Measuring Generalization with Optimal Transport

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Abstract

Understanding the generalization of deep neural networks is one of the most important tasks in deep learning. Although much progress has been made, theoretical error bounds still often behave disparately from empirical observations. In this work, we develop margin-based generalization bounds, where the margins are normalized with optimal transport costs between independent random subsets sampled from the training distribution. In particular, the optimal transport cost can be interpreted as a generalization of variance which captures the structural properties of the learned feature space. Our bounds robustly predict the generalization error, given training data and network parameters, on large scale datasets. Theoretically, we demonstrate that the concentration and separation of features play crucial roles in generalization, supporting empirical results in the literature. The code is available at https://github.com/chingyaoc/kV-Margin.

1 Introduction

Motivated by the remarkable empirical success of deep learning, there has been significant effort in statistical learning theory toward deriving generalization error bounds for deep learning, i.e, complexity measures that predict the gap between training and test errors. Recently, substantial progress has been made, e.g., [3, 4, 7, 14, 22, 45, 59]. Nevertheless, many of the current approaches lead to generalization bounds that are often vacuous or not consistent with empirical observations [15, 26, 40].

In particular, Jiang et al. [26] present a large scale study of generalization in deep networks and show that many existing approaches, e.g., norm-based bounds [4, 44, 45], are not predictive of generalization in practice. Recently, the Predicting Generalization in Deep Learning (PGDL) competition described in [27] sought complexity measures that are predictive of generalization error given training data and network parameters. To achieve a high score, the predictive measure of generalization had to be robust to different hyperparameters, network architectures, and datasets. The participants [34, 42, 51] achieved encouraging improvement over the classic measures such as VC-dimension [57] and weight norm [4]. Unfortunately, despite the good empirical results, these proposed approaches are not yet supported by rigorous theoretical bounds [28].

In this work, we attempt to decrease this gap between theory and practice with margin bounds based on optimal transport. In particular, we show that the expected optimal transport cost of matching two independent random subsets of the training distribution is a natural alternative to Rademacher complexity. Interestingly, this optimal transport cost can be interpreted as the $k$-variance [52], a generalized notion of variance that captures the structural properties of the data distribution. Applied to latent space, it captures important properties of the learned feature distribution. The resulting $k$-variance normalized margin bounds can be easily estimated and correlate well with the generalization error on the PGDL datasets [27]. In addition, our formulation naturally encompasses the gradient...
normalized margin proposed by Elsayed et al. [16], further relating our bounds to the decision boundary of neural networks and their robustness.

Theoretically, our bounds reveal that the concentration and separation of learned features are important factors for the generalization of multiclass classification. In particular, the downstream classifier generalizes well if (1) the features within a class are well clustered, and (2) the classes are separable in the feature space in the Wasserstein sense.

In short, this work makes the following contributions:

- We develop new margin bounds based on $k$-variance [52], a generalized notion of variance based on optimal transport, which better captures the structural properties of the feature distribution;
- We propose $k$-variance normalized margins that predict generalization error well on the PGDL challenge data;
- We provide a theoretical analysis to shed light on the role of feature distributions in generalization, based on our $k$-variance normalized margin bounds.

## 2 Related Work

### Margin-based Generalization Bounds

Classic approaches in learning theory bound the generalization error with the complexity of the hypothesis class [5, 57]. Nevertheless, previous works show that these uniform convergence approaches are not able to explain the generalization ability of deep neural networks given corrupted labels [63] or on specific designs of data distributions as in [40]. Recently, substantial progress has been made to develop better data-dependent and algorithm-dependent bounds [3, 6, 7, 11, 46, 55, 59]. Among them, we will focus on margin-based generalization bounds for multi-class classification [31, 33]. Bartlett et al. [4] show that margin normalized with the product of spectral norms of weight matrices is able to capture the difficulty of the learning task, where the conventional margin struggles. Concurrently, Neyshabur et al. [45] derive spectrally-normalized margin bounds via weight perturbation within a PAC-Bayes framework [36]. However, empirically, spectral norm-based bounds can correlate negatively with generalization [40, 26]. Elsayed et al. [16] present a gradient-normalized margin, which can be interpreted as the first order approximation to the distance to the decision boundary. Jiang et al. [25] further show that gradient-normalized margins, when combined with the total feature variance, are good predictors of the generalization gap. Despite the empirical progress, gradient-normalized margins are not yet supported by theoretical bounds.

### Empirical Measures of Generalization

Large scale empirical studies have been conducted to study various proposed generalization predictors [25, 26]. In particular, Jiang et al. [26] measure the average correlation between various complexity measures and generalization error under different experimental settings. Building on their study, Dziugaite et al. [15] emphasize the importance of the robustness of the generalization measures to the experimental setting. These works show that well-known complexity measures such as weight norm [39, 44], spectral complexity [4, 45], and their variants are often negatively correlated with the generalization gap. Recently, Jiang et al. [27] hosted the Predicting Generalization in Deep Learning (PGDL) competition, encouraging the participants to propose robust and general complexity measures that can rank networks according to their generalization errors. Encouragingly, several approaches [34, 42, 51] outperformed the conventional baselines by a large margin. Nevertheless, none of these are theoretically motivated with rigorous generalization bounds. Our $k$-variance normalized margins are good empirical predictors of the generalization gap, while also being supported with strong theoretical bounds.

## 3 Optimal Transport and $k$-Variance

Before presenting our generalization bounds with optimal transport, we first give a brief introduction to the Wasserstein distance, a distance function between probability distributions defined via an optimal transport cost. Letting $\mu$ and $\nu \in \text{Prob} (\mathbb{R}^d)$ be two probability measures, the $p$-Wasserstein distance with Euclidean cost function is defined as

$$ W_p(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \left( \mathbb{E}_{(X,Y) \sim \pi} \| X - Y \|^p \right)^{1/p}, $$
where $\Pi(\mu, \nu) \subseteq \text{Prob}(\mathbb{R}^d \times \mathbb{R}^d)$ denotes the set of measure couplings whose marginals are $\mu$ and $\nu$, respectively. The 1-Wasserstein distance is also known as the Earth Mover distance. Intuitively, Wasserstein distances measure the minimal cost to transport the distribution $\mu$ to $\nu$.

Based on the Wasserstein distance, Solomon et al. [52] propose the $k$-variance, a generalization of variance, to measure structural properties of a distribution beyond variance.

**Definition 1 (Wasserstein-p $k$-variance).** Given a probability measure $\mu \in \text{Prob}(\mathbb{R}^d)$ and a parameter $k \in \mathbb{N}$, the Wasserstein-p $k$-variance is defined as

$$\text{Var}_{k,p}(\mu) = c_p(k, d) \cdot \mathbb{E}_{S,S \sim \mu^k} \left[ \mathcal{W}_p^k(\mu_S, \mu_{S}) \right],$$

where $\mu_S = \frac{1}{k} \sum_{i=1}^{k} \delta_{x_i}$, for $x_i \sim \mu$ and $c_p(k, d)$ is a normalization term described in [52].

When $k = 1$ and $p = 2$, the $k$-variance is equivalent to the variance $\text{Var}[X]$ of the random variable $X \sim \mu$. For $k > 1$ and $d \geq 3$, Solomon et al. [52] show that when $p = 2$, the $k$-variance provides an intuitive way to measure the average intra-cluster variance of clustered measures. In this work, we use the unnormalized version ($c_p(k, d) = 1$) of $k$-variance and $p = 1$, and drop the $p$ in the notation:

(Wasserstein-1 $k$-variance): $\text{Var}_{k}(\mu) = \mathbb{E}_{S,S \sim \mu^k} \left[ \mathcal{W}_1(\mu_S, \mu_{S}) \right].$

Note that setting $c_p(k, d) = 1$ is not an assumption, but instead an alternative definition of $k$-variance. The change in constant has no effect on any part of our paper, as we could reintroduce the constant of Solomon et al. [52] and simply include a premultiplication term in the generalization bounds to cancel it out. In Section 6, we will show that this unnormalized Wasserstein-1 $k$-variance captures the concentration of learned features. Next, we use it to derive generalization bounds.

### 4 Generalization Bounds with Optimal Transport

We present our generalization bounds in the multi-class setting. Let $\mathcal{X}$ denote the input space and $\mathcal{Y} = \{1, \ldots, K\}$ denote the output space. We will assume a compositional hypothesis class $F \circ \Phi$, where the hypothesis $f \circ \phi$ can be decomposed as a feature (representation) encoder $\phi \in \Phi$ and a predictor $f \in F$. This includes dividing multilayer neural networks at an intermediate layer.

We consider the score-based classifier $f = [f_1, \ldots, f_K]$, $f_c \in F_c$, where the prediction for $x \in \mathcal{X}$ is given by $\arg \max_{y \in \mathcal{Y}} f_y(\phi(x))$. The margin of $f$ for a datapoint $(x, y)$ is defined by

$$\rho_f(\phi(x), y) := f_y(\phi(x)) - \max_{y' \neq y} f_{y'}(\phi(x)), \quad (1)$$

where $f$ misclassifies if $\rho_f(\phi(x), y) \leq 0$. The dataset $S = \{x_i, y_i\}_{i=1}^{m}$ is drawn i.i.d. from distribution $\mu$ over $\mathcal{X} \times \mathcal{Y}$. Define $m_c$ as the number of samples in class $c$, yielding $m = \sum_{c=1}^{K} m_c$. We denote the marginal over a class $c \in \mathcal{Y}$ as $\mu_c$ and the distribution over classes by $\mu$. The pushforward measure of $\mu$ with respect to $\phi$ is denoted as $\phi \# \mu$. We are interested in bounding the expected zero-one loss of a hypothesis $f \circ \phi$: $R_{\mu}(f \circ \phi) = \mathbb{E}_{(x,y) \sim \mu} [\mathbf{1}_{\rho_f(\phi(x), y) \leq 0}]$ by the corresponding empirical $\gamma$-margin loss $\hat{R}_{\gamma,m}(f \circ \phi) = \mathbb{E}_{(x,y) \sim S} [\mathbf{1}_{\rho_f(\phi(x), y) \leq \gamma}]$.

#### 4.1 Feature Learning and Generalization: Margin Bounds with $k$-Variance

Our theory is motivated by recent progress in feature learning, which suggests that imposing certain structure on the feature distribution improves generalization [8, 10, 30, 60, 62]. The participants [34, 42] of the PGDL competition [27] also demonstrate nontrivial correlation between feature distribution and generalization.

To study the connection between learned features and generalization, we derive generalization bounds based on the $k$-variance of the feature distribution. In particular, we first derive bounds for a fixed encoder and discuss the generalization error of the encoder at the end of the section. Theorem 2 provides a generalization bound for neural networks via the concentration of $\mu_c$ in each class.

**Theorem 2.** Let $f = [f_1, \ldots, f_K] \in F = F_1 \times \cdots \times F_K$ where $F_i : \mathcal{X} \rightarrow \mathbb{R}$. Fix $\gamma > 0$. The following bound holds for all $f \in F$ with probability at least $1 - \delta > 0$:

$$R_{\mu}(f \circ \phi) \leq \hat{R}_{\gamma,m}(f \circ \phi) + \mathbb{E}_{c \sim \mu} \left[ \frac{\text{Lip}(\rho_f(\cdot, c))}{\gamma} \text{Var}_{m_c}(\phi \# \mu_c) \right] + \sqrt{\frac{\log(1/\delta)}{2m}},$$

where $\text{Lip}(\cdot) = \sup_{x \neq x'} |f(x) - f(x')|$.
where $\text{Lip} (\rho_f (\cdot, c)) = \sup_{x,x' \in \mathcal{X}} \frac{|\rho_f (\phi(x), c) - \rho_f (\phi(x'), c)|}{\|\phi(x) - \phi(x')\|_2}$ is the margin Lipschitz constant w.r.t $\phi$.

We give a proof sketch here and defer the full proof to the supplement. For a given class $c$ and a given feature map $\phi$, let $\mathcal{H}_c = \{ h(x) = \rho_f (\phi(x), c) | f = (f_1 \ldots f_K), f_k \in \mathcal{F} \}$. The last step in deriving Rademacher-based generalization bounds [5] amounts to bounding for each class $c$:

$$
\Delta_c = \mathbb{E}_{S, \tilde{S} \sim \mu_{c \circ}^n} \left[ \sup_{h \in \mathcal{H}_c} \frac{1}{m_c} \sum_{i=1}^{m_c} h(\tilde{x}_i) - \frac{1}{m_c} \sum_{i=1}^{m_c} h(x_i) \right],
$$

(2)

where $S, \tilde{S} \sim \mu_{c}^n$. Typically we would plug in the Rademacher variable and arrive at the standard Rademacher generalization bound. Instead, our key observation is that the Kantorovich-Rubinstein duality [24] implies

$$
\mathcal{W}_1 (\mu, \nu) = \sup_{\text{Lip}(h) \leq 1} \mathbb{E}_{x \sim \mu} h(x) - \mathbb{E}_{x \sim \nu} h(x),
$$

where the supremum is over the 1-Lipschitz functions $h : \mathbb{R}^d \rightarrow \mathbb{R}$. Suppose $\mathcal{H}_c$ is a subset of $L$-Lipschitz functions. By definition of the supremum, the duality result immediately implies that (2) can be bounded with $k$-variance for $k = m_c$:

$$
\Delta_c \leq L \cdot \mathbb{E}_{S, \tilde{S} \sim \mu_{c}^n} [\mathcal{W}_1 (\phi#\mu_S , \phi#\mu_{\tilde{S}})] = L \cdot \text{Var}_{m_c} (\phi#\mu_c).
$$

(3)

This connection suggests that $k$-variance is a natural alternative to Rademacher complexity if the margin is Lipschitz. The following lemma shows that this holds when the functions $f_j$ are Lipschitz:

**Lemma 3.** The margin $\rho_f (\cdot, y)$ is Lipschitz in its first argument if each of the $f_j$ is Lipschitz.

The bound in Theorem 2 is minimized when (a) the $k$-variance of features within each class is small, (b) the classifier has large margin, and (c) the Lipschitz constant of $f$ is small. In particular, (a) and (b) express the idea of concentration and separation of the feature distribution, which we will further discuss in Section 6.

Compared to the margin bound with Rademacher complexity [33], Theorem 2 studies a fixed encoder, allowing the bound to capture the structure of the feature distribution. Although the Rademacher-based bound is also data-dependent, it only depends on the distribution over inputs and therefore can neither capture the effect of label corruption nor explain how the structure of the feature distribution $\phi#(\mu)$ affects generalization. Importantly, it is also non-trivial to estimate the Rademacher complexity empirically, which makes it hard to apply the bound in practice.

### 4.2 Gradient Normalized (GN) Margin Bounds with $k$-Variance

We next extend our theorem to use the gradient-normalized margin, a variation of the margin (1) that empirically improves generalization and adversarial robustness [16, 25]. Elsayed et al. [16] proposed it to approximate the minimum distance to a decision boundary, and Jiang et al. [25] simplified it to

$$
\tilde{\rho}_f (\phi(x), y) := \rho_f (\phi(x), y) / (\|\nabla_{\phi} \rho_f (\phi(x), y)\|_2 + \epsilon),
$$

where $\epsilon$ is a small value ($10^{-6}$ in practice) that prevents the margin from going to infinity. The gradient here is $\nabla_{\phi} \rho_f (\phi(x), y) := \nabla_{\phi} f(y \circ \phi(x)) - \nabla_{\phi} f_{\max} (\phi(x))$, where ties among the $y_{\text{max}}$ are broken arbitrarily as in [16, 25] (ignoring subgradients). The gradient-normalized margin $\tilde{\rho}_f (x, y)$ can be interpreted as the first order Taylor approximation of the minimum distance of the input $x$ to the decision boundary for the class pair $(y, y')$ [16]. In particular, the distance is defined as the norm of the minimal perturbation in the input or feature space to make the prediction change. See also Lemma 20 in the supplement for an interpretation of this margin in terms of robust feature separation. Defining the margin loss $\tilde{R}^{\gamma}_{\gamma, m}(f) = \mathbb{E}_{(x,y) \sim S} [\mathbb{I}_{\tilde{\rho}_f (\phi(x), y) \leq \gamma}]$, we extend Theorem 2 to the gradient-normalized margin.

**Theorem 4** (Gradient-Normalized Margin Bound). Let $f = [f_1, \ldots, f_K] \in \mathcal{F} = [\mathcal{F}_1, \ldots, \mathcal{F}_K]$ where $\mathcal{F}_i : \mathcal{X} \rightarrow \mathbb{R}$. Fix $\gamma > 0$. Then, for any $\delta > 0$, the following bound holds for all $f \in \mathcal{F}$ with probability at least $1 - \delta > 0$:

$$
R_{\mu} (f \circ \phi) \leq \tilde{R}^{\gamma}_{\gamma, m} (f \circ \phi) + \mathbb{E}_{c \sim p} \left[ \text{Lip} (\tilde{\rho}_{f_j}(\cdot, c)) \right] \text{Var}_{m_c} (\phi#\mu_c) + \sqrt{\frac{\log (1/\delta)}{2m}},
$$

where $\text{Lip} (\tilde{\rho}_{f_j}(\cdot, c)) = \sup_{x,x' \in \mathcal{X}} \frac{|\tilde{\rho}_{f_j}(\phi(x), c) - \tilde{\rho}_{f}(\phi(x'), c)|}{\|\phi(x) - \phi(x')\|}$ is the Lipschitz constant defined w.r.t $\phi$. 

4
4.3 Estimation Error of $k$-Variance

So far, our bounds have used the $k$-variance, which is an expectation. Lemma 5 bounds the estimation error when estimating the $k$-variance from data. This may be viewed as a generalization error for the learned features in terms of $k$-variance, motivated by the connections of $k$-variance to test error.

**Lemma 5** (Estimation Error of $k$-Variance / “Generalization Error” of the Encoder). Given a distribution $\mu$ and $n$ empirical samples $\{S^j, \tilde{S}^j\}_{j=1}^n$ where each $S^j, \tilde{S}^j \sim \mu^k$, define the empirical Wasserstein-1 $k$-variance:

$$\text{Var}_k(\phi) = \frac{1}{n} \sum_{j=1}^n W_1(\phi_{\# \mu S^j}, \phi_{\# \mu \tilde{S}^j}).$$

Suppose the encoder satisfies $\sup_{x,x'} ||\phi(x) - \phi(x')|| \leq B$, then with probability at least $1 - \delta > 0$, we have

$$\text{Var}_k(\phi_{\# \mu}) \leq \text{Var}_{k,n}(\phi_{\# \mu}) + \sqrt{\frac{2B^2 \log(1/\delta)}{nk}}.$$

We can then combine Lemma 5 with our margin bounds to obtain full generalization bounds. The following corollary states the empirical version of Theorem 2:

**Corollary 6.** Given the setting in Theorem 2 and Lemma 5, with probability at least $1 - \delta$, for $m = \sum_{c=1}^K \lceil \frac{m_c}{2n} \rceil$, $R_\mu(f \circ \phi)$ is upper bounded by

$$\hat{R}_{\gamma,m}(f \circ \phi) + \mathbb{E}_{c \sim \rho_c} \left[ \frac{\text{Lip}(\rho_f(\cdot, c))}{\gamma} \left( \text{Var}_{\lceil \frac{m_c}{2n} \rceil, n}(\phi_{\# \mu_c}) + 2B \sqrt{\frac{\log(2K/\delta)}{n \lceil \frac{m_c}{2n} \rceil}} \right) \right] + \frac{\log(\frac{2}{\delta})}{2m}.$$

Note that the same result holds for the gradient normalized margin $\hat{\rho}_f$. The proof of this corollary is a simple application of a union bound on the concentration of the $k$-variance for each class and the concentration of the empirical risk. We end this section by bounding the variance of the empirical $k$-variance. While Solomon et al. [52] proved a high-probability concentration result using McDiarmid’s inequality, we here use the Efron-Stein inequality to directly bound the variance.

**Theorem 7** (Empirical variance). Given a distribution $\mu$ and an encoder $\phi$, we have

$$\text{Var} \left[ \text{Var}_{k,n}(\phi_{\# \mu}) \right] \leq \frac{4 \text{Var}_n(\phi(X))}{nk},$$

where $\text{Var}_n(\phi(X)) = \mathbb{E}_{x \sim \mu} \|\phi(x) - \mathbb{E}_{x \sim \mu} \phi(x)\|^2$ is the variance of $\phi_{\# \mu}$.

Theorem 7 implies that if the feature distribution $\phi_{\# \mu}$ has bounded variance, the variance of the empirical $k$-variance decreases as $k$ and $n$ increase. The values of $k$ we used in practice were large enough that the empirical variance of $k$-variance was small even when we set $n = 1$.

5 Measuring Generalization with Normalized Margins

We now empirically compare the generalization behavior of neural networks to the predictions of our margin bounds. To provide a unified view of the bound, we set the second term in the right-hand side of the bound to a constant. For instance, for Theorem 2, we choose $\gamma = \gamma_0 \cdot \mathbb{E}_{c \sim \rho} \left[ \text{Lip}(\rho_f(\cdot, c)) \cdot \text{Var}_{m_c}(\phi_{\# \mu_c}) \right]$, yielding $R_\mu(f \circ \phi) \leq \hat{R}_{\gamma,m}(f \circ \phi) + 1/\gamma_0 + O(m^{-1/2})$, where

$$\hat{R}_{\gamma,m}(f \circ \phi) = \mathbb{E}_{(x,y) \sim S} \left[ 1 \left( \rho_f(\phi(x), y) / \mathbb{E}_{c \sim \rho} \left[ \text{Lip}(\rho_f(\cdot, c)) \cdot \text{Var}_{m_c}(\phi_{\# \mu_c}) \right] \right) \leq \gamma_0 \right].$$

and $1(\cdot)$ is the indicator function. This implies the model generalizes better if the normalized margin is larger. We therefore consider the distribution of the $k$-variance normalized margin, where each data point is transformed into a single scalar via

$$\frac{\rho_f(\phi(x), y)}{\mathbb{E}_{c \sim \rho} \left[ \text{Var}_{\lceil \frac{m_c}{2n} \rceil, 1}(\phi_{\# \mu_c}) \cdot \text{Lip}(\rho_f(\cdot, c)) \right]}$$

and

$$\frac{\hat{\rho}_f(\phi(x), y)}{\mathbb{E}_{c \sim \rho} \left[ \text{Var}_{\lceil \frac{m_c}{2n} \rceil, 1}(\phi_{\# \mu_c}) \cdot \text{Lip}(\hat{\rho}_f(\cdot, c)) \right]}.$$

respectively. For simplicity, we set $k$ and $n$ as $k = \lfloor m_c/2 \rfloor$ and $n = 1$. We refer to these normalized margins as $k$-Variance normalized Margin ($kV$-Margin) and $k$-Variance Gradient Normalized Margin ($kV$-GN-Margin), respectively.
We evaluate our margin bounds on the Predicting Generalization in Deep Learning (PGDL) dataset. (TV-GN-Margin) of [25] corresponds to (CMI). Intuitively, CMI measures the minimal mutual information between complexity measure and generalization error conditioned on different sets of hyperparameters. To achieve high CMI, the complexity measure must be robust to all possible settings including different architectures, learning rates, batch sizes, etc. Please refer to [27] for details.

It is NP-hard to compute the exact Lipschitz constant of ReLU networks [50, 29]. Various approaches have been proposed to estimate the Lipschitz constant for ReLU networks [29, 17], however they remain computationally expensive. As we show in Appendix B.4, a naive spectral upper bound on the Lipschitz constant leads to poor results in predicting generalization. On the other hand, as observed by [29], a simple lower bound can be obtained for the Lipschitz constant of ReLU networks by taking the supremum of the norm of the Jacobian on the training set.† Letting \( y^* = \arg \max_{y \neq c} f_y(\phi(x)) \), the Lipschitz constant of the margin can therefore be empirically approximated as

\[
\hat{\text{Lip}}(\rho_f(\cdot, c)) := \max_{x \in S_c} \| \nabla_x f_x(\phi(x)) - \nabla_x f_{y^*}(\phi(x)) \|,
\]

where \( S_c = \{(x_i, y_i) \in S \mid y_i = c\} \) is the set of empirical samples for class \( c \) (as noted in [29], although this does not lead to correct computation of Jacobians for ReLU networks, it empirically performs well). In practice, we take the maximum over samples in the training set. We refer the reader to [41] and [54] for an analysis of the estimation error of the Lipschitz constant from finite subsets. In the supplement (App. C.1), we show that for piecewise linear hypotheses such as ReLU networks, the norm of the Jacobian of the gradient-normalized margin is very close to \( 1 \). Although this does not lead to correct computation of Jacobians for ReLU networks, it empirically performs well. In practice, we take the maximum over samples in the training set. We refer the reader to [41] and [54] for an analysis of the estimation error of the Lipschitz constant from finite subsets. In the supplement (App. C.1), we show that for piecewise linear hypotheses such as ReLU networks, the norm of the Jacobian of the gradient-normalized margin is very close to \( 1 \) almost everywhere. We thus simply set the Lipschitz constant to \( 1 \) for the gradient-normalized margin.

### 5.1 Experiment: Predicting Generalization in Deep Learning

We evaluate our margin bounds on the Predicting Generalization in Deep Learning (PGDL) dataset [27]. The dataset consists of 8 tasks, each task contains a collection of models trained with different hyperparameters. The models in the same task share the same dataset and model type, but can have different depths and hidden sizes. The goal is to find a complexity measure of networks that correlates with their generalization error. In particular, the complexity measure maps the model and training dataset to a real number, where the output should rank the models in the same order as the generalization error. The performance is then measured by the Conditional Mutual Information (CMI). Intuitively, CMI measures the minimal mutual information between complexity measure and generalization error conditioned on different settings of hyperparameters. To achieve high CMI, the measure must be robust to all possible settings including different architectures, learning rates, batch sizes, etc. Please refer to [27] for details.

| Margin \( ^1 \) | CIFAR VGG | SVHN NiN | CINIC FCN bn | CINIC FCN | Flowers NiN | Pets NiN | Fashion VGG | CIFAR NiN |
|-----------------|-----------|---------|-------------|-----------|-------------|---------|------------|----------|
| SN-Margin \( ^1 \) [4] | 13.59     | 16.32   | 2.03        | 2.99      | 0.33        | 1.24    | 0.45       | 5.45     |
| GN-Margin 1st [25] | 5.28      | 3.11    | 0.24        | 2.89      | 0.10        | 1.00    | 0.49       | 6.15     |
| GN-Margin 8th [25] | 3.53      | 35.42   | 26.69       | 6.78      | 4.43        | 1.61    | 1.04       | 13.49    |
| TV-GN-Margin 1st [25] | 0.39      | 31.81   | 7.17        | 1.70      | 0.17        | 0.79    | 2.12       | 1.16     |
| TV-GN-Margin 8th [25] | 19.22     | 36.90   | 31.70       | 16.56     | 4.67        | 4.20    | 0.16       | 25.06    |

Table 1: Mutual information scores on PGDL tasks. We compare different margins across tasks in PGDL. The first and second rows indicate the datasets and the architecture types used by tasks. The methods that are supported with theoretical bounds are marked with \( ^\dagger \). Our \( k \)-variance normalized margins outperform the baselines in 6 out of 8 tasks in PGDL dataset.

$\dagger$ In general, the Lipschitz constant of smooth, scalar valued functions is equal to the supremum of the norm of the input Jacobian in the domain [18, 29, 50].
of networks, we present the results with respect to the shallow layer (first layer) and the deep layer (8th layer if the number of convolutional layers is greater than 8, otherwise the deepest convolutional layer). To produce a scalar measurement, we use the median to summarize the margin distribution, which can be interpreted as finding the margin $\gamma$ that makes the margin loss $\approx 0.5$. We found that using expectation or other quantiles leads to similar results. The Wasserstein-1 distance in $k$-variance is computed exactly, with the linear program in the POT library [19]. All of our experiments are run on 6 TITAN X (Pascal) GPUs.

To ease the computational cost, all margins and $k$-variances are estimated with random subsets of size $\min(200 \times \#\text{classes}, \text{data\_size})$ sampled from the training data. The average results over 4 subsets are shown in Table 1. Standard deviations are given in App. B.2, as well as the effect of varying the size of the subset in App. B.3. Our $k$-variance normalized margins outperform the baselines in 6 out of 8 tasks. Notably, our margins are the only ones achieving good empirical performance while being supported with theoretical bounds.

**Margin Visualization.** To provide a qualitative comparison, we select four models from the first task of PGDL (CIFAR10/VGG), which have generalization error 24.9%, 26.2%, 28.6%, and 31.8%, respectively. We visualize margin distributions for each in Figure 1. Without proper normalization, Margin and GN-Margin struggle to discriminate these models. Similar to the observation in [26], SN-Margin even negatively correlates with generalization. Among all the approaches, $kV$-GN-Margin is the only measure that correctly orders and distinguishes between all four models. This is consistent with Table 1, where $kV$-GN-Margin achieves the highest score.

![Margin Visualization of PGDL Models](image)

Figure 1: Margin Visualization of PGDL Models. From left to right, the correct order of the margin distributions should be red, green, orange, and blue. $kV$-GN-Margin is the only measure that behaves consistently with the generalization error.

Next, we compare our approach against the winning solution of the PGDL competition: Mixup*DBI [42]. Mixup*DBI uses the geometric mean of the Mixup accuracy [64] and Davies Bouldin Index (DBI) to predict generalization. In particular, they use DBI to measure the clustering quality of intermediate representations of neural networks. For fair comparison, we calculate the geometric mean of the Mixup accuracy and the median of the $k$-variance normalized margins and show the results in Table 2. Following [42], all approaches use the representations from the first layer. Our Mixup*$kV$-GN-Margin outperforms the state-of-the-art [42] in 5 out of the 8 tasks.

### 5.2 Experiment: Label Corruption

A sanity check proposed in [63] is to examine whether the generalization measures are able to capture the effect of label corruption. Following the experiment setup in [63], we train two Wide-ResNets [61], one with true labels (generalization error $= 12.9\%$) and one with random labels (generalization error $= 89.7\%$) on CIFAR-10 [32]. Both models achieve 100% training accuracy. We select the
Table 2: Mutual information scores on PGDL tasks with Mixup. We compare with the winner (Mixup*DBI) of the PGDL competition [27]. Scores of Mixup*DBI from [42].

| Feature         | CIFAR  | SVHN  | CINIC | CINIC | Flowers | Pets | Fashion | VGG | NiN |
|-----------------|--------|-------|-------|-------|---------|------|---------|-----|-----|
| VGG             | 0.00   | 42.31 | 31.79 | 15.92 | 43.99   | 12.59| 9.24    |     |     |
| NiN             | 7.37   | 27.76 | 39.77 | 20.87 | 9.14    | 4.83 | 1.32    | 22.30|     |
| Mixup* kV-Margin| 20.73  | 48.99 | 36.27 | 22.15 | 4.91    | 11.56| 0.51    | 25.86|     |
| Mixup* kV-GN-Margin| 43.77  | 39.77 | 20.87 | 9.14  | 4.83    | 1.32 | 22.30   | 25.86|     |

5.3 Experiment: Task Hardness

Next, we demonstrate our margins are able to measure the “hardness” of learning tasks. We say that a learning task is hard if the generalization error appears large for well-trained models. Different from the PGDL benchmark, where only models trained on the same dataset are compared, we visualize the margin distributions of Wide-ResNets trained on CIFAR-10 [32], SVHN [43], and MNIST [35], which have generalization error 12.9%, 5.3%, and 0.7%, respectively. The margins are measured on the respective datasets. In Figure 3, we again see that k-variance normalized margins reflect the hardness better than the baselines. For instance, CIFAR-10 and SVHN are indicated to be harder than MNIST as the margins are smaller.

Figure 2: Margin distributions with clean or random labels. Without k-variance normalization, Margin and GN-Margin struggle to distinguish the models trained with clean labels or random labels.

Figure 3: CIFAR-10, SVHN, and MNIST have different hardness. Although models achieve 100% training accuracy on each task, the test accuracy differs. With k-variance normalization, the margin distributions of the models are able to recognize the hardness of the tasks.

6 Analysis: Concentration and Separation of Representations

6.1 Concentration of Representations

In this section, we study how the structural properties of the feature distributions enable fast learning. Following the Wasserstein-2 k-variance analysis in [52], we apply bounds by Weed and Bach [58] to demonstrate the fast convergence rate of Wasserstein-1 k-variance when (1) the distribution has low intrinsic dimension or (2) the support is clusterable.
Assume $f$.

We show a similar relation for the gradient-normalized margin [16] in the supplement (Lemma 20):

We showed in the previous section that the concentration of the representations is captured by the variance $\operatorname{Var}_m(\phi_{\#}) \leq O(m^{-1/d})$ where $d' < d$. We obtain a better rate: $\operatorname{Var}_m(\phi_{\#}) \leq O(m^{-1/d'}).$

We defer the complete statement to the supplement. Without any assumption, the rate gets significantly worse as the feature dimension $d$ increases. Nevertheless, for an intrinsically $d'$-dimensional measure, the variance decreases with a faster rate. For clustered features, we can obtain an even stronger rate:

**Proposition 9. (Clusterable Measures)** A distribution $\mu$ is $(n, \Delta)$-clusterable if $\operatorname{supp}(\mu)$ lies in the union of $n$ balls of radius at most $\Delta$. If $\phi_{\#} \mu$ is $(n, \Delta)$-clusterable, then for all $m \leq n(2\Delta)^{-2}$,

\[
\operatorname{Var}_m(\phi_{\#} \mu) \leq 24 \sqrt{\frac{n}{m}}.
\]

We arrive at the parametric rate $O(m^{-1/2})$ if the cluster radius $\Delta$ is sufficiently small. In particular, the fast rate holds for large $m$ when the clusters are well concentrated. Different from conventional studies that focus on the complexity of a complete function class (such as Rademacher complexity [5]), our $k$-variance bounds capture the concentration of the feature distribution.

### 6.2 Separation of Representations

We showed in the previous section that the concentration of the representations is captured by the $k$-variance and that this notion translates the properties of the underlying probability measures into generalization bounds. Next, we show that maximizing the margin sheds light on the separation of the underlying representations in terms of Wasserstein distance.

**Lemma 10. (Large Margin and Feature Separation)** Assume there exist $f_{y,y'} = 1 \ldots K$ that are $L$-Lipschitz and satisfy the maximum margin constraint $y \phi(x) \geq \gamma$ for all $(x,y) \sim D$, i.e. $f_y(\phi(x)) \geq f_{y'}(\phi(x)) + \gamma$, $\forall y' \neq y$, $\forall x \in \operatorname{supp}(\mu_y)$. Then $\forall y \neq y'$, $W_1(\phi_{\#}(\mu_y), \phi_{\#}(\mu_{y'})) \geq \frac{\gamma}{L}$.

Lemma 10 states that large margins imply Wasserstein separation of the representations of each class. It also sheds light on the Lipschitz constant of the downstream classifier $F$: $L \geq \gamma/\min_{y,y'} W_1(\phi_{\#}(\mu_y), \phi_{\#}(\mu_{y'}))$. One would need more complex classifiers, i.e., those with a larger Lipschitz constant, to correctly classify classes that are close to other classes, by Wasserstein distance, in feature space. We further relate the margin loss to Wasserstein separation:

**Lemma 11.** Define the pairwise margin loss $R_{y,y'}^\phi$ for $y, y' \in \mathcal{Y}$ as

\[
R_{y,y'}^\phi(f \circ \phi) = \frac{1}{2} \left( \mathbb{E}_{x \sim \mu_y}[\gamma - f_y(\phi(x))] + \mathbb{E}_{x \sim \mu_{y'}}[\gamma - f_{y'}(\phi(x))] + \mathbb{E}_{x \sim \mu_y}[\gamma - f_y(\phi(x))] + f_y(\phi(x))] \right).
\]

Assume $f_c$ is $L$-Lipschitz for all $c \in \mathcal{Y}$. Given a margin $\gamma > 0$, for all $y \neq y'$, we have:

\[
W_1(\phi_{\#}(\mu_y), \phi_{\#}(\mu_{y'})) \geq \frac{1}{L} \left( \gamma - R_{y,y'}^\phi(f \circ \phi) \right).
\]

We show a similar relation for the gradient-normalized margin [16] in the supplement (Lemma 20): gradient normalization results in a robust Wasserstein separation of the representations, making the feature separation between classes robust to adversarial perturbations.

**Example: Clean vs. Random Labels.** Finally, we provide an illustrative example on how concentration and separation are associated with generalization. For the label corruption setting from Section 5.2, Figure 4 shows t-SNE visualizations [56] of the representations learned with true or random labels on CIFAR-10. Training with clean labels leads to well-clustered representations. Although the model trained with random labels has 100% training accuracy, the resulting feature distribution is less concentrated and separated, implying worse generalization.

![Figure 4: t-SNE visualization of representations. Classes are indicated by colors.](image-url)
7 Conclusion

In this work, we present $k$-variance normalized margin bounds, a new data-dependent generalization bound based on optimal transport. The proposed bounds predict the generalization error well on the large scale PGDL dataset [27]. We use our theoretical bounds to shed light on the role of the feature distribution in generalization. Interesting future directions include (1) trying better approximations to the Lipschitz constant such as [29, 50], (2) exploring the connection between contrastive representation learning [8, 10, 23, 30, 49] and generalization theory, and (3) studying the generalization of adversarially robust deep learning akin to [13].

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Appendix

A Broader Impact

We work on generalization in deep learning, a fundamental learning theory problem, which does not have an obvious negative societal impact. Nevertheless, in many applications of societal interest, such as medical data analysis [37] or drug discovery [53], predicting the generalization could be very important, where our work can potentially benefit related applications. Understanding and measuring the generalization are also important directions for machine learning fairness [12] and AI Safety [2].

B Additional Experiment Results

B.1 Summary of Margins

| Margin                  | Definition                                                                 |
|-------------------------|-----------------------------------------------------------------------------|
| Margin                  | \(\rho_f(\phi(x), y)\)                                                     |
| SN-Margin [4]           | \(\rho_f(\phi(x), y)/SC(f \circ \phi)\)                                    |
| GN-Margin [25]          | \(\tilde{\rho}_f(\phi(x), y) = \rho_f(\phi(x), y)/(\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon)\) |
| TV-GN-Margin [25]       | \(\tilde{\rho}_f(\phi(x), y)/\sqrt{\text{Var}_{x \sim \mu}(\|\phi(x)\|^2)}\)  |
| \(kV\)-Margin (Ours)   | \(\rho_f(\phi(x), y)/\text{E}_{c \sim p}[\text{Var}_{m_c}(\phi \# \mu_c) \cdot \text{Lip}(\rho_f(\cdot, c))]\) |
| \(kV\)-GN-Margin (Ours)| \(\tilde{\rho}_f(\phi(x), y)/\text{E}_{c \sim p}[\text{Var}_{m_c}(\phi \# \mu_c) \cdot \text{Lip}(\tilde{\rho}_f(\cdot, c))]\) |

Table 3: Definitions of margins. The SC stands for the spectral complexity defined in [4]. We use the empirical estimation of \(k\)-variance and Lipschitz constant defined in section 5 to calculate \(kV\)-Margin and \(kV\)-GN-Margin.

B.2 Variance of Empirical Estimation

In Table 1, we show the average scores over 4 random sampled subsets. We now show the standard deviation in Table 4. Overall, the standard deviation of the estimation is fairly small, consistent to the observation in Theorem 7.

|                | CIFAR | SVHN | CINIC | CINIC | Flowers | Pets | Fashion | CIFAR |
|----------------|-------|------|-------|-------|---------|------|---------|-------|
| Margin†        | 0.25  | 0.84 | 0.16  | 0.13  | 0.01    | 0.04 | 0.06    | 0.59  |
| SN-Margin† [4] | 0.07  | 0.06 | 0.01  | 0.03  | 0.00    | 0.01 | 0.01    | 0.00  |
| GN-Margin 1st [25] | 0.18 | 0.17 | 0.27  | 0.15  | 0.06    | 0.02 | 0.10    | 0.52  |
| GN-Margin 8th [25] | 0.03 | 1.44 | 0.09  | 0.04  | 0.01    | 0.00 | 0.05    | 0.14  |
| TV-GN-Margin 1st [25] | 0.26 | 0.78 | 0.49  | 0.62  | 0.03    | 0.05 | 0.03    | 1.29  |
| TV-GN-Margin 8th [25] | 0.31 | 0.35 | 0.18  | 0.19  | 0.01    | 0.14 | 0.09    | 0.73  |
| \(kV\)-Margin† 1st | 0.40 | 1.57 | 0.55  | 0.45  | 0.07    | 0.03 | 0.23    | 2.78  |
| \(kV\)-Margin† 8th | 0.64 | 0.89 | 0.24  | 0.21  | 0.02    | 0.03 | 0.07    | 0.84  |
| \(kV\)-GN-Margin† 1st | 0.15 | 0.56 | 0.47  | 0.72  | 0.02    | 0.04 | 0.06    | 1.70  |
| \(kV\)-GN-Margin† 8th | 0.81 | 0.93 | 0.16  | 0.33  | 0.03    | 0.01 | 0.04    | 0.44  |

Table 4: Standard deviation of CMI score on PGDL tasks.

B.3 The effect of \(k\) in \(k\)-Variance

We next show the ablation study with respect to \(m\) (data size) in Table 5. In particular, we draw \(m_c \times \#\text{classes}\) samples where \(m_c = 50, 100,\) and \(200\). Note that if the class distribution \(p\) is not uniform, \(m_c\) could be different for each class. The scores are computed with one subset for computational efficiency. Since the sample size per class of Flowers and Pets datasets are smaller than 50, the ablation study is not applicable.
Table 5: The role of data size in estimating $k$-variance. The number between brackets denotes the average class size $\bar{m}_c$.

B.4 Spectral Approximation to Lipschitz Constant

In section 5, we use the supermum of the norm of the jacobian on the training set as an approximation to Lipschitz constant, which is a simple lower bound of Lipschitz constant for ReLU networks [29]. It is well known that the spectral complexity, the multiplication of spectral norm of weights, is an upper bound on the Lipschitz constant of ReLU networks [38]. We replace the $\hat{L}_{ij}$ in $k$-V-Margin with the spectral complexity of the network and show the results in Table 6. The norm of the jacobian yields much better results than spectral complexity, which aligns with the observations in [15, 26].

Table 6: $k$-variance normalized margins with spectral complexity. We show the score of $k$-V-Margin with different approximations to Lipschitz constant. Empirically, gradient norm of data points yields better results.

B.5 Experiment Details

PGDL Dataset The models and datasets are accessible with Keras API [9] (integrated with TensorFlow [1]): https://github.com/google-research/google-research/tree/master/pgdl (Apache 2.0 License). We use the official evaluation code of PGDL competition [27]. All the scores can be computed with one TITAN X (Pascal) GPUs. The intuition behind the sample size $\min(200 \times \#\text{classes}, \text{data}_\text{size})$ is that we want the average sample size for each class is 200. Note that if the class distribution $p$ is not uniform, the sample size for each class could be different. However, the sample size per class of Flowers and Pets datasets are smaller than $200 \times \#\text{classes}$, we constrain the sample size to be dataset size at most. We follow the setting in [42] to calculate the mixup accuracy with label-wise mixup.

Other Experiments The experiments in section 5.2 are run with the code from [63]: https://github.com/pluskid/fitting-random-labels (MIT License). We trained the models with the exact same code and visualize the margins with our own implementation via PyTorch [47]. For the experiments in section 5.3, we only change the data loader part of the code. The models of MNIST and SVHN are trained for 10 and 20 epochs, respectively. To visualize the t-SNE in section 6, we use the default parameter in scikit-learn [48] (sklearn.manifold.TSNE) with the output from the 4th residual block of the network.
C Proofs

C.1 Estimating the Lipschitz Constant of the GN-Margin

\[ \hat{\text{Lip}}(\hat{\rho}_f(\cdot, c)) = \max_{x \in S_c} \left\| \nabla_\phi \frac{\rho_f(\phi(x), c)}{\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon} \right\|_2 = \max_{x \in S_c} \frac{\|\nabla_\phi \rho_f(\phi(x), y)\|_2}{\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon} \approx 1 \] (4)

Proof of equation 4 We first expand the derivative as follows:

\[ \hat{\text{Lip}}(\hat{\rho}_f(\cdot, c)) = \max_{x \in X} \left\| \nabla_\phi \frac{\rho_f(\phi(x), c)}{\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon} \right\|_2 = \max_{x \in X} \frac{\|\nabla_\phi \rho_f(\phi(x), c)\|\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon - \rho_f(\phi(x), c)\|\nabla_\phi \nabla_\phi \rho_f(\phi(x), y)\|_2}{\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon} \].

Note that \(\rho_f\) is piecewise linear as \(f\) is ReLU networks. For points where \(\rho_f\) is differentiable i.e. that do not lie on the boundary between linear regions, the second order derivative is zero. In particular, we have \(\nabla_\phi \nabla_\phi \rho_f(\phi(x), y)\|_2 = 0\). Therefore, excluding from \(X\) non differentiable points of \(\rho_f\), the empirical Lipschitz estimation (lower bound) can be written as

\[ \hat{\text{Lip}}(\hat{\rho}_f(\cdot, c)) = \max_{x \in X} \left\| \nabla_\phi \frac{\rho_f(\phi(x), c)\|\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon - \rho_f(\phi(x), c)\|\nabla_\phi \nabla_\phi \rho_f(\phi(x), y)\|_2}{\|\nabla_\phi \rho_f(\phi(x), y)\|_2 + \epsilon} \right\|_2 \]

\[ = \max_{x \in X} \|\nabla_\phi \rho_f(\phi(x), c)\|_2 \leq 1. \]

We can see that \(\hat{\text{Lip}}\) is tightly upper bounded by 1 when \(\epsilon\) is a very small value.

Discussion of Lower and Upper Bounds on the Lipschitz constant Note that the approximation of the lipchitz constant will result in additional error in the generalization bound as follows:

\[ \hat{R}_{\gamma,m}(f \circ \phi) + \mathbb{E}_{c \sim p_y} \left[ \frac{\text{Lip}(\rho_f(\cdot, c))}{\gamma} \left( \mathbb{V} \left[ \frac{\mathbb{P}_c(\phi}{n(\phi \# \mu_c)} + 2B\sqrt{\frac{\log(2K/\delta)}{n(\mu_c/2n)}} \right] \right) \right] \]

\[ + \mathbb{E}_{c \sim p_y} \left[ \frac{\text{Lip}(\rho_f(\cdot, c)) - \hat{\text{Lip}}(\rho_f(\cdot, c))}{\gamma} \left( \mathbb{V} \left[ \frac{\mathbb{P}_c(\phi}{n(\phi \# \mu_c)} + 2B\sqrt{\frac{\log(2K/\delta)}{n(\mu_c/2n)}} \right] \right) + \sqrt{\frac{\log(2)}{2m}}. \]

While for an upper bound on the lipschitz constant the third term is negative and can be ignored in the generalization bound. For a lower bound this error term \(\text{Lip}(\rho_f(\cdot, c)) - \hat{\text{Lip}}(\rho_f(\cdot, c))\) results in additional positive error term. Bounding this error term is beyond the scope of this work and we leave it for a future work.

C.2 Proof of the Margin Bound

Proof of Theorem 2. Recall the margin definition:

\[ \rho_f(\phi(x), y) = f_y(\phi(x)) - \max_{y' \neq y} f_{y'}(\phi(x)) \]

Let \(\mu_c(x) = \mathbb{P}(x|y = c)\), and let \(p(y) = \mathbb{P}(Y = y) = \pi_y\). Given \(f \in \mathcal{F}\) and \(\phi \in \Phi = \{\phi : \mathcal{X} \to \mathcal{Z},||\phi(x)|| \leq R\}\), we are interested in bounding the class-average zero-one loss of a hypothesis \(f \circ \phi:\)

\[ R_\mu(f \circ \phi) = \sum_{c=1}^{K} \pi_k \mu_c(f(\circ \phi)) = \sum_{c=1}^{K} \pi_k \mathbb{E}_{x \sim \mu_c} [\mathbb{I}_{\rho_f(\phi(x), c) \leq 0}], \]
where we will bound the error of each class \( c \in \mathcal{Y} \) separately. To do so, the margin loss defined by \( \ell_{\gamma} \) by \( L_{\gamma}(u) = 1_{u \leq 0} + (1 - \frac{u}{\gamma})1_{0 < u \leq \gamma} \) would be handy.

Note that :
\[
R_{\mu}(f \circ \phi) \leq \mathbb{E}(x,y)L_{\gamma}(\rho_{f}(\phi(x), y))
\]
(see for example Lemma A.4 in [4] for a proof of this claim.)

By McDiarmid Inequality, we have with probability at least \( 1 - \delta \),
\[
R_{\mu}(f \circ \phi) \leq \mathbb{E}(x,y)L_{\gamma}(\rho_{f}(\phi(x), y)) \leq \sum_{c=1}^{K} \pi_{c} \mathbb{E}_{S_{c} \sim \mu_{c}}[L_{\gamma}(\rho_{f}(\phi(x), c))] + \mathbb{D}(f \circ \phi, \mu) + \sqrt{\log(1/\delta) \over 2m}.
\]

where
\[
\mathbb{D}(f \circ \phi, \mu) = \mathbb{E}_{S_{1} \sim \mu_{1}} \ldots \mathbb{E}_{S_{K} \sim \mu_{K}} \left[ \sup_{f \in F} \left( \sum_{c=1}^{K} \pi_{c} \left( \mathbb{E}_{S_{c} \sim \mu_{c}}[L_{\gamma}(\rho_{f}(\phi(x), c))] - \hat{\mathbb{E}}_{S_{c} \sim \mu_{c}}[L_{\gamma}(\rho_{f}(\phi(x), c))] \right) \right) \right].
\]

Note that the \( \sup \) here is taken only on the classifier function class and not on the classifier and the function map together. For a given class \( c \) and feature map \( \phi \) define:
\[
\mathcal{G}_{c} = \{ h|h(z) = L_{\mu} \circ \rho_{f}(z, c) : f \in F, z \in \mathcal{Z} \}.
\]

Using the fact that \( \sup(a + b) \leq \sup a + \sup b \), we have:
\[
\mathbb{D}(f \circ \phi, \mu) \leq \sum_{c=1}^{K} \pi_{c} \mathbb{E}_{S_{c} \sim \mu_{c}} \sup_{f \in F} \left( \mathbb{E}_{S_{c} \sim \mu_{c}}[L_{\gamma}(\rho_{f}(\phi(x), c))] - \hat{\mathbb{E}}_{S_{c} \sim \mu_{c}}[L_{\gamma}(\rho_{f}(\phi(x), c))] \right)
\]
\[
= \sum_{c=1}^{K} \pi_{c} \mathbb{E}_{S_{c} \sim \mu_{c}} \left( \sup_{h \in \mathcal{U}_{c}} \left( \mathbb{E}_{S_{c} \sim \mu_{c}}[h(\phi(x))] - \hat{\mathbb{E}}_{S_{c} \sim \mu_{c}}[h(\phi(x))] \right) \right),
\]
where the last equality follows from the definition of the function class \( \mathcal{G}_{c} \).

We are left now with bounding each class dependent deviation. We drop the index \( c \) from \( S_{c} \) in what follows in order to avoid cumbersome notations. Considering an independent sample of same size \( \hat{S} \) from \( \mu_{c} \), we have:
\[
\mathbb{E}_{\hat{S} \sim \mu_{c}} \left[ \sup_{h \in \mathcal{U}_{c}} \left( \mathbb{E}_{\mu_{c}}[h(\phi(x))] - \hat{\mathbb{E}}_{\hat{S} \sim \mu_{c}}[h(\phi(x))] \right) \right] \leq \mathbb{E}_{\hat{S},\hat{S} \sim \mu_{c}} \left[ \sup_{h \in \mathcal{U}_{c}} \hat{\mathbb{E}}_{\hat{S}}[h(\phi(x))] - \hat{\mathbb{E}}_{\hat{S}}[h(\phi(x))] \right].
\]

Note that \( h(z) = L_{\gamma}(\rho_{f}(z, c)) \) is lipchitz with lipchitz constant \( \frac{1}{\gamma} \text{Lip}(\rho_{f}(\cdot, c)) \), since \( L_{\gamma} \) is lipchitz with lipchitz constant \( \frac{1}{\gamma} \) and by assumption the margin \( \rho_{f}(z, c) \) is lipchitz in its first argument. By the dual of the Wasserstein 1 distance we have:
\[
\mathcal{W}_{1}(\phi_{\#}p_{\hat{S}}, \phi_{\#}p_{\hat{S}}) = \sup_{h, \text{Lip}(h) \leq 1} \hat{\mathbb{E}}_{\hat{S}}[h(\phi(x))] - \hat{\mathbb{E}}_{\hat{S}}[h(\phi(x))]
\]

Since \( \mathcal{G}_{c} \) are subset of lipchitz of functions with lipchitz constant \( \frac{\text{Lip}(\rho_{f}(\cdot, c))}{\gamma} \), it follows that:
\[
\sup_{h \in \mathcal{U}_{c}} \hat{\mathbb{E}}_{\hat{S}}[h(\phi(x))] - \hat{\mathbb{E}}_{\hat{S}}[h(\phi(x))] \leq \frac{\text{Lip}(\rho_{f}(\cdot, c))}{\gamma} \mathcal{W}_{1}(\phi_{\#}p_{\hat{S}}, \phi_{\#}p_{\hat{S}})
\]

It follows from (7) and (8), that:
\[
\mathbb{E}_{\hat{S} \sim \mu_{c}} \left[ \sup_{h \in \mathcal{U}_{c}} \left( \mathbb{E}_{\mu_{c}}[h(\phi(x))] - \hat{\mathbb{E}}_{\hat{S} \sim \mu_{c}}[h(\phi(x))] \right) \right] \leq \frac{\text{Lip}(\rho_{f}(\cdot, c))}{\gamma} \mathbb{E}_{\hat{S},\hat{S} \sim \mu_{c}} \mathcal{W}_{1}(\phi_{\#}p_{\hat{S}}, \phi_{\#}p_{\hat{S}})
\]
\[
= \frac{\text{Lip}(\rho_{f}(\cdot, c))}{\gamma} \text{Var}_{\mu_{c}}(\phi_{\#}c).
\]
we finally have by (5), the following generalization bound, that holds with probability $1 - \delta$:

$$D(f \circ \phi, \mu) \leq \sum_{c \in \gamma} \pi_c \text{Lip}(\rho_f (\cdot, c)) \text{Var}_{m_c}(\phi_{\#} \mu_c)$$

Using (10) and noting that,

$$L_\gamma(\rho_f (\phi(x), c)) \leq 1_{\rho_f (\phi(x), c) \leq \gamma}$$

we finally have by (5), the following generalization bound, that holds with probability $1 - \delta$:

$$R_{\mu}(f \circ \phi) \leq \sum_{c \in \gamma} \pi_c \hat{E}_{S \sim \mu_S} [1_{\rho_f (\phi(x), c) \leq \gamma}] + \frac{1}{\gamma} \sum_{c \in \gamma} \pi_c \text{Lip}(\rho_f (\cdot, c)) \text{Var}_{m_c}(\phi_{\#} \mu_c) + \sqrt{\frac{\log(1/\delta)}{2m}}$$

Finally Plugging (9) in (6) we obtain finally:

$$\hat{D}(f \circ \phi, \mu) \leq \sum_{c \in \gamma} \pi_c \text{Lip}(\rho_f (\cdot, c)) \text{Var}_{m_c}(\phi_{\#} \mu_c)$$

Proof of Theorem 4. It is enough to show that:

$$\hat{R}_{\mu}(f \circ \phi) \leq \hat{E}_{(x, y) \sim \mu} [L_\gamma(\hat{\rho}_f (\phi(x), y))],$$

and the rest of the proof is the same as in Theorem 2. For any $\xi(x, y) > 0$, and $\gamma > 0$

$$R_{\mu}(f \circ \phi) = \mathbb{P}_{(x, y)}(\arg \max_{c} f_c(\phi(x)) \neq y)$$

$$\leq \mathbb{P}(f_y(\phi(x)) - \max_{y' \neq y} f_{y'}(\phi(x)) \leq 0)$$

$$= \mathbb{P} \left( \frac{f_y(\phi(x)) - \max_{y' \neq y} f_{y'}(\phi(x))}{\xi(x)} \leq 0 \right)$$

$$\leq \mathbb{E} \left[ 1_{f_y(\phi(x)) - \max_{y' \neq y} f_{y'}(\phi(x)) \leq 0} \right]$$

$$\leq \mathbb{E} \left[ L_\gamma \left( \frac{f_y(\phi(x)) - \max_{y' \neq y} f_{y'}(\phi(x))}{\xi(x, y)} \right) \right].$$

Setting $\xi(x, y) = \| \nabla_{\phi} \rho_f (\phi(x), y) \|_2 + \epsilon$, gives the result.
C.3 Proof of the Estimation Error of $k$-Variance (Generalization Error of the Encoder)

Proof of Lemma 5. We would like to estimation to the $k$-variance with $\hat{\text{Var}}_k(\phi_#\mu) = \frac{1}{n} \sum_{j=1}^n W_1(\phi_#p_{S_j}, \phi_#p_{\tilde{S}_j})$ as a function of the $nk$ independent samples from which it is computed, each sample being a pair $(x_i, \tilde{x}_i)$. To apply the McDiarmid’s Inequality, we have to examine the stability of the empirical $k$-variance.

The Kantorovich–Rubinstein duality gives us the general formula of $W_1$ distance:

$$W_1(P, Q) = \sup_{\text{Lip}(f) \leq 1} \mathbb{E}_P[f] - \mathbb{E}_Q[f]$$

In our case, separately for each $j$, we can write

$$W_1(\phi_#p_{S_j}, \phi_#p_{\tilde{S}_j}) = \sup_{\text{Lip}(f) \leq 1} \frac{1}{k} \sum_{\ell=1}^k (f(\phi(x_i^\ell)) - f(\phi(\tilde{x}_i^\ell))).$$

Recall that the $(x_i, \tilde{x}_i)$ are independent across $\ell$ and $j$. Consider replacing one of the elements $(x_i^\ell, \tilde{x}_i^\ell)$ with some $(x_i^{'\ell}, \tilde{x}_i^{'\ell})$, forming $p_{\tilde{S}_j}$ and $p_{\tilde{S}_j}$. Since the $(x_i^\ell, \tilde{x}_i^\ell)$ are identically distributed, by symmetry we can set $i = 1$. We then bound

$$W_1(\phi_#p_{S_1}, \phi_#p_{\tilde{S}_1}) - W_1(\phi_#p_{S_1}, \phi_#p_{\tilde{S}_1})$$

$$= \sup_{\text{Lip}(f) \leq 1} \frac{1}{k} \left( (f(\phi(x_1^1)) - f(\phi(x_1^1))) + \sum_{\ell=2}^k (f(\phi(x_1^\ell)) - f(\phi(\tilde{x}_1^\ell))) \right)$$

$$\leq \frac{1}{k} \sup_{\text{Lip}(f) \leq 1} \left( (f(\phi(x_1^1)) - f(\phi(x_1^1)) + f(\phi(x_1^{'\ell})) - f(\phi(\tilde{x}_1^{'\ell}))) \right)$$

$$\leq \frac{1}{k} \sup_{\text{Lip}(f) \leq 1} \left( (f(\phi(x_1^1)) - f(\phi(x_1^1))) + \frac{1}{k} \sup_{\text{Lip}(f) \leq 1} \left( (f(\phi(x_1^{'\ell})) - f(\phi(\tilde{x}_1^{'\ell}))) \right) \right)$$

$$\leq \frac{\|\phi(x_1^1) - \phi(x_1^{'\ell})\| + \|\phi(x_1^{'\ell}) - \phi(\tilde{x}_1^{'\ell})\|}{k},$$

where we have used in the third inequality the fact that the $\sup$ is a contraction ($\sup_h A(h) - \sup_h B(h) \leq \sup_h (A(h) - B(h))$), and the definition of the Lipschitizity in the fourth inequality.

By symmetry and scaling the right hand side with $\frac{1}{n}$, we have:

$$\left| \frac{1}{n} \sum_{j=1}^n W_1(\phi_#p_{S_j}, \phi_#p_{\tilde{S}_j}) - \frac{1}{n} \sum_{j=1}^n W_1(\phi_#p_{S_j}, \phi_#p_{\tilde{S}_j}) \right| \leq \frac{2B}{nk}.$$ 

We are now ready to apply the McDiarmid Inequality with $nk$ samples, which yields:

$$\mathbb{P}(\text{Var}_k(\phi_#\mu) - \hat{\text{Var}}_{k,n}(\phi_#\mu) \geq t) \leq \exp \left( -\frac{t^2nk}{2B^2} \right).$$

Setting the probability to be less than $\delta$ and solving for $t$, we can see that this probability is less than $\delta$ if and only if $t \geq \sqrt{\frac{2B^2 \log(1/\delta)}{nk}}$. Therefore, with probability at least $1 - \delta$,

$$\mathbb{E}_{S,S}[W_1(\phi_#p_{S}, \phi_#p_{\tilde{S}})] \leq \frac{1}{n} \sum_{j=1}^n W_1(\phi_#p_{S_j}, \phi_#p_{\tilde{S}_j}) + \sqrt{\frac{2B^2 \log(1/\delta)}{nk}}.$$ 

Proof of Corollary 6. For each class $c \in \mathcal{Y}$, we obtain $m_c$ samples $\{(x_i, y_i)\}_{i=1}^n$. Therefore, to compute $\hat{\text{Var}}_{k,n}(\phi_#\mu_c)$, the largest $k$ for a specific $n$ is $\lfloor m_c/2n \rfloor$. By Lemma 5 and applying union bounds for each class (using confidence $\delta/2K$ for each) and completes the proof.

\[ \square \]
C.4  Proof of Empirical Variance

Proof of Theorem 7. We use the Efron Stein inequality:

**Lemma 13 (Efron Stein Inequality).** Let $X := (X_1, \ldots, X_m)$ be an $m$-tuple of $X$-valued independent random variables, and let $X'_i$ be independent copies of $X_i$ with the same distribution. Suppose $g : \mathcal{X}^m \to \mathbb{R}$ is a map, and define $X^{(i)} = (X_1, \ldots, X_{i-1}, X'_i, X_{i+1} \ldots X_m)$. Then

$$\text{Var}(g(X)) \leq \frac{1}{2} \sum_{i=1}^{m} \mathbb{E} \left[ (g(X) - g(X^{(i)}))^2 \right]. \quad (11)$$

Consider $\frac{1}{n} \sum_{j=1}^{n} W_1(\hat{\mu}_k^j, \hat{\mu}_k)$ as a function of the $nk$ independent samples from which it is computed, each sample being a pair $(x_i^j, y_i^j)$. Using Kantorovich–Rubinstein duality, we have the general formula:

$$W_1(P, Q) = \sup_{\|f\|_{\text{Lip}} \leq 1} \mathbb{E}_P[f] - \mathbb{E}_Q[f]$$

where $\| \cdot \|_{\text{Lip}}$ is the Lipschitz norm. In our case, separately for each $j$, we can write

$$W_1(\hat{\mu}_k^j, \hat{\mu}_k) = W_1\left(\frac{1}{k} \sum_{\ell=1}^{k} \delta_{x_i^j}, \frac{1}{k} \sum_{\ell=1}^{k} \delta_{y_i^j}\right) = \sup_{\|f\|_{\text{Lip}} \leq 1} \frac{1}{k} \sum_{\ell=1}^{k} (f(x_i^j) - f(y_i^j)).$$

Recall that the $(x_i^j, y_i^j)$ are independent across $\ell$ and $j$. Consider replacing one of the elements $(x_i^j, y_i^j)$ with some $(x_i^{j'}, y_i^{j'})$, forming $\hat{\mu}_k$ and $\hat{\mu}_k^j$. Since the $(x_i^j, y_i^j)$ are identically distributed, by symmetry we can set $i = 1$. We then bound

$$W_1(\hat{\mu}_k^j, \hat{\mu}_k) - W_1(\hat{\mu}_k, \hat{\mu}_k^j) = \sup_{\|f\|_{\text{Lip}} \leq 1} \frac{1}{k} \left( (f(x_1^j) - f(y_1^j)) + \sum_{\ell=2}^{k} (f(x_1^\ell) - f(y_1^\ell)) \right)$$

$$- \sup_{\|f\|_{\text{Lip}} \leq 1} \frac{1}{k} \left( (f(x_1^{j'}) - f(y_1^{j'})) + \sum_{\ell=2}^{k} (f(x_1^\ell) - f(y_1^\ell)) \right)$$

$$\leq \frac{1}{k} \sup_{\|f\|_{\text{Lip}} \leq 1} (f(x_1^j) - f(x_1^{j'})) + (f(y_1^j) - f(y_1^{j'}))$$

$$\leq \frac{\|x_1^j - x_1^{j'}\| + \|y_1^j - y_1^{j'}\|}{k},$$

where we have used the definition of the Lipschitz norm. By symmetry, this yields (scaling by $\frac{1}{n}$ as in the expression in the theorem)

$$\left| \frac{1}{n} W_1(\hat{\mu}_k^j, \hat{\mu}_k) - \frac{1}{n} W_1(\hat{\mu}_k^j, \hat{\mu}_k^j) \right| \leq \frac{\|x_1^j - x_1^{j'}\| + \|y_1^j - y_1^{j'}\|}{kn}$$

It follows that:

$$\mathbb{E} \left[ \left( \frac{1}{n} W_1(\hat{\mu}_k^j, \hat{\mu}_k) - \frac{1}{n} W_1(\hat{\mu}_k^j, \hat{\mu}_k^j) \right)^2 \right] \leq \frac{\mathbb{E} \left[ (\|x_1^j - x_1^{j'}\| + \|y_1^j - y_1^{j'}\|)^2 \right]}{kn^2}$$

$$= \frac{2(\mathbb{E}_{x,x' \sim \mu} \|x - x'\|^2 + (\mathbb{E}_{x,x' \sim \mu} \|x - x'\|)^2)}{kn^2}$$

20
for each of the independent $nk$ random variables $(x_i^j, y_i^j)$, where we have used the fact that $x_i^j$ and $y_i^j$ are i.i.d. We can substitute this into the Efron Stein inequality above to obtain

\[
\Var \left[ \hat{W}_{k,n}(\mu) \right] \leq \frac{E_{x,x' \sim \mu} \|x - x'\|^2 + (E_{x,x' \sim \mu} \|x - x'\|)^2}{kn} = \frac{2 \Var_{\mu}(X) + (E_{x,x' \sim \mu} \|x - x'\|)^2}{kn} \leq \frac{2 \Var_{\mu}(X) + E_{x,x' \sim \mu} \|x - x'\|^2}{kn} \leq 4 \Var_{\mu}(X)
\]

where used that the variance $\Var_{\mu}(X) = \frac{1}{2} E_{x,x' \sim \mu} \|x - x'\|^2$, and Jensen inequality.

\[\square\]

### C.5 Proof of Proposition 8

We will prove these two arguments separately with the following two propositions.

**Proposition 14.** For any $\phi_{\#} \mu \in \Prob(\mathbb{R}^d)$, we have $\Var_m(\phi_{\#} \mu) \leq O(m^{-1/d})$ for $d > 2$.

**Proof.** The result is an application of Theorem 1 of [20].

**Theorem 15 ((Fournier and Guillin [20])).** Let $\mu \in \Prob(\mathbb{R}^d)$ and let $p > 0$. Define $M_q(\mu) = \int_{\mathbb{R}^d} |x|^q \mu(dx)$ be the $q$-th moment for $\mu$ and assume $M_q(\mu) \leq \infty$ for some $q > p$. There exists a constant $C$ depending only on $p, d, q$ such that, for all $m \geq 1$, $p \in (0, d/2)$ and $q \neq d/(d - p)$,

\[
E_{S \sim \mu^m}[W_p(\mu_S, \mu)] \leq CM_{q/(d-q)}^{p/q}(m^{-p/d} + m^{-(q-p)/q}).
\]

By the triangle inequality and setting $p = 1$, we have

\[
\Var_m(\phi_{\#} \mu) = E_{S,S' \sim \mu^m}[W_1(\phi_{\#} \mu_S, \phi_{\#} \mu_{S'})] \leq 2E_{S \sim \mu^m}[W_1(\mu_S, \mu_S)] \leq 2CM_{q/(d-q)}^{1/q}(m^{-1/d} + m^{-(q-1)/q}).
\]

Note that the term $m^{-(q-1)/q}$ is small and can be removed. For instance, plugging $q = 2$, we can see that the first term dominates the second term which completes the proof for the first argument. \[\square\]

We then demonstrate the case when the measure has low-dimensional structure.

**Definition 16. (Low-dimensional Measures)** Given a set $S \subseteq X$, the $\epsilon$-covering number of $S$, denoted as $\mathcal{N}_\epsilon(S)$, is the minimum $n$ such that there exists $n$ closed balls $B_1, \cdots, B_n$ of diameter $\epsilon$ such that $S \subseteq \bigcup_{1 \leq i \leq n} B_i$. For any $S \subseteq X$, the $\epsilon$-fattening of $S$ is $S_\epsilon := \{y : D(y, S) \leq \epsilon\}$, where $D$ denotes the Euclidean distance.

**Proposition 17.** Suppose $\supp(\phi_{\#} \mu) \subseteq S$, for some $\epsilon > 0$, where $S$ satisfies $\mathcal{N}_\epsilon(S) \leq (3\epsilon')^{-d}$ for all $\epsilon' \leq 1/27$ and some $d > 2$. Then, for all $m \leq (3\epsilon')^{-d}$, we have $\Var_m(\phi_{\#} \mu) \leq 2C_1 m^{-1/d}$, where $C_1 = 54 + 27/(3^{3/4} - 1)$.

**Proof.** an application of Weed and Bach [58]'s Proposition 15 for $p = 1$.

**Proposition 18 ((Weed and Bach [58])).** Suppose $\supp(\mu) \subseteq S$, for some $\epsilon > 0$, where $S$ satisfies $\mathcal{N}_\epsilon(S) \leq (3\epsilon')^{-d}$ for all $\epsilon' \leq 1/27$ and some $d > 2p$. Then, for all $m \leq (3\epsilon')^{-d}$, we have

\[
E_{S \sim \mu^m}[W_p(\mu_S, \mu_S)] \leq C_1 m^{-p/d},
\]

where

\[
C_1 = 27^p \left( 2 + \frac{1}{3^{3/4} - p - 1} \right).
\]

By the triangle inequality and setting $p = 1$, we have

\[
\Var_m(\phi_{\#} \mu) = E_{S,S' \sim \mu^m}[W_1(\phi_{\#} \mu_S, \phi_{\#} \mu_{S'})] \leq 2E_{S \sim \mu^m}[W_p(\mu_S, \mu_S)] \leq 2C_1 m^{-1/d},
\]

where $C_1 = 54 + 27/(3^{3/4} - 1)$. \[\square\]
C.6 Proof of Proposition 9

Proof. The results is an application of Weed and Bach [58]’s Proposition 13 for \( p = 1 \).

Proposition 19 (Weed and Bach [58]). If \( \mu \) is \((n, \Delta)\)-clusterable, then for all \( m \leq n(2\Delta)^{-2p} \),

\[
\mathbb{E}_{S \sim \mu} [W_p^p(\mu, \mu_S)] \leq (9^p + 3) \frac{n}{m}.
\]

Similarly, by the triangle inequality, we have

\[
\text{Var}_m(\phi_{\#} \mu) = \mathbb{E}_{S, \tilde{S} \sim \mu} [W_1(\phi_{\#} \mu_S, \phi_{\#} \mu_{\tilde{S}})] \leq 2\mathbb{E}_{S \sim \mu} [W_p^p(\mu, \mu_S)] \leq 24 \frac{n}{m}.
\]

\(\square\)

D Feature Separation and Margin

Proof of Lemma 10. Since \( f_y \) and \( f_y' \) are \( L \) lipchitz, it follows that \( g(z) = f_y(z) - f_y'(z) \) is \( 2L \)
Lipchitz, and hence \( \frac{g}{2L} \) is \( Lip_1 \).

\[
W_1(\phi_{\#}(\mu_y), \phi_{\#}(\mu_{y'})) = \sup_{f \in Lip_1} \mathbb{E}_{x \sim p_y} f(\phi(x)) - \mathbb{E}_{x \sim \mu_y} f(\phi(x))
\geq \frac{1}{2L} \left( \mathbb{E}_{x \sim p_y} g(\phi(x)) - \mathbb{E}_{x \sim \mu_y} g(\phi(x)) \right)
= \frac{1}{2L} \left( \mathbb{E}_{x \sim p_y} [f_y(\phi(x)) - f_y'(\phi(x))] + \mathbb{E}_{x \sim \mu_y} [f_y'(\phi(x)) - f_y(\phi(x))] \right)
\geq \frac{1}{2L} (2 \gamma) \quad \text{(By Assumption on } f \text{)}
= \frac{\gamma}{L}
\]

\(\square\)

Proof of Lemma 11. We follow the same notation of the proof above but we don’t make any assumption
on \( f_y, f_y' \) except that they are \( Lip_L \):

\[
W_1(\phi_{\#}(\mu_y), \phi_{\#}(\mu_{y'})) = \sup_{f \in Lip_1} \mathbb{E}_{x \sim p_y} f(\phi(x)) - \mathbb{E}_{x \sim \mu_y} f(\phi(x))
\geq \frac{1}{2L} \left( \mathbb{E}_{x \sim p_y} g(\phi(x)) - \mathbb{E}_{x \sim \mu_y} g(\phi(x)) \right)
= \frac{1}{2L} \left( \int [f_y(z) - f_y'(z)] d\phi_{\#}(\mu_y)(z) + \int [f_y'(z) - f_y(z)] d\phi_{\#}(\mu_{y'})(z) \right)
\geq \frac{1}{2L} \left( \gamma - \int [\gamma - (f_y(z) - f_y'(z))] d\phi_{\#}(\mu_y)(z) + \gamma - \int [\gamma - (f_y'(z) - f_y(z))] d\phi_{\#}(\mu_{y'})(z) \right)
\geq \frac{1}{2L} \left( 2 \gamma - \int [\gamma - (f_y(z) - f_y'(z))] + d\phi_{\#}(\mu_y)(z) - \int [\gamma - (f_y'(z) - f_y(z))] + d\phi_{\#}(\mu_{y'})(z) \right)
\]

where the last inequality follows from the fact that for \( t \in \mathbb{R} \), we have \( t \leq |t|_+ = \max(t, 0) \) Hence we have:

\[
W_1(\phi_{\#}(\mu_y), \phi_{\#}(\mu_{y'})) \geq \frac{1}{L} \left( \gamma - \frac{1}{2} \left( \mathbb{E}_{\mu_y} [\gamma - f_y(\phi(x)) + f_y'(\phi(x))]_+ + \mathbb{E}_{\mu_{y'}} [\gamma - f_y'(\phi(x)) + f_y(\phi(x))]_+ \right) \right).
\]

\(\square\)

Lemma 20 (Robust Feature Separation and Max-Gradient-Margin classifiers). Let \( \mathcal{F} \) be function
class satisfying assumption 1 and assumption 2 (ii) in [21] (piece-wise smoothness and growth and
Then:

\[ f_y(\phi(x)) > f_{y'}(\phi(x)) + \gamma + \delta_n \| \nabla_z f_y(\phi(x)) - \nabla_z f_{y'}(\phi(x)) \|_2, \forall x \in \text{supp}(\hat{\mu}_y), \forall y' \neq y \]

Then:

\[ \sup_{\mu, W_{\infty}(\mu, \hat{\mu}) \leq \delta_n} W_1(\phi \# \mu, \phi \# \hat{\mu}_y) \geq \frac{\gamma}{L} - \delta_n M - \epsilon_n. \]

where \( \epsilon_n = O(1/\sqrt{n}) \) \( \hat{\mu} \) is defined as follows: \( \hat{\mu}(x, c) \) be such that \( \hat{\mu}(x|c = 1) = \hat{\mu}_{\mu}(x) \) and \( \hat{\mu}(x|c = -1) = \hat{\mu}_{y'}(x) \), let \( \hat{\mu}(c = 1) = \hat{\mu}(c = -1) = \frac{1}{2} \) (similar definition holds for \( \mu \)).

**Proof.** Without Loss of generality assume \( \phi(x) = x \).

\[ W_1(\mu_y, \mu_{y'}) = \sup_{f \in \text{Lip}_1} \mathbb{E}_{\mu_y} f(x) - \mathbb{E}_{\mu_{y'}} f(x) \]

\[ = \sup_{f \in \text{Lip}_1} \mathbb{E}_{(c,x) \sim \mu} 2c f(x) \]

\[ = - \inf_{f \in \text{Lip}_1} -2\mathbb{E}_{(c,x) \sim \mu} c f(x) \]

This form of \( W_1 \) suggests studying the following robust risk, for technical reason we will use another functional class \( \mathcal{F} \subset \text{Lip}_1 \) instead of \( \text{Lip}_1 \):

\[ \inf_{f \in \mathcal{F}} \sup_{\mu, W_{\infty}(\mu, \hat{\mu}) \leq \delta_n} -2\mathbb{E}_{(c,x) \sim \mu} c f(x) \]

Applying here theorem 1 (1) of Gao et al [21] see also example 12, for \( \mathcal{F} \) of function satisfying assumption 1 and assumption 2 in Gao et al in addition to being lipchitz we have:

\[ \sup_{\mu, W_{\infty}(\mu, \hat{\mu}) \leq \delta_n} -2\mathbb{E}_{(c,x) \sim \mu} c f(x) \leq -2\mathbb{E}_{(c,x) \sim \mu} c f(x) + \delta_n 2\mathbb{E}_{\hat{\mu}} |\nabla_{(c,x)} c f(x)| + \epsilon_n \]

Note that:

\[ 2\mathbb{E}_{(c,x) \sim \mu} c f(x) = \mathbb{E}_{\mu_y} f(x) - \mathbb{E}_{\mu_{y'}} f(x) \]

and

\[ \nabla_{(c,x)} c f(x) = (f(x), c \nabla_x f(x)) \]

and

\[ |\nabla_{(c,x)} c f(x)| = \sqrt{f(x)^2 + |\nabla_x f(x)|^2} \leq |f(x)| + |\nabla_x f(x)| \leq M + |\nabla_x f(x)| \]

where we used

\[ \sqrt{a + b} \leq \sqrt{a} + \sqrt{b}, \text{ and } |f(x)| \leq M \]

Hence we have:

\[ \inf_{f \in \mathcal{F}} \sup_{\mu, W_{\infty}(\mu, \hat{\mu}) \leq \delta_n} -2\mathbb{E}_{(c,x) \sim \mu} c f(x) = \inf_{f \in \mathcal{F}} -2\mathbb{E}_{(c,x) \sim \mu} c f(x) + \delta_n 2\mathbb{E}_{\hat{\mu}} |\nabla_{(c,x)} c f(x)| + \epsilon_n \]

\[ \leq - \inf_{f \in \mathcal{F}} \mathbb{E}_{\mu_y} f(x) + \mathbb{E}_{\mu_{y'}} f(x) + \delta_n \mathbb{E}_{\mu_y} (|\nabla_x f(x)| + |f(x)|) + \delta_n \mathbb{E}_{\mu_{y'}} (|\nabla_x f(x)| + |f(x)|) + \epsilon_n \]

\[ \leq - \inf_{f \in \mathcal{F}} \mathbb{E}_{\mu_y} (f(x) - \delta_n ||\nabla_x f(x)||) + \mathbb{E}_{\mu_{y'}} (f(x) + \delta_n ||\nabla_x f(x)||) + \delta_n M + \epsilon_n \]

Let \( g(x) = \frac{f_y(x) - f_{y'}(x)}{2L} \) we have:

\[ \inf_{f \in \mathcal{F}} -\mathbb{E}_{\mu_y} (g(x) - \delta_n ||\nabla x g(x)||) + \mathbb{E}_{\mu_{y'}} (g(x) + \delta_n ||\nabla x g(x)||) \]

\[ \leq -\mathbb{E}_{\mu_y} (g(x) - \delta_n ||\nabla x g(x)||) + \mathbb{E}_{\mu_{y'}} (g(x) + \delta_n ||\nabla x g(x)||) \]

\[ = -\mathbb{E}_{\mu_y} (g(x) - \delta_n ||\nabla x g(x)||) - \mathbb{E}_{\mu_{y'}} (-g(x) - \delta_n ||\nabla x g(x)||) \]

\[ \leq -\frac{2\gamma}{2L} = -\frac{\gamma}{L}. \]
It follows that there exists a robust classifier between the two classes $y, y'$:

$$\inf_{f \in \mathcal{F}} \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} -2\mathbb{E}_{(c,x) \sim \mu} cf(x) \leq -\frac{\gamma}{L} + \delta_n M + \varepsilon_n$$

Note that:

$$-\inf_{f \in \mathcal{F}} \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} -2\mathbb{E}_{(c,x) \sim \mu} cf(x) = \sup_{f \in \mathcal{F}} \inf_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} 2\mathbb{E}_{(c,x) \sim \mu} cf(x)$$

Hence:

$$\sup_{f \in \mathcal{F}} \inf_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} 2\mathbb{E}_{(c,x) \sim \mu} cf(x) \geq \frac{\gamma}{L} - \delta_n M - \varepsilon_n.$$  

On the other hand we have:

$$\sup_{f \in \mathcal{F}} \inf_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} 2\mathbb{E}_{(c,x) \sim \mu} cf(x) \leq \sup_{f \in \mathcal{F}} \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} 2\mathbb{E}_{(c,x) \sim \mu} cf(x) \geq \frac{\gamma}{L} - \delta_n M - \varepsilon_n.$$  

Note that $\mathcal{F} \subset \text{Lip}_1$

$$\sup_{f \in \text{Lip}_1} \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} 2\mathbb{E}_{(c,x) \sim \mu} cf(x) \geq \sup_{f \in \mathcal{F}} \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} 2\mathbb{E}_{(c,x) \sim \mu} cf(x) \geq \frac{\gamma}{L} - \delta_n M - \varepsilon_n.$$  

We can now swap the two sups and obtain:

$$\sup_{f \in \text{Lip}_1} \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} 2\mathbb{E}_{(c,x) \sim \mu} cf(x) = \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} \sup_{f \in \text{Lip}_1} 2\mathbb{E}_{(c,x) \sim \mu} cf(x) = \sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} W_1(\mu_y, \mu_{y'})$$

and finally we have:

$$\sup_{\mu, \mathcal{W}_\infty(\mu, \hat{\mu}) \leq \delta_n} W_1(\mu_y, \mu_{y'}) \geq \frac{\gamma}{L} - \delta_n M - \varepsilon_n.$$  

□