the single-label assumption. However, we can still empirically compare the MI estimators by the relative size of their final MI estimation. We conduct a demo experiment on ImageNet in the Appendix.

**Evaluation** To verify the performance of MI estimators, we perform our benchmark tasks on the CIFAR10 and CIFAR100 dataset [Krizhevsky 2009]. As both CIFAR10 and CIFAR100 have a uniform label distribution, ideal MI is log $10$ and log $100$, respectively. In addition, to check whether this MI estimation task is actually helpful for downstream tasks, we evaluate each estimator on both dimensions: MI estimation and test set accuracy. Similar to the existing settings in the contrastive learning literature [Chen et al. 2020] He et al. 2020], we design the test accuracy of CLB by defining the label estimate $\hat{y}$ of each test set sample $x_{\text{Test}}$ to be the label of $x = \arg\max_{y \in X_{\text{Train}}} f(x) \cdot f(x_{\text{Test}})$ of the train dataset $X_{\text{Train}}$. Similarly for SLB, we chose...
We observe in Table 2 that additional regularization generally induces better performance on both the MI estimation task and the downstream task (test accuracy). Hence, adding the regularizer to a pre-existing supervised or contrastive learning loss seems to be a viable option to increase the performance further. Even when the performance of the regularized loss slightly degrades, its negative impact is minimal. This implies that even for the case where the regularizer is not greatly helpful, it does not greatly hinder optimization. Especially, it is intriguing that many losses, $I_{\text{MINE}}$, $I_{\text{SMILE}}$, and $I_{\text{TUBA}}$, are better than $I_{\text{InfoNCE}}$ in SLB, which is used as the de facto standard in classification. Also, $I_{\text{MINE}}$, $I_{\text{NWJ}}$, and $I_{\text{TUBA}}$ fail to converge in CLB, where simply adding a regularization term solves the issue altogether, yielding a competitive or even better performance than all the other losses. Given the fact that numerous contrastive learning literature suffers from instability [Caron et al., 2021; Bardes et al., 2021; Chen et al., 2020; He et al., 2020; Bardes et al., 2021], we emphasize that adding our regularization term can be a simple yet effective method to stabilize training.

Additionally, to observe the impact of regularization strength $\lambda$, we plot the benchmark performance for each $\lambda$ in Fig. 6. We compare the losses on CLB as experimental results suggest that CLB is a more difficult task than SLB, showing significant performance differences between various losses. On CIFAR-10, $\lambda$ acts as a trade-off parameter between test accuracy and MI estimation quality. Performance trade-off has also been reported in other literature, where better MI estimation does not necessarily deliver better downstream performance [Tschannen et al., 2020; Tian et al., 2020b]. However, compared to CIFAR-100, test accuracy differences are minimal, where MI differences are apparent. $I_{\text{ReMINE}}$ and $I_{\text{ReSMILE}}$ show excellent MI estimation quality in CIFAR-10 compared to other losses. In contrast, test accuracy and MI estimation quality align well in the CIFAR-100 case. $I_{\text{ReSMILE}}$ shows good overall performance, albeit its sensitivity towards regularization strength. $I_{\text{ReInfoNCE}}$, on the other hand, shows stable performance in the downstream task, sacrificing the MI estimation quality. This result is further supported by the prominence of $I_{\text{InfoNCE}}$ in the contrastive learning domain. It is yet unclear where the difference between CIFAR-10 and CIFAR-100 comes from, whether it is due to the difference in the level of difficulty of the dataset or the batch size used throughout the training. We leave further analysis as future work.

5.3 COMPARISON WITH THE STANDARD TOY PROBLEM

We provide the quality of MI-based losses on the 20D Correlated Gaussian task [Belghazi et al. 2018; Poole et al. 2019] where the true MI is increased 5 times during optimization in Fig. 7. This experiment demonstrates how stable the MI-based losses estimate MI in a dynamically changing environment. We apply the same settings from

\[
y = \arg\max_x f(x_{\text{true}}) \cdot o(y) \text{ where } o(y) \text{ is the one-hot encoding of } y.\]
Table 2: Our supervised and contrastive learning benchmark results. We provide the 95% confidence interval of 5 runs for both MI estimation and test accuracy, where we clip the negative MI estimations to 0. We compare the performance of original and regularized loss. Bold text and blue text indicates the better performance with overlapping and non-overlapping confidence interval, respectively.

Table 1 where we fix the regularization strength $\lambda = 1.0$ for all the losses. With the exception of $I_{\text{InfoNCE}}$, regularized losses show clear superiority over the original losses. Regularization facilitates $I_{\text{MINE}}$ and $I_{\text{SMILE}}$ to avoid the instability which is mentioned in Section 3. Also, regularization greatly enhances the MI estimation quality of $I_{\text{JS}}$ and lessens the variance of both $I_{\text{NWJ}}$ and $I_{\text{TUBA}}$.

6 CONCLUSION

In this paper, we identify the two symptoms behind the instability: The statistics network was not converging even after the loss seemed to converge, and its outputs from the product of marginal distribution explode during training. We propose a novel regularization term to mitigate the instability during training by adding to various existing MI-based losses. We theoretically and experimentally demonstrate that the added regularizer directly alleviates the two instability symptoms. Finally, we present a benchmark that evaluates both the MI estimation power and its capability on the downstream tasks by imitating the supervised or contrastive learning settings. We compare six different losses and their regularized counterparts on various benchmarks to show the method’s effectiveness and broad applicability.

Figure 7: Estimation performance on 20-D Gaussian. The estimated MI (light) and the smoothed estimation with exponential moving average (dark) are plotted for each methods with its regularized counterparts. Black line represents the true MI. Dotted line shows the bound of $I_{\text{InfoNCE}}$ due to the limited batch size of 64.
LIMITATIONS AND FUTURE WORKS

We suspect that the instability of MI estimators can also be related to the collapse problem [Bardes et al., 2021] [Caron et al., 2021]. Further loss-based approaches to combat this problem by regularizing the network outputs may be helpful. We expect that extending our methods to various contrastive learning losses may yield fruitful results for self-supervised learning, notably for other domains such as text or audio. Also, our mathematical analysis is mainly focused on the drifting problem of $I_{\text{MINE}}$, not the explosion problem of $I_{\text{NWJ}}$. For $I_{\text{NWJ}}$, we suspect that the absence of the log function wrapping the exponential values makes the second term much more susceptible to output explosion due to its numerical instability. The added regularizer gives additional hints for the second term to converge to a specific value. However, we did not expand the discussion further in this paper.

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Combating the Instability of Mutual Information-based Losses via Regularization (Supplementary material)

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A PROOFS

In this section, we provide proof of all theoretical results mentioned in the manuscript.

A.1 PROOF OF THE $D_{\text{REDV}}$ REPRESENTATION

In this subsection, we consider two probability distributions $P$ and $Q$, with $P$ absolutely continuous with respect to $Q$. In addition, assume that both distributions are absolutely continuous with respect to Lebesgue measure $\mu$ on some compact domain $\Omega$.

We first show that there exists the family of optimal function for the DV representation [Donsker and Varadhan, 1975].

**Lemma 9.** All functions of the form $T = \log \frac{dP}{dQ} + C^*$ is optimal for the DV representation $D_{\text{DV}}$.

**Proof.** To show this theorem, we borrow the proof of the dual representation for the KL divergence [Belghazi et al., 2018].

For a function $T$, let $\Delta_T$ be the gap

$$ \Delta_T := D_{\text{KL}}(P||Q) - (\mathbb{E}_P(T) - \log \mathbb{E}_Q(e^T)). $$

By Theorem 1 of MINE [Donsker and Varadhan, 1975], we already knew that there exists an optimal function $T^* = \log \frac{dP}{dQ} + C$ for some $C \in \mathbb{R}$ such that $\Delta_{T^*} = 0$.

Consider a function $T = \log \frac{dP}{dQ} + C^*$ for $C^* \in \mathbb{R}$. The function $T$ can be rewritten as $(T^* - C) + C^*$.

Since

$$ \mathbb{E}_P(T) = \mathbb{E}_P(T^* - C + C^*) $$

$$ = \mathbb{E}_P(T^*) - C + C^*, $$

and

$$ \log(\mathbb{E}_Q(e^T)) = \log(\mathbb{E}_Q(e^{T^*} - C + C^*)) $$

$$ = \log(e^{C^* - C} \mathbb{E}_Q(e^{T^*})) $$

$$ = (C^* - C) + \log(\mathbb{E}_Q(e^{T^*})), $$

$$ \mathbb{E}_P(T) - \log(\mathbb{E}_Q(e^T)) = \mathbb{E}_P(T^*) - \log(\mathbb{E}_Q(e^{T^*})). $$

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Accepted for the 38th Conference on Uncertainty in Artificial Intelligence (UAI 2022).
Therefore, for the function $T$,
\[
\Delta_T = D_{KL}(P||Q) - (\mathbb{E}_P(T) - \log \mathbb{E}_Q(e^T)) = D_{KL}(P||Q) - \left(\mathbb{E}_P(T^*) - \log \mathbb{E}_Q(e^{T^*})\right) = \Delta_{T^*} = 0. \tag{28}
\]

As a result, optimal functions takes the form $T = \log \frac{dP}{dQ} + C^*$ for some constant $C^* \in \mathbb{R}$.

**Theorem.** (Theorem 1 restated) Let $d$ be a distance function on $\mathbb{R}$. For any constant $C^* \in \mathbb{R}$ and any class of functions $T$ mapping from $\Omega$ to $\mathbb{R}$, we have a novel dual representation of KL divergence

\[
D_{RDV} := \sup_{T \in \mathcal{T}} \mathbb{E}_P(T) - \log(\mathbb{E}_Q(e^T)) - d(\log(\mathbb{E}_Q(e^T)), C^*) = D_{KL}(P||Q). \tag{29}
\]

**Proof.** i) For any $T$,
\[
\mathbb{E}_P(T) - \log(\mathbb{E}_Q(e^T)) - d(\log(\mathbb{E}_Q(e^T)), C^*) \leq \mathbb{E}_P(T) - \log(\mathbb{E}_Q(e^T)). \tag{30}
\]

Therefore, $\sup_{T: \Omega \rightarrow \mathbb{R}} \mathbb{E}_P(T) - \log(\mathbb{E}_Q(e^T)) - d(\log(\mathbb{E}_Q(e^T)), C^*) \leq D_{KL}(P||Q)$.

ii) By the lemma above, there exists $T^* = \log \frac{dP}{dQ} + C^*$ such that
\[
D_{KL}(P||Q) = \mathbb{E}_P(T^*) - \log(\mathbb{E}_Q(e^{T^*})) \tag{31}
\]

and
\[
\log(\mathbb{E}_Q(e^{T^*})) = \log(\mathbb{E}_Q(e^{C^*})) = \log(\int e^{C^*} \frac{dP}{dQ} dQ) = C^*. \tag{32}
\]

Therefore,
\[
\sup_{T: \Omega \rightarrow \mathbb{R}} \mathbb{E}_P(T) - \log(\mathbb{E}_Q(e^T)) - d(\log(\mathbb{E}_Q(e^T)), C^*) \geq \mathbb{E}_P(T^*) - \log(\mathbb{E}_Q(e^{T^*})) - d(\log(\mathbb{E}_Q(e^{T^*})), C^*) \tag{33}
\]

\[
= D_{KL}(P||Q). \tag{34}
\]

Combining i) and ii) finishes the proof.

\[
\square
\]

### A.2 EXTENSION TO NWJ REPRESENTATION

In this subsection, we show that our regularizer can also be applied to the NWJ representation [Nguyen et al., 2010].

**Theorem.** Let $d$ be a distance function on $\mathbb{R}$. We have another dual representation such that

\[
D_{RDNWJ} := (P||Q) = \sup_{T: \Omega \rightarrow \mathbb{R}} \mathbb{E}_P(T) - \mathbb{E}_Q(e^{T-1}) - d(\mathbb{E}_Q(e^{T-1}), 1) = D_{KL}(P||Q). \tag{35}
\]

**Proof.** As $d$ is a distance function, $d(\mathbb{E}_Q(e^{T-1}), 1) \geq 0$.

i) For any $T$,
\[
\mathbb{E}_P(T) - \mathbb{E}_Q(e^{T-1}) - d(\mathbb{E}_Q(e^{T-1}), 1) \leq \mathbb{E}_P(T) - \mathbb{E}_Q(e^{T}). \tag{36}
\]

Therefore, $\sup_{T: \Omega \rightarrow \mathbb{R}} \mathbb{E}_P(T) - \mathbb{E}_Q(e^{T-1}) - d(\mathbb{E}_Q(e^{T-1}), 1) \leq D_{KL}(P||Q)$.

ii) By Poole et al. [2019], there exists $T^* = \log \frac{dP}{dQ} + 1$ such that
\[
D_{KL}(P||Q) = \mathbb{E}_P(T^*) - \mathbb{E}_Q(e^{T^*-1}). \tag{37}
\]

\[
\mathbb{E}_P(T^*) = \mathbb{E}_P(1 + \log \frac{dP}{dQ}) = 1 + D_{KL}(P||Q). \tag{38}
\]
and
\[ E_Q(e^{T^*-1}) = E_Q\left(\frac{dP}{dQ}\right) = 1. \] (39)

Therefore,
\[ \sup_{T: \Omega \to \mathbb{R}} E_P(T) - E_Q(e^{T^*-1}) - d(E_Q(e^{T^*-1}), 1) \geq E_P(T^*) - E_Q(e^{T^*-1}) - d(E_Q(e^{T^*-1}), 1) \]
\[ = D_{KL}(P \parallel Q). \] (41)

Combining i) and ii) finishes the proof. \(\square\)

### A.3 Mathematical Properties of \(I_{\text{ReMINE}}\)

This subsection presents the proof of the consistency and the sample complexity of \(I_{\text{ReMINE}}\). To show these properties, we assume that the input space of the functions below is a compact domain, and all measures are absolutely continuous with respect to the Lebesgue measure. We will restrict to families of feedforward functions with continuous activations, with a single output neuron. To avoid unnecessary heavy notation, we denote \(P = P_{X,Y}\) and \(Q = P_X \otimes P_Y\) as the joint distribution and the product of marginals unless specified.

First, we define the sample complexity of the MI estimator. As mentioned by Belghazi et al. [2018], this property is related to the approximation problem, which addresses the size of the family of function \(T_\theta\), and the estimation problem, which addresses whether it is a reliable estimator.

**Definition 1.** The MI estimator \(\hat{I}(X,Y)_n\) is strongly consistent if for all \(\epsilon > 0\), there exists a positive integer \(N\) and a choice of statistics networks such that \(\forall n \geq N, |I(X,Y) - \hat{I}(X,Y)_n| \leq \epsilon\), where the probability is over a set of samples.

**Consistency Proof**

**Lemma 10.** (Approximation) Let \(\eta > 0\). There exists a neural network function \(T_\theta\) with parameters \(\theta \in \Theta\) such that
\[ |\hat{I}_{\text{ReMINE}}(X,Y) - I_{\text{ReMINE}}(X,Y)| \leq \eta, \] (42)
where
\[ \hat{I}_{\text{ReMINE}}(X,Y) = \sup_{\theta \in \Theta} E_P(T_\theta) - \log(E_Q(e^{T_\theta})) - d(\log(E_Q(e^{T_\theta})), C^*). \] (43)

**Proof.** Without loss of generality, we set \(T^* = \log \frac{dP}{dQ}\). By construction, \(T^*\) satisfies:
\[ E_P(T^*) = I(X,Y), \quad E_Q(e^{T^*}) = 1, \quad \log(E_Q(e^{T^*})) = 0 \] (44)

For a function \(T\),
\[ I_{\text{ReMINE}}(X,Y) - \hat{I}_{\text{ReMINE}}(X,Y) \]
\[ \leq E_P(T^* - T) + \log(E_Q(e^{T^*})) + d(\log(E_Q(e^{T^*})), C^*) - d(\log(E_Q(e^{T^*})), C^*) \]
\[ \leq E_P(T^* - T) + \log(E_Q(e^{T^*})) + d(\log(E_Q(e^{T^*})), \log(E_Q(e^{T^*})) \]
\[ \leq E_P(T^* - T) + E_Q(e^{T^*} - e^{T^*}) + d(\log(e^{T^*} - 1), 0) \] (48)

where we used the inequality \(\log x \leq x - 1\) and \(d(\cdot, \cdot)\) is the distance function induced by norm on \(\mathbb{R}\) (e.g., absolute or square error). Fix \(\eta > 0\). By the universal approximation theorem, we may choose a feedforward network function \(T_\theta \leq M\) such that
\[ E_P|T^* - T_\theta| \leq \frac{\eta}{3}, \quad E_Q|T^* - T_\theta| \leq \frac{\eta}{3} e^{-M}, \quad \text{and} \quad d(E_Q|T_\theta - T^*|, 0) \leq \frac{\eta}{3} \cdot d(e^M, 0) \] (49)

Since exp is Lipschitz continuous with constant \(e^M\) on \((-\infty, M]\), we have
\[ E_Q|e^{T^*} - e^{T_\theta}| \leq e^M E_Q|T^* - T_\theta| \leq \frac{\eta}{3}, \] (50)
and
\[ d(\mathbb{E}_Q(e^T) - 1, 0) = d(\mathbb{E}_Q(e^{T_\theta}) - \mathbb{E}_Q(e^{T^*}), 0) = d(\mathbb{E}_Q|e^{T_\theta} - e^{T^*}|, 0) \]
\[ \leq d(e^M |e^{T_\theta} - T^*|, 0) \leq d(e^M, 0) \cdot d(\mathbb{E}_Q|T_\theta - T^*|, 0) \leq \frac{\eta}{3}. \]  
(51)

From Eq. (48), Eq. (49), Eq. (50), Eq. (51) and the triangular inequality, we then obtain:
\[ |\hat{I}_{\text{ReMINE}}(X, Y) - I_{\text{ReMINE}}(X, Y)| < \eta. \]  
(53)

\[ \square \]

**Lemma 11.** (Estimation) Let \( \eta > 0 \). Given a neural network function \( T_\theta \) with parameters \( \theta \in \Theta \), there exists \( N \in \mathbb{N} \) such that
\[ \forall n \geq N, \mathbb{P}(|\hat{I}_{\text{ReMINE}}(X, Y)_n - \hat{I}_{\text{ReMINE}}(X, Y)| \leq \eta) = 1, \]  
(54)
where \( \hat{I}_{\text{ReMINE}}(X, Y)_n \) is the ReMINE representation which is empirically obtained by \( n \) samples.

**Proof.** We start by using the triangular inequality to write,
\[ |\hat{I}_{\text{ReMINE}}(X, Y)_n - \sup_{\theta \in \Theta} \hat{I}_{\text{ReMINE}}(T_\theta)| \leq \sup_{\theta \in \Theta} |\mathbb{E}_\varphi(T_\theta) - \mathbb{E}_{\varphi_n}(T_\theta)| + \sup_{\theta \in \Theta} |\mathbb{E}_Q(e^{T_\theta}) - \log \mathbb{E}_{Q_n}(e^{T_\theta})| \]
\[ + \sup_{\theta \in \Theta} d(|\log \mathbb{E}_Q(e^{T_\theta}) - \log \mathbb{E}_{Q_n}(e^{T_\theta})|, 0). \]  
(55)

Since the function \( T_\theta \) is uniformly bounded by a constant \( M \) and \( \log \) is Lipschitz continuous with constant \( e^M \), we have
\[ |\log \mathbb{E}_Q(e^{T_\theta}) - \log \mathbb{E}_{Q_n}(e^{T_\theta})| \leq e^M |\mathbb{E}_Q(e^{T_\theta}) - \mathbb{E}_{Q_n}(e^{T_\theta})| \]  
(56)
and
\[ d(|\log \mathbb{E}_Q(e^{T_\theta}) - \log \mathbb{E}_{Q_n}(e^{T_\theta})|, 0) \leq d(e^M, 0) \cdot d(|\mathbb{E}_Q(e^{T_\theta}) - \mathbb{E}_{Q_n}(e^{T_\theta})|, 0). \]  
(57)

Since \( \Theta \) is compact and the feedforward network function is continuous, \( T_\theta \) and \( e^{T_\theta} \) satisfy the uniform law of large numbers [Belghazi et al. 2018]. Given \( \epsilon > 0 \), we can thus choose \( N \in \mathbb{N} \) such that \( \forall n \geq N \) and with probability 1,
\[ \sup_{\theta \in \Theta} |\mathbb{E}_\varphi(T_\theta) - \mathbb{E}_{\varphi_n}(T_\theta)| \leq \frac{\eta}{3}, \]  
(58)
\[ \sup_{\theta \in \Theta} |\mathbb{E}_Q(e^{T_\theta}) - \mathbb{E}_{Q_n}(e^{T_\theta})| \leq e^{-M} \frac{\eta}{3}, \]  
(59)
\[ \sup_{\theta \in \Theta} d(|\mathbb{E}_Q(e^{T_\theta}) - \mathbb{E}_{Q_n}(e^{T_\theta})|, 0) \leq \frac{1}{d(e^M, 0)} \frac{\eta}{3}. \]  
(60)

Hence, this leads to
\[ |\hat{I}_{\text{ReMINE}}(X, Y)_n - \hat{I}_{\text{ReMINE}}(X, Y)| \leq \frac{\eta}{3} + \frac{\eta}{3} + \frac{\eta}{3} = \eta. \]  
(61)

\[ \square \]

**Theorem.** ReMINE is strongly consistent.

**Proof.** Let \( \epsilon > 0 \). We apply Lemma 10 and Lemma 11 to find a neural network function \( T_\theta \) and \( N \in \mathbb{N} \) such that Eq. (42) and Eq. (54) hold with \( \eta = \epsilon/2 \). By the triangular inequality, for all \( n \geq N \) and with probability one, we have:
\[ |I(X, Y) - \hat{I}_{\text{ReMINE}}(X, Y)_n| = |\hat{I}_{\text{ReMINE}}(X, Y) - \hat{I}_{\text{ReMINE}}(X, Y)_n| \quad (\therefore \text{Theorem 1}) \]
\[ \leq |\hat{I}_{\text{ReMINE}}(X, Y) - \hat{I}_{\text{ReMINE}}(X, Y)| + |\hat{I}_{\text{ReMINE}}(X, Y)_n - \hat{I}_{\text{ReMINE}}(X, Y)| \leq \epsilon \]  
(62)
which proves the consistency.  
\[ \square \]
Sample complexity proof

**Theorem.** Assume that the function \( T_\theta \) are \( M \)-bounded and \( \mathcal{L} \)-lipschitz with respect to the parameter \( \theta \). The domain \( \theta \) is bounded, so that \( \| \theta \| \leq K \) for some constant \( K \). When using \( k \) mini-batches to estimate \( MI \), we have

\[
P(|\hat{I}_{\text{ReMINE}}(X, Y) - I(X, Y)| \leq \epsilon) \geq 1 - \delta
\]

whenever the number of samples \( n \) for each batch satisfies

\[
n \geq \frac{2M^2(d \log(24Kd\sqrt{d}/\epsilon) + 2dM + \log(2/\delta))}{\epsilon^2 k}
\]

**Proof.** As the optimal \( T^* \) of \( I_{\text{ReMINE}} \) is also the solution of \( I_{\text{MINE}} \), we can use the same proof process of the Theorem 6 in [Belghazi et al., 2018]. Contrast to MINE [Belghazi et al., 2018], we start from \( P(\|E_Q[f] - E_Q[\hat{f}]\| > \epsilon/6) \leq 2 \exp(-\frac{\epsilon^2 nk}{2M^2}) \) by the Hoeffding inequality, because we use \( n \cdot k \) samples and our loss function consists of three terms including the regularization term. \( \square \)

### A.4 MATHEMATICAL PROPERTIES OF \( I_{\text{ReNWJ}} \)

**Consistency Proof** We show the proof of the consistency for the ReNWJ based estimator. Same to the proof of ReMINE consistency, we assume that the input space of the functions below is a compact domain, and all measures are absolutely continuous with respect to the Lebesgue measure. We will also restrict to families of feedforward functions with continuous activations, with a single output neuron. We provide a proof for the case where \( d(\cdot, \cdot) \) is the log-Euclidean distance in this subsection.

**Lemma 12.** (Approximation) Let \( \eta > 0 \). There exists a neural network function \( T_\theta \) with parameters \( \theta \in \Theta \) such that

\[
|\hat{I}_{\text{ReNWJ}}(X, Y) - I_{\text{ReNWJ}}(X, Y)| \leq \eta \tag{65}
\]

where

\[
\hat{I}_{\text{ReNWJ}}(X, Y) = \sup_{\theta \in \Theta} \mathbb{E}_\theta(T_\theta) - \mathbb{E}_Q(e^{T_\theta - 1}) - d(\mathbb{E}_Q(e^{T_\theta - 1}), 1). \tag{66}
\]

**Proof.** Without loss of generality, we set \( T^* = \log \frac{d^2}{\delta^2} + 1 \). By construction, \( T^* \) satisfies

\[
\mathbb{E}_p(T^*) = 1 + I(X, Y), \quad \mathbb{E}_Q(e^{T^* - 1}) = 1. \tag{67}
\]

For a function \( T \),

\[
I_{\text{ReNWJ}}(X, Y) - \hat{I}_{\text{ReNWJ}}(X, Y) \leq \mathbb{E}_p(T^* - T) + \mathbb{E}_Q(e^{T^* - 1} - e^{T^* - 1}) + d(\mathbb{E}_Q(e^{T^* - 1}), 1) - d(\mathbb{E}_Q(e^{T^* - 1}), 1) \tag{68}
\]

\[
\leq \mathbb{E}_p(T^* - T) + \mathbb{E}_Q(e^{T^* - 1} - e^{T^* - 1}) + d(\mathbb{E}_Q(e^{T^* - 1}), 1) \tag{69}
\]

\[
\leq \mathbb{E}_p(T^* - T) + e^{T^* - 1}\mathbb{E}_Q(e^{T^* - 1}) + d(\mathbb{E}_Q(e^{T^* - 1}), 1) \tag{70}
\]

where \( d(\cdot, \cdot) \) is the log-Euclidean distance on \( \mathbb{R} \). Fix \( \eta > 0 \). By the universal approximation theorem, we may choose a feedforward network function \( T_\theta \leq M \) with \( M > 1 \) such that

\[
\mathbb{E}_p|T^* - T_\theta| \leq \frac{\eta}{3}, \quad \mathbb{E}_Q|T^* - T_\theta| \leq \frac{\eta}{3} e^{1-M}, \quad \text{and} \quad d(\mathbb{E}_Q(e^{T_\theta}), e) \leq \frac{\eta}{3}. \tag{72}
\]

Since \( \exp \) is Lipschitz continuous with constant \( e^M \) on \((-\infty, M]\), we have

\[
\mathbb{E}_Q|e^{T^*} - e^{T_\theta}| \leq e^M \mathbb{E}_Q|T^* - T_\theta| \leq \frac{\eta}{3} e. \tag{73}
\]

And

\[
d(\mathbb{E}_Q(e^{T^* - 1}), 1) = d(\mathbb{E}_Q(e^{T_\theta}), \mathbb{E}_Q(e^{T^* - 1})) \leq d(\mathbb{E}_Q(e^{T_\theta}), e) \leq \frac{\eta}{3}. \tag{74}
\]
From Eq. (71), Eq. (73), Eq. (74) and the triangular inequality, we then obtain

\[ |\hat{I}_{\text{ReNWJ}}(X, Y) - I_{\text{ReNWJ}}(X, Y)| < \eta. \]  

(75)

**Lemma 13.** (Estimation) Let \( \eta > 0 \). Given a neural network function \( T_{\theta} \) with parameters \( \theta \in \Theta \), there exists \( N \in \mathbb{N} \) such that

\[ \forall n \geq N, \mathbb{P}(|\hat{I}_{\text{ReNWJ}}(X, Y)_n - \hat{I}_{\text{ReNWJ}}(X, Y)| \leq \eta) = 1, \]  

(76)

where \( \hat{I}_{\text{ReNWJ}}(X, Y)_n \) is the ReNWJ representation which is empirically obtained by \( n \) samples.

**Proof.** We start by using the triangular inequality to write,

\[
|\hat{I}_{\text{ReNWJ}}(X, Y)_n - \sup_{\theta \in \Theta} \hat{I}_{\text{ReNWJ}}(T_{\theta})| \leq \sup_{\theta \in \Theta} |E_P(T_{\theta}) - E_{P_n}(T_{\theta})| + \sup_{\theta \in \Theta} |E_Q(e^{T_{\theta} - 1})| \nonumber
\]

\[ + \sup_{\theta \in \Theta} d(E_Q(e^{T_{\theta} - 1}), E_{Q_n}(e^{T_{\theta} - 1})). \]  

(77)

Since \( \Theta \) is compact and the feedforward network \( T_{\theta} \) is continuous and uniformly bounded by a constant \( M \), \( T_{\theta} \) and \( e^{T_{\theta}} \) satisfy the uniform law of large numbers [Belghazi et al., 2018]. Given \( \epsilon > 0 \), we can thus choose \( N \in \mathbb{N} \) such that \( \forall n \geq N \) and with probability 1,

\[ \sup_{\theta \in \Theta} |E_P(T_{\theta}) - E_{P_n}(T_{\theta})| \leq \frac{\eta}{3}, \]  

(78)

\[ \sup_{\theta \in \Theta} e^{T_{\theta} - 1}|E_Q(e^{T_{\theta}}) - E_{Q_n}(e^{T_{\theta}})| \leq \frac{\eta}{3} e^{-M}, \]  

(79)

\[ \sup_{\theta \in \Theta} d(E_Q(e^{T_{\theta}}), E_{Q_n}(e^{T_{\theta}})) \leq \frac{\eta}{3}. \]  

(80)

Hence, this leads to

\[ |\hat{I}_{\text{ReNWJ}}(X, Y)_n - \hat{I}_{\text{ReNWJ}}(X, Y)| \leq \frac{\eta}{3} + \frac{\eta}{3} + \frac{\eta}{3} = \eta. \]  

(81)

**Theorem.** The ReNWJ estimator is strongly consistent.

**Proof.** Let \( \epsilon > 0 \). We apply Lemma 12 and Lemma 13 to find a neural network function \( T_{\theta} \) and \( N \in \mathbb{N} \) such that Eq. (65) and Eq. (76) hold with \( \eta = \epsilon/2 \). By the triangular inequality, for all \( n \geq N \) and with probability one, we have

\[ |I(X, Y) - \hat{I}_{\text{ReNWJ}}(X, Y)_n| = |I_{\text{ReNWJ}}(X, Y) - \hat{I}_{\text{ReNWJ}}(X, Y)| \quad \text{(\because ReNWJ representation)} \]

\[ \leq |I_{\text{ReNWJ}}(X, Y) - \hat{I}_{\text{ReNWJ}}(X, Y)| + |\hat{I}_{\text{ReNWJ}}(X, Y)_n - \hat{I}_{\text{ReNWJ}}(X, Y)| \leq \epsilon \]  

(82)

which proves the consistency.

**Sample complexity proof**

**Theorem.** Assume that the function \( 1 \leq |T_{\theta}| < M \) is \( \mathcal{L} \)-lipschitz with respect to the parameter \( \theta \). The domain \( \theta \) is bounded, so that \( ||\theta|| \leq K \) for some constant \( K \). When using \( k \) mini-batches to estimate MI and \( d(x, 1) \leq |x - 1| \), we have

\[ \mathbb{P}(|\hat{I}_{\text{ReNWJ}}(X, Y) - I(X, Y)| \leq \epsilon) \geq 1 - \delta \]  

(83)

whenever the number of samples \( n \) for each batch satisfies

\[ n \geq \frac{2M^2(24KL\sqrt{d}/\epsilon + 2dM + \log(2/\delta))}{\epsilon^2k}. \]  

(84)
We now choose that ball radius to be \( \eta \)
\( \Theta \subset \mathbb{R}^d \) by a finite set of small balls of radius \( \eta \).
\( \Theta \subset \bigcup_j B_\eta(\theta_j) \), and the union bound. The minimal cardinality of such covering is bounded by the covering number \( N_\eta(\Theta) \) of \( \Theta \),
\[
N_\eta(\Theta) \leq \left( \frac{2K \sqrt{d}}{\eta} \right)^d.
\] (86)

Successively applying a union bound in Eq. (85) with the set of functions \( \{T_\theta\}_j \), and \( \{e^{T_\theta}\}_j \). We have
\[
P \left( \max_j |E_Q(T_\theta) - E_{\hat{Q}}(T_\theta)| \geq \frac{\epsilon}{6} \right) \leq 2N_\eta(\Theta) \exp\left(-\frac{\epsilon^2(n \cdot k)}{2M^2}\right),
\] (87)
\[
P \left( \max_j |E_Q(e^{T_\theta}) - E_{\hat{Q}}(e^{T_\theta})| \geq \frac{\epsilon}{6} \right) \leq 2N_\eta(\Theta) \exp\left(-\frac{\epsilon^2(n \cdot k)}{2M^2}\right).
\] (88)

We now choose that ball radius to be \( \eta = \frac{\epsilon}{12} e^{-2M} \). Solving for \( n \) the inequation,
\[
2N_\eta(\Theta) \exp\left(-\frac{\epsilon^2 n}{2M^2}\right) \leq \delta,
\] (89)
we deduce from Eq. (87) that, whenever Eq. (84) holds, with probability at least \( 1 - \delta \), for all \( \theta \in \Theta \),
\[
|E_Q(T_\theta) - E_{\hat{Q}}(T_\theta)| \leq |E_Q(T_\theta) - E_Q(T_{\theta_j})| + |E_Q(T_{\theta_j}) - E_{\hat{Q}}(T_{\theta_j})| + |E_{\hat{Q}}(T_{\theta_j}) - E_Q(T_{\theta_j})| \leq \frac{\epsilon}{12} e^{-2M} + \frac{\epsilon}{6} + \frac{\epsilon}{12} e^{-2M} \leq \frac{\epsilon}{3}.
\] (90)

Similarly, using Eq. (88), we get that with probability at least \( 1 - \delta \),
\[
|E_Q(e^{T_\theta-1}) - E_{\hat{Q}}(e^{T_\theta-1})| \leq \frac{\epsilon}{3} < e \cdot \frac{\epsilon}{3}.
\] (91)

Hence,
\[
|I_{\text{ResNVI}}(X, Y) - I(X, Y)| \leq |E_Q(T_{\theta_j}) - E_{\hat{Q}}(T_{\theta_j})| + |E_{\hat{Q}}(e^{T_{\theta_j}-1}) - E_Q(e^{T_{\theta_j}-1})| + d(E_{\hat{Q}}(e^{T_{\theta_j}}), E_Q(e^{T_{\theta_j}})) \leq |E_Q(T_{\theta_j}) - E_{\hat{Q}}(T_{\theta_j})| + e^{-1} |E_{\hat{Q}}(e^{T_{\theta_j}}) - E_Q(e^{T_{\theta_j}})| + |E_{\hat{Q}}(e^{T_{\theta_j}}) - E_Q(e^{T_{\theta_j}})| \leq \epsilon.
\] (92)

**A.5 THE PROPERTY OF MI ESTIMATORS**

The variance of the exponential value of the statistic network’s output according to the bias of optimal functions on the distribution \( Q \).

**Theorem.** Let \( Q^{(n)} \) be the empirical distributions of \( n \) i.i.d. samples from \( Q \). For the optimal \( T_1 = \log \frac{dp}{dq} + C_1 \) and \( T_2 = \log \frac{dp}{dq} + C_2 \) where \( C_1 \geq C_2 \),
\[
\begin{align*}
\text{Var}_Q(E_{Q^{(n)}}(e^{T_1})) &\geq \text{Var}_Q(E_{Q^{(n)}}(e^{T_2})).
\end{align*}
\] (93)
When the number of batch is $B$, when used on DV representation, the two averaging strategies below produce a biased MI estimate if the drifting problem occurs.

We start from the definition of $I_{D蔬}$, where

$$I_{D蔬}(X, Y) = E_p(T(x, y)) - \log(E_Q(e^{T(x,y)}))$$

becomes the objective function to estimate MI, i.e. MINE.

Let $T_{ij}^{(j)}$ and $T_{ij}^{(M)}$ denote the $ij$-th element of outputs for $P_m$ and $Q_n$, respectively, where $i$ is the index of batch and $j$ is the index of sample inside the batch, and the non-drifting output as $T_{ij}^{*}$, and the drifting constant for each batch $C_i$. Then, $T_{ij} = T_{ij}^{*} + C_i$.

When the number of batch is $B$ and each batch size is $N$,

1. Macro averaging:

$$\frac{1}{B} \sum \left[ \frac{1}{N} \sum_j T_{ij}^{(j)} - \log(\frac{1}{N} \sum_j e^{T_{ij}^{(M)}}) \right]$$

$$= \frac{1}{B} \sum \left[ \frac{1}{N} \sum_j (T_{ij}^{(j)} + C_i) - \log(\frac{1}{N} \sum_j e^{T_{ij}^{(M)} + C_i}) \right]$$

$$= \frac{1}{B} \sum \left[ \frac{1}{N} \sum_j (T_{ij}^{(j)} + C_i) - \log(\frac{1}{N} e^{C_i} \sum_j e^{T_{ij}^{(M)}}) \right]$$

$$= \frac{1}{B} \sum \left[ \frac{1}{N} \sum_j T_{ij}^{(j)} - \log(\frac{1}{N} e^{C_i} \sum_j e^{T_{ij}^{(M)}}) \right]$$

$$= \frac{1}{B} \sum \left[ \frac{1}{N} \sum_j T_{ij}^{(j)} - \log(\frac{1}{N} \sum_j e^{T_{ij}^{(M)}}) \right]$$

$$\neq \frac{1}{NB} \sum_{ij} T_{ij}^{(j)} - \frac{1}{B} \sum \left[ \log(\frac{1}{N} \sum_j e^{T_{ij}^{(M)}}) \right]$$

2. Micro-averaging: Calculate the DV representation using the average of the each individual network outputs.

Proof. We start from the definition of $I_{D蔬}$, where

$$I_{D蔬}(X, Y) = E_p(T(x, y)) - \log(E_Q(e^{T(x,y)}))$$

becomes the objective function to estimate MI, i.e. MINE.

Consider that

$$\text{Var}_Q(e^{T_1}) = e^{2C_1} \left( \mathbb{E}_Q \left( \frac{dP}{dQ} \right)^2 - \left( \mathbb{E}_Q \left( \frac{dP}{dQ} \right) \right)^2 \right)$$

and

$$\text{Var}_Q(e^{T_2}) = e^{2C_2} \left( \mathbb{E}_Q \left( \frac{dP}{dQ} \right)^2 - \left( \mathbb{E}_Q \left( \frac{dP}{dQ} \right) \right)^2 \right)$$

By [Song and Ermon 2020], the variance of the mean of $n$ i.i.d. random variable then gives us

$$\text{Var}_Q(\mathbb{E}_{Q^n}(e^{T_1})) = \frac{\text{Var}_Q(e^{T_1})}{n} = \frac{\text{Var}_Q(e^{T_2})}{n}$$

Since $e^x \geq 1$ for all $x \geq 0$,

$$\frac{\text{Var}_Q(\mathbb{E}_{Q^n}(e^{T_1}))}{\text{Var}_Q(\mathbb{E}_{Q^n}(e^{T_2}))} = \frac{\text{Var}_Q(e^{T_1})}{\text{Var}_Q(e^{T_2})} = e^{2(C_1 - C_2)} \geq 1.$$  

Therefore, the variance of $T_1$ is equal to or less than the that of $T_2$ on $Q$.

Proof of estimation bias caused by drifting

Theorem. When used on DV representation, the two averaging strategies below produce a biased MI estimate if the drifting problem occurs.

1. Macro-averaging (similar to that of Poole et al. 2019): Establish a single estimate through the average of estimated MI from each batch.

2. Micro-averaging: Calculate the DV representation using the average of the each individual network outputs.
2. Micro averaging:

\[
\frac{1}{NB} \sum_{ij} T_{ij}^{(J)} - \log \left( \frac{1}{NB} \sum_{ij} e^{T_{ij}^{(M)}} \right) \quad (106)
\]

\[
= \frac{1}{NB} \sum_{ij} (T_{ij}^{(J*)} + C_i) - \log \left( \frac{1}{NB} \sum_{ij} e^{(T_{ij}^{(M*)} + C_i)} \right) \quad (107)
\]

\[
= \frac{1}{NB} \sum_{ij} T_{ij}^{(J*)} - \log \left[ \frac{1}{NB} \sum_{ij} e^{(T_{ij}^{(M*)} + C_i)} \right] \quad (108)
\]

\[\neq \frac{1}{NB} \sum_{ij} T_{ij}^{(J*)} - \log \left( \frac{1}{NB} \sum_{ij} e^{T_{ij}^{(M*)}} \right) \quad (109)\]

We emphasize that we have to stop the drifting via the regularization term of ReDV.

Wrong estimation derived from biased values According to the theorem above, the MI estimate derived from the average of the values estimated from the mini-batch in DV representation-based estimators will lead to erroneous results. However, the micro-averaging strategy is often used to measure the performance of MI estimators (MINE or InfoNCE), as shown in Fig. 6 of Cheng et al. [2020].

### A.6 THE PROOF FOR THE VALIDITY OF OUR BENCHMARK

We assume that the dataset used for our benchmark satisfies the single label assumption where there exists exactly one label for every sample inside the dataset. Note that the assumption implies that \( p(y|x) = 1 \). In other words, we assume statistical dependence between \( X \) and \( Y \) [Tishby and Zaslavsky, 2015].

**Theorem.** *(Supervised Learning Benchmark)* Consider a dataset \( D = (X, Y) \) where \( Y \) is the label for sample \( X \), and \( H(Y) \) is the entropy of \( Y \).

\[
I(X, Y) = H(Y) \quad (110)
\]

**Proof.**

\[
I(X; Y) = \int_{X,Y} P(X, Y) \log \frac{P(X, Y)}{P(X)P(Y)} \quad (111)
\]

\[
= \int_x \int_y P(x, y) \log \frac{P(y|x)}{P(y)} dydx \quad (112)
\]

\[
= \int_x \int_y P(x)P(y|x) \log \frac{P(y|x)}{P(y)} dydx \quad (113)
\]

\[
= \int_x P(x) \left( \int_y P(y|x) \log \frac{P(y|x)}{P(y)} dy \right) dx \quad (114)
\]

\[
= \int_R P(x^*) \log \frac{1}{P(y^*)} \quad \text{(where } R \text{ is the region where } y^* \text{ is a correct label for the given } x^*) \quad (115)
\]

\[
= \sum_c \int_{R_c} P(x^*, c) \log \frac{1}{P(c)} \quad \text{(where } R \text{ is partitioned by the label } c \text{ to yield } R_c) \quad (116)
\]

\[
= \sum_c \log \frac{1}{P(c)} \int_{R_c} P(x^*, c) \quad (\therefore P(c) \text{ is constant inside the } R_c) \quad (117)
\]

\[
= \sum_c \log \frac{1}{P(c)} P(c) \quad (\therefore \int_{R_c} P(x^*, c) = P(c), \text{ i.e., marginalization}) \quad (118)
\]

\[
= H(Y) \quad (119)
\]
**Theorem. (Contrastive Learning Benchmark)** Consider a dataset $D = (X, Y)$. Let $X_1$ be a sample drawn from the dataset with the label $Y$ and $X_2$ be another sample drawn from the subset of $D$ where all the samples inside the subset are with the same label $Y$. Assume that $D$ also satisfies the single label assumption.

$$I(X_1, X_2) = I(X_1, Y) = I(X_2, Y) = H(Y)$$  \hfill (120)

**Proof.**

$$P(X_1, X_2) = \sum_{y_i} P(X_1, X_2, Y) \quad (\therefore \text{marginalization})$$

$$= \sum_{y_i} P(X_1)P(Y|X_1)P(X_2|Y, X_1) \quad (\therefore \text{factorization})$$

$$= \sum_{y_i} P(Y)P(X_1|Y)P(X_2|Y) \quad (\therefore X_1 \text{ and } X_2 \text{ are independent for given } Y)$$

$$= \sum_{y_i} P(y_i)P(X_1|y_i)P(X_2|y_i)$$

$$P(X_1) = \sum_{y_i} P(X_1, Y) = \sum_{y_i} P(Y)P(X_1|Y) = \sum_{i} P(y_i)P(X_1|y_i)$$

$$P(X_2) = \sum_{y_i} P(X_2, Y) = \sum_{y_i} P(Y)P(X_2|Y) = \sum_{i} P(y_i)P(X_2|y_i)$$

$$\frac{P(X_1, X_2)}{P(X_1)P(X_2)} = \frac{\sum_{i} P(y_i)P(X_1|y_i)P(X_2|y_i)}{\sum_{i} P(y_i)P(X_1|y_i) \sum_{y_i} P(y_i)P(X_2|y_i)}$$

$$= \frac{\sum_{i} P(y_i)P(X_1|y_i)P(X_2|y_i)}{\sum_{i} P(y_i)^2P(X_1|y_i)P(X_2|y_i)} \quad (\therefore X_1 \text{ and } X_2 \text{ has the same label})$$

Let $R_i$ be the region where $(X, y_i)$ such as $i$-th class label $y_i$ is a correct label for the given $X_1$.

$$I(X_1, X_2) = \int_{X_1, X_2} P(X_1, X_2) \log \frac{P(X_1, X_2)}{P(X_1)P(X_2)}$$

$$= \int_{X_1, X_2} \left( \sum_{i} P(y_i)P(X_1|y_i)P(X_2|y_i) \right) \log \frac{\sum_{i} P(y_i)P(X_1|y_i)P(X_2|y_i)}{\sum_{i} P(y_i)^2P(X_1|y_i)P(X_2|y_i)}$$

$$= \sum_{i} P(y_i) \int_{X_2} P(X_2|y_i) \left( \int_{R_i} P(X_1|y_i) \log \frac{P(y_i)P(X_1|y_i)P(X_2|y_i)}{P(y_i)^2P(X_1|y_i)P(X_2|y_i)} dx_1 \right) dx_2$$

$$= \sum_{i} P(y_i) \int_{X_2} P(X_2|y_i) \left( \int_{R_i} P(X_1|y_i) \log \frac{1}{P(y_i)} dx_1 \right) dx_2$$

$$= \sum_{i} P(y_i) \log \frac{1}{P(y_i)} \int_{X_2} P(X_2|y_i) \left( \int_{R_i} P(X_1|y_i) dx_1 \right) dx_2$$

$$= \sum_{i} P(y_i) \log \frac{1}{P(y_i)}$$

$$= H(Y)$$

$\square$
Figure 8: Histogram of the exponential of the network outputs $e^T(x,y)$ which is trained with CLB CIFAR10. Training samples and unseen samples are fed to (a) and (b), respectively.

**B DIRECTLY UTILIZING THE STATISTICS NETWORK OUTPUTS FOR OUT-OF-DISTRIBUTION TASK**

We observe the SLB CIFAR10-trained network outputs when seen or unseen samples are fed to the statistics network $T$ in Fig. 8. Note that we can take $e^T(x,y) = \frac{dP_{XY}}{dP_X \otimes P_Y}$ for granted, thanks to regularization. Fig. 8 (a) shows the distribution of $e^T(x,y)$ for the training set samples $(x,y) \sim P_{X\text{Train}}Y_{\text{Train}}$. As 90% of $(x,y) \sim P_X \otimes P_Y$ is wrongly labeled, the majority yields $e^T(x,y) = 0$. The likelihood ratio for the $(x,y) \sim P_{XY}$ is 10, and all the samples are centered around the ideal value as expected. CIFAR10 test set samples $(x,y) \sim P_{X\text{Test}}Y_{\text{Test}}$ also yield similar results, where some of the samples are wrongly positioned, being the test error of $T$. Surprisingly, when we feed MNIST [LeCun et al., 1998] training samples $(x,y) \sim P_{X\text{MNIST}}Y_{\text{MNIST}}$, model successfully classifies nearly all the samples to be less likely to occur in $P_{X\text{Train}}Y_{\text{Train}}$. This implies that exploiting the network outputs with the viewpoints of MI may show usefulness in out-of-distribution detection.

Figure 9: Training $T_\theta$ using $I_{\text{MINE}}$ and $I_{\text{ReMINE}}$ with batch size 100 for 20 epochs. We breakdown the MI loss into two components. We split both losses into first term $E_{P_{XX}}(T)$ and second term $\log E_{P_X \otimes P_X}(e^T)$.

**C EXPERIMENTS ON IMAGENET**

We test on the ImageNet dataset with 1000 classes, where we use the batch size of 100. We set the batch size to be relatively small to observe how different losses behave, whereas multiple contrastive learning literature such as Chen et al. [2020], He et al. [2020] uses large batch sizes to avoid instability. We train for 20 epochs to observe the early stages of training.

First, we can observe in Fig. 9 that the regularizer successfully solves the drifting problem of $I_{\text{MINE}}$. Also, Table 3 shows that $I_{\text{NWJ}}$ fails in the contrastive learning benchmark. $I_{\text{NWJ}}$ explodes within a few steps of training, where the regularizer successfully avoids the problem to yield a feasible output. Note that we did not observe the losses till convergence; we have to train much longer to obtain a more accurate performance of MI estimation and test accuracy. However, we can see
| Task                             | Loss | MI Estimation       | Test Accuracy     |
|---------------------------------|------|---------------------|-------------------|
|                                 |      | Original | Regularized | Original | Regularized |
| Supervised Learning Benchmark   | CE   | -        | -           | 0.0795   | -           |
|                                 | MINE | 6.147    | 6.110       | 0.1056   | 0.1081      |
|                                 | NWJ  | 6.072    | 6.075       | 0.1020   | 0.1005      |
| Contrastive Learning Benchmark  | MINE | 1.095    | 1.140       | 0.0103   | 0.0098      |
|                                 | NWJ  | 0.000    | 1.008       | 0.0010   | 0.0072      |

Table 3: Our supervised and contrastive learning benchmark results on ImageNet dataset. We provide the MI estimation and test accuracy, where we clip the negative MI estimations to 0. We compare the performance of original and regularized loss. We also add the accuracy of standard cross-entropy loss (CE) for comparison. Similar to Section 5.2, we choose the regularization weight $\lambda \in \{0.1, 0.01, 0.001\}$ that shows the best MI estimation results.

that in the supervised learning benchmark, which is the relatively easier benchmark, all the losses are already close to the optimal MI even in the earlier epochs. We can also observe a similar trade-off between the MI estimation and test accuracy in Table 3. Future works on large-scale datasets are needed to observe the behaviors further.

D EXPERIMENTAL DETAILS

D.1 HARDWARE SPECIFICATION

We use a single NVIDIA DGX A100 machine with 8 GPUs for all the experiments. All the experiments except for our benchmark experiments take less than 10 minutes and a single GPU to compute. It takes less than 2 days to compute all the benchmark experiments: 4 settings, 12 losses, and 5 seeds running on 8 GPUs and 4 processes per GPU.

D.2 DETAILED SETTINGS FOR ONE-HOT DATASET EXPERIMENTS

We describe the detailed settings for Fig. 1, Fig. 2, Fig. 3, Fig. 4, and Fig. 5. We choose $N = 16$ for the one-hot discrete dataset $X \sim U(1, N)$. We use a simple statistics network $T$ with a concatenated vector of dimension $N \times 2 = 32$ as input. We pass the input through two fully connected layers with ReLU activation by widths: $32 \rightarrow 256 \rightarrow 1$. The last layer outputs a single scalar with no bias and activation. We use stochastic gradient descent (SGD) with learning rate 0.1 to optimize the statistics network unless specified.

D.3 DETAILED SETTINGS FOR OUR BENCHMARK

We describe the detailed settings for Table 2 and Fig. 6. We use ResNet-18 [He et al., 2016] as the backbone network and use Adam optimizer with the default learning rate $0.001$, $\beta_1 = 0.9$ and $\beta_2 = 0.999$. We use batch size 100 for CIFAR10 and 10 for CIFAR10. We train for different epochs per each benchmark: 40 epochs (SLB CIFAR10), 100 epochs (SLB CIFAR100), 100 epochs (CLB CIFAR10), and 150 epochs (CLB CIFAR100). We choose enough number of epochs for all the losses to be fully converged for each of the benchmarks. We rerun the same experiment 5 times with different seeds.

D.4 DETAILED SETTINGS FOR THE 20D CORRELATED GAUSSIAN TASK

We describe the detailed settings for Fig. 7. We sampled $(x, y)$ from $d$-dimensional correlated Gaussian dataset where $X \sim N(0, I_d)$ and $Y \sim N(\rho X, (1 - \rho^2)I_d)$ given the correlation parameter $0 \leq \rho < 1$, which is taken from Belghazi et al. [2018]. The true MI for the dataset is $I(X, Y) = -\frac{d}{2} \log(1 - \rho^2)$. For the statistics network architecture, we consider the architecture similar to Appendix D.2, where we concatenate the inputs $(x, y)$ to pass through three fully connected layers with ReLU activation (excluding the output layer) by widths $40 \rightarrow 256 \rightarrow 256 \rightarrow 1$, same as the network used in Poole et al. [2019]. We used the same optimizer with Appendix D.3.