The Many Faces of 1-Lipschitz Neural Networks

Louis Béthune
Université Paul-Sabatier, IRIT
ANITI
Toulouse, France

Alberto González-Sanz
Université Paul-Sabatier, IMT
ANITI
Toulouse, France

Franck Mamalet
IRT Saint-Exupéry
Toulouse, France

Mathieu Serrurier
Université Paul-Sabatier, IRIT
Toulouse, France

Abstract

Lipschitz constrained models have been used to solve specific deep learning problems such as the estimation of Wasserstein distance for GAN, or the training of neural networks robust to adversarial attacks. Regardless the novel and effective algorithms to build such 1-Lipschitz networks, their usage remains marginal, and they are commonly considered as less expressive and less able to fit properly the data than their unconstrained counterpart. The goal of this paper is to demonstrate that, despite being empirically harder to train, 1-Lipschitz neural networks are theoretically better grounded than unconstrained ones when it comes to classification. We recall some results about 1-Lipschitz functions in the scope of deep learning and we extend and illustrate them to derive general properties for classification. We propose and demonstrate several new properties of 1-Lipschitz neural networks for classification. First, we show they can fit arbitrarily difficult frontiers, making them as expressive as classical ones, in addition to provide robustness certificates. We prove that when minimizing cross entropy loss the optimization problem under Lipschitz constraint is well posed and its solution generalizes well in the limit of big datasets, whereas regular neural networks can diverge even on remarkably simple situations. Then, we study the link between classification with 1-Lipschitz network and optimal transport thanks to regularized versions of Kantorovich-Rubinstein duality theory. Last, we derive preliminary bounds on their VC dimensions.

1 Introduction

The Lipschitz constant of neural networks has drawn a great attention in the last decade, with motivation ranging from adversarial robustness to Wasserstein distance computation. Deep neural networks are known to be vulnerable to adversarial attacks [1]: a carefully chosen small noise added to the input, usually indistinguishable, can change the class prediction. This is mainly due to the Lipschitz constant of neural networks which can grow arbitrarily high when unconstrained. One possible defense against adversarial attacks is to constraint the Lipschitz constant of the network [2], which provides provable robustness guarantees, together with an improvement of generalization [3] and interpretability of the model [4].

1-Lipschitz Neural Networks (1-Lip NN) have also used to estimate the Wasserstein distance between two probability distributions, thanks to Kantorovich-Rubinstein duality, in the seminal work of [5]. These approaches propose different ways to control precisely the Lipschitz constant of the network such as gradient penalty [6], spectral normalization [7] and orthogonalization of the matrix weights [8]. These algorithms facilitate greatly the learning of 1-Lip NN. Lipschitz constrained functions are
known to have some desirable properties for machine learning. Although they are primarily used in the previously described area, they are not applied widely on deep learning applications. A belief commonly invoked against the 1-Lipschitz networks is that they are much more difficult to train and far less expressive, making them rarely competitive on challenging benchmarks.

The goal of this paper is to demonstrate that, despite being empirically harder to train, 1-Lipschitz neural networks are theoretically better grounded than unconstrained ones when it comes to classification. First, even if they are obviously less expressive than their unconstrained counterpart for regression tasks, we will prove this intuition fades when it comes to classification. High accuracy and robustness certificates are not necessarily antagonist objectives, corroborating the findings of [9]. We also explore the statistical and optimization properties of 1-Lipschitz networks in Section 4 and their VC dimension in Section 5.

The main contribution of the paper is to propose a general view of the multiple interest of the 1-Lip NN for deep learning, gathering known results, and demonstrating new ones. The first section is devoted to the related work on 1-Lipschitz neural network. In Section 3, we show that 1-Lip NN are able to learn arbitrary complex decision frontiers and are naturally robust. In the third section, we prove that unconstrained optimization of binary cross entropy is an ill-posed optimization problem that becomes well posed when restricting to the class of 1-Lipschitz networks: we demonstrate that even on very simple toy example, unconstrained neural networks may have an arbitrarily high Lipschitz constant which leads to overfitting. In the last sections, we outline the link between classification with 1-Lipschitz functions and optimal transport and we show that the class of 1-Lipschitz functions with margin have a finite VC dimension and then provable error bounds.

2 Notations and related work

2.1 Notations

This work will deal with the classification over $\mathbb{R}^n$. The label set is $\mathcal{Y} = \{-1, +1\}$ for binary classification and $\mathcal{Y} = \{1, 2, \ldots, K\}$ with $K > 2$ for multi-class. Let $(X, Y)$ be a random variable taking values on $\mathcal{X} \times \mathcal{Y}$, where $\mathcal{X} \subseteq \mathbb{R}^n$, such a pair follows the joint distribution $P_{XY}$, defined on the space of probability measures over $\mathcal{X} \times \mathcal{Y}$, i.e. $P_{XY} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$. The marginal distribution of
$X$ is denoted by $\mathbb{P}_X \in \mathcal{P}(X)$ and its support by $\text{supp } \mathbb{P}_X$. We suppose the observation of a sample $(x_1, y_1), \ldots, (x_p, y_p)$ i.i.d. with common law $P_{X,Y}$, and the goal is to learn a classifier $c : \mathcal{X} \to \mathcal{Y}$ modeling the optimal Bayes classifier $\arg \max_{y \in \mathcal{Y}} P_{Y|X}(y|x)$. For binary classification $P$ (resp. $Q$) denotes the input distribution of label +1 (resp. −1).

The Lipschitz constant of function $f : \mathbb{R}^n \to \mathbb{R}^K$ is defined as the smallest $L$ such that for all $x, y \in \mathbb{R}^n$ we have $\|f(x) - f(y)\| \leq L \|x - y\|$, in this case $f$ is said $L$-Lipschitz. For simplicity we will focus on euclidean norm $\| \cdot \|_2$ in the rest of the paper. The set of $L$-Lipschitz functions over $\mathcal{X} \subset \mathbb{R}^n$ with image in $\mathbb{R}^K$ will be denoted $\text{Lip}_L(\mathcal{X}, \mathcal{R}^K)$. The gradient of $f$ w.r.t $x$ will be written $(\nabla_x f)$, and its Jacobian $(J_c f)$. The norm of any matrix must be understood as operator norm. The proof of every Proposition can be found in Appendix.

In the rest of the paper, “unconstrained neural network” must be understood as any feed forward network of fixed depth (without recurrent mechanisms) with parametrized affine layers (including convolutions), and Lipschitz activation functions (such as ReLU, sigmoid, tanh, and other popular variants). Such neural networks are known to be Lipschitz [10] but with no knowledge on their constant $L$. The last layer is assumed without activation function (to produce logits in $\mathbb{R}$), any further non linearity being merged into the loss function.

### 2.2 Related work

It is known that evaluating exactly the Lipschitz constant is a NP-hard problem [11] and many approaches have been proposed to estimate it. A neural network is a composition of linear and non-linear functions. As a composition of functions, the Lipschitz constant of a multilayer network is upper bounded by the product of the individual Lipschitz constants of each layer.

Clipping the weights of a networks as in Wasserstein GAN [5], or $L_2$ regularisation are a way to constraint the Lipschitz constant of a network, however it gives no guarantee about its real value, only a very crude upper bound. Gradient penalty [6] and spectral regularization [7] allow for a better control of the constant but still without guarantees. Normalizing the weights by their Frobenius norm [12] leads to a tighter upper singular value, and spectral normalization, as proposed in [13], allows each dense layer to be exactly 1-Lipschitz. However, spectral normalization results in neural networks with effective Lipschitz constant far smaller than 1, leading to vanishing gradient. Most activation function are 1-Lipschitz, the popular including ReLU, sigmoid, tanh, softplus, and others. some other layers such as Attention are not even Lipschitz [14], and cannot benefit to 1-Lipschitz neural networks in straightforward manner. Some attempts have been made to propose Lipschitz recurrent units [15]. Even on residual connections, appropriate scaling can yields Lipschitz bounds but no necessarily gradient preservation (Appendix [D] remark [10]). Alternatives need to be found.

In [6], authors shows that the optimal solution $f$ of the Kantorovich-Rubinstein dual transport problem verifies $\|\nabla_x f(x)\| = 1$ almost everywhere. [8] proved that such functions are dense in the set of 1-Lipschitz functions w.r.t uniform convergence. They also establish that if a neural network verifies $\|\nabla_x f(x)\| = 1$ almost everywhere and uses monotone elementwise non linearities, then $f$ is an affine function. They proposed sorting activation function to circumvent this issue, in combination with Björck orthonormalization [16] to ensure that all eigenvalues are close to 1. Afterward GroupSort [17] revealed to be as useful as sorting.

Orthogonal convolutions are still an active research area. The constraint is enforced by using appropriate regularization [18], by expressing convolutions in Fourrier space [19], by using Block Convolution Orthogonal Parameterization (BCOP) [2] or by optimizing over the set of orthogonal convolutions directly [20].

Orthogonal kernels are of special interest in the context of normalizing flows [21]. The optimization over the orthogonal group (known as Stiefel manifold) has been extensively studied in [22], while [23] or [24] focus on neural networks with tools like Cayley transform. There is also approaches based on stochastic flows and graph matching [25].

Adversarial attacks (see [26] and references therein) are small perturbations in input space, invisible to humans, but nonetheless able to change class prediction. This is a vulnerability of modern deep neural networks making them not suitable for critical applications. Adversarial training [27] leads to empirical improvements but fails to provide certificates. Certificates can be produced by bounding the Lipschitz constant, using extreme value theory [28], linear approximations [29] or polynomial
optimization. In [31], the control of Lipschitz constant and margins is used to guarantee robustness against attacks. In [32], the authors link classification with optimal transport by considering a hinge regularized version of the Kantorovich-Rubinstein optimization. They built provably robust classifiers using 1-Lipschitz neural networks with \( \|\nabla_x f(x)\| = 1 \) almost everywhere.

In [33] Lipschitz classifiers are shown to be isometrically isomorphic to linear large margin classifiers over some Banach space, into which the data have been embedded. Generalization bounds for large class of Lipschitz classifiers are provided by the work of [34] using Vapnik–Chervonenkis theory. Other generalization bounds related to large margin classifiers can be found in [35]. Links between adversarial robustness, large margins classifiers and optimization bias is studied in [36].

2.3 Experimental setting

All the experiments done in the paper uses the Deel.Lip library developed for [32]. The network verifies \( \|\nabla_x f\| = 1 \) almost everywhere thanks to 1) orthogonal matrices in affine layers 2) layerwise sort activation function. GroupSort2 [17] is defined such that \( \text{GroupSort2}(x)_{2i, 2i+1} = [\min(x_{2i}, x_{2i+1}), \max(x_{2i}, x_{2i+1})] \) for all \( i \). Spectral normalization and Björck orthonormalization algorithm ensures that most singular values are equal to 1. This implementation is based on the seminal work of [8], who first proved that those functions are dense in the space of 1-Lipschitz functions. With dilation by a constant \( L \in \mathbb{R} \) we can parameterize the set \( \text{Lip}_L(X, \mathbb{R}) \). We minimize losses using Adam optimizer. In this paper we will not use convolutions because we could not guarantee formally that \( \|\nabla_x f\| = 1 \) in the current implementation.

3 1-Lipschitz classifier

In this section, we show that 1-Lipschitz functions are as powerful as any other classifier, like their unconstrained counterpart. In particular, when classes are separable they can achieve 100% accuracy. Even in the non separable case the optimal Bayes classifier can nonetheless be imitated. We also recall the main property of 1-Lipschitz neural networks: their ability to produce robustness radius certificates against adversarial examples.

3.1 Frontier decision fitting

**Proposition 1** (Lipschitz Binary classification). For any binary classifier \( c : \mathcal{X} \rightarrow \mathcal{Y} \) with closed pre-images \( c^{-1}(\{y\}) \) is a closed set for any \( y \in \mathcal{Y} \) there exists a 1-Lipschitz function \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) such that \( \text{sign}(f(x)) = c(x) \) on \( \mathcal{X} \). Moreover we have \( \|\nabla_x f\|_2 = 1 \) almost everywhere (w.r.t Lebesgue measure). Note that the classifier \( c \) does not need to be defined everywhere on \( \mathbb{R}^n \), while \( f \) is.

**Proof.** The function \( f \) introduced below in Definition[1] verifies the aforementioned properties. Full proof detailed in Appendix.

**Definition 1** (Highest Mountain Function)

Let \( \partial \) the maximum margin frontier: the set of points equidistant to \( c^{-1}(\{-1\}) \) and \( c^{-1}(\{+1\}) \). We define the binary **Highest Mountain Function (HMF)** as \( f(x) = c(x)d(x, \partial) \) on \( \mathcal{X} \), which implicitly depends of \( c \).

\[ \square \]

Similar results can be obtained for multiclass classification.

**Proposition 2** (Lipschitz Multiclass classification). For any multiclass classifier \( c : \mathcal{X} \rightarrow \mathcal{Y} \) with closed pre-images there exists a 1-Lipschitz function \( f : \mathbb{R}^n \rightarrow \mathbb{R}^K \) such that \( \arg \max_k f_k(x) = c(x) \) on \( \mathcal{X} \). Moreover \( \|J_x f\| = 1 \) almost everywhere (w.r.t Lebesgue measure).

For simplicity in the following sections we will focus on the binary classification case only (\( K = 2 \)).

With these propositions in mind, we can deduce Corollary[1]

[1] https://github.com/deel-ai/deel-lip
Corollary 1 (1-Lipschitz Networks are as powerful as unconstrained ones). For any neural network \( f : \mathbb{R}^n \to \mathbb{R} \) there exists 1-Lipschitz neural network \( \tilde{f} : \mathbb{R}^n \to \mathbb{R} \) such that \( \text{sign}(f(x)) = \text{sign}(\tilde{f}(x)) \).

Proof. Indeed, every unconstrained neural network is \( L \)-Lipschitz for some (generally unknown) \( L \). If \( g : \mathbb{R}^n \to \mathbb{R} \) is \( L \)-Lipschitz neural network, then \( \frac{1}{L} g \) is a 1-Lipschitz neural network with the same decision frontier. \( \square \)

The Error of a classifier \( c \) is defined as \( E(c) = \mathbb{E}_{(x,y) \sim P_{X,Y}}[\mathbb{I}\{c(x) \neq y\}] \). The Risk of a classifier is defined as \( R(c) = E(c) - E(b) \) where \( b \) denotes the optimal Bayes classifier. Some empirical studies shows that indeed most datasets are separated \([9]\) such as CIFAR10 or MNIST.

Corollary 2 (Separable classes implies zero error). The distributions \( P \) and \( Q \) are \( \epsilon \)-separated if it exists \( \epsilon > 0 \) such that the distance between \( \text{supp} P \) and \( \text{supp} Q \) exceeds \( \epsilon \). In this case 1-Lipschitz neural networks can achieve zero error.

Furthermore, even if the classes are not separable, 1-Lipschitz neural network can nonetheless approximate the optimal Bayes classifier under mild assumptions.

The hypothesis class contains a classifier with optimal accuracy, despite having hugely constrained Lipschitz constant. The difficulty lies in the optimization (see Section 4) over such class of functions.

Example 1 (Highest Mountain Function). An example of HMF is depicted in Figures 1(a) and (b), with \( \theta \) chosen to be the fourth iteration of Von Koch Snowflake. We train a 6-layers (5 hidden layers of width 128) 1-Lipschitz NN by regression to fit the HMF (160 000 pixels, 20 epochs) and we obtain the function in Figure 1(c), with mean absolute error inferior to 1. The green strip corresponds to the zone \( |f(x)| \leq 0.5 \). It proves empirically that this classification task, associated to a very sharp (almost fractal) decision frontier, can be solved by a NN verifying \( \|\nabla_x f\| = 1 \) almost everywhere. There is not constraint on the shape of the frontier: only on the “speed” at which we move away from it.

3.2 Robustness

One of the most appealing properties of 1-Lipschitz neural networks is their ability to provide robustness radius certificates against adversarial attacks.

Definition 2 (Adversarial Example) For any classifier \( c : X \to Y \), any \( x \in \mathbb{R}^n \), consider the following problem:

\[
\delta \in \arg \min_{\delta^* \in \mathbb{R}^n} ||\delta^*|| \quad \text{subject to} \quad c(x + \delta^*) \neq c(x)
\]

\( \delta \) is an adversarial attack, \( \hat{x} = x + \delta \) is an adversarial example, and \( ||\delta|| \) is the robustness radius of \( x \).
While unconstrained neural networks have usually very small robustness radius \(1\) whose exact computation is often intractable, 1-Lipschitz neural networks can provide certificates \(31\).

**Property 1 (Robustness Certificates \(2\)).** For any 1-Lipschitz neural network, the robustness radius \(\|\delta\|\) at example \(x\) verifies \(\|\delta\| \geq |f(x)|\).

Computing the certificate is straightforward and do not increase runtime, contrary to methods based on bounding boxes or abstract interpretation. There is no need for adversarial training \(27\) that fails to produce guarantees, or for randomized smoothing \(37\) which can be costly.

The HMF(b) function associated to the Bayes classifier \(b\) is the one providing the largest certificate among the classifiers of maximum accuracy.

**Corollary 3.** For the HMF(b), the bound of Property \([1]\) is tight: \(\|\delta\| = |f(x)|\). In particular \(\delta = - f(x) \nabla_x f(x)\) is guaranteed to be an adversarial attack. The risk is the smallest possible. There is no classifier with the same risk and better certificates. Said otherwise the HMF(b) is the solution to:

\[
\max_{f \in Lip_1(\mathbb{R}^n, \mathbb{R})} \min_{x \in X} \min_{\delta \in \mathbb{R}^n} \|\delta\| \quad \text{under the constraint } R(\text{sign}(f)) \text{ minimal}
\]

Unfortunately the HMF(b) cannot be explicitly constructed since it relies on the (generally unknown) optimal Bayes classifier. We deduce that a robust 1-Lipschitz classifier must certainly aims to maximize \(|f(x)|\) for each \(x\) in the training set, in order to achieve maximum robustness. One question remains: which loss should we chose to achieve this goal?

### 4 Binary Cross Entropy and 1-Lipschitz neural networks

The Binary Cross Entropy (BCE) loss (also called logloss) is among the most popular choices within the deep learning community. In the next section we highlight some of its properties w.r.t the Lipschitz constant.

Let \(f : \mathbb{R}^n \rightarrow \mathbb{R}\) a neural network. For an example \(x \in \mathbb{R}^n\) with label \(y \in \{-1, +1\}\), with \(\sigma(x) = \frac{1}{1+ \exp(-x)}\) the logistic function mapping logits to probabilities, the BCE is written \(L(f(x), y) = - \log \sigma(y f(x))\).

On unconstrained neural networks, minimization of this loss leads to saturation of the logits and uncontrolled growth of Lipschitz constant.

**Proposition 3 (Saturated Neural Networks have high Lipschitz constant).** Let \(f_t\) be a sequence of neural networks, that minimizes the BCE over a non trivial (with more than one class) training set of size \(p\), i.e:

\[
\lim_{t \rightarrow \infty} \frac{1}{p} \sum_{i=1}^{p} L(f_t(x_i), y_i) = 0
\]

Let \(L_t\) the Lipschitz constant of \(f_t\). Then \(\lim_{t \rightarrow \infty} L_t = +\infty\).

This issue is specially important since the high Lipschitz constant of neural networks have been identified as the main cause of adversarial vulnerabilities. With saturated logits the probability \(\sigma(f(x))\) will be either 0 or 1 which do not carry any useful information on the true confidence of the classifier, specially in the out-of-distribution setting.

**Example 2** (Illustration on linear classifier). Consider binary classification task on \(\mathbb{R}^n\), with, for simplicity, classes that are linearly separable. We use an affine model \(f(x) = W x + b\) for the logits (with \(W \in \mathbb{R}^n\) and \(b \in \mathbb{R}\)), that can be seen as a one-layer neural network. Since the classes are linearly separable it exits \(W, b\) such that \(f\) achieves 100\% accuracy. However, as noticed in \(39\) (Section 4.3.2) the cross entropy loss will not be null. The loss can be minimized only with the diverging sequence of parameters \((\lambda W, \lambda b)\) as \(\lambda \rightarrow \infty\). Turn out the infimum is not a minimum!

Even on this trivial example, with a hugely constrained model the minimization problem is ill-defined. Without \(l_1\) or \(l_2\) regularization the minimizer can not be attained. Moreover there is an issue of vanishing gradient with BCE: \(\lim_{y f(x) \rightarrow \infty} \| \nabla_y f(x) L(y f(x), y) \| = 0\). Most order-1 methods struggle to saturate the logits, even on unconstrained neural networks as depicted in Figure 2a whereas
**Proposition 4** (BCE minimization for $L$-Lipschitz functions). Let $\mathcal{X} \subset \mathbb{R}^n$ be a compact and $L > 0$. Then the minimum of Equation 4 is attained.

$$f^*_L \in \arg \min_{f \in \text{Lip}_L(\mathcal{X}, \mathbb{R})} \mathbb{E}_{(x,y) \sim P_{XY}} \left[ \mathcal{L}(f(x), y) \right]$$  \hspace{1cm} (4)

Proposition 4 shows that the minimum exists. The upperbound on Lipschitz constant is turned into a lower bound on the norm of the gradient of BCE (see Appendix D). Combined with Gradient Preserving layers (including orthogonal matrices and GroupSort activation function), this preserves 1-Lip NN to suffer from vanishing gradient.

Machine learning practitioners are mostly interested by the minimization of the empirical risk (i.e maximization of the accuracy). However one cannot guarantees that the minimizer of BCE will maximize accuracy (see Example 3). Besides, if $f^*_L$ is a minimum of Equation 4 for some $L$, in general $\frac{1}{L} f^*_L$ is not necessarily a minimum of Equation 4 for $L = 1$.

**Example 3.** We illustrate this phenomenon in Figure 2b by training various neural networks with different Lipschitz constants $L$. We chose a simple setting with only four training points in $\mathbb{R}^2$. The inputs are $\{-2, -1, 1, 2\}$ respectively. Their sampling weights are $\{0.9, 0.1, 0.1, 0.9\}$ respectively and their labels $\{+1, -1, +1, -1\}$. We plot the value of $f(x)$ to highlight the different shapes of the minimizer $f$ as function of $L$. High values of $L$ leads to better fitting.

We observe the same phenomenon on CIFAR10 (“dogs” versus “cats”) with Lipschitz contrained NN, see Figure 3a. We place ourselves in over-parameterized regime with five hidden layers of width 512. We compare the loss and the error on the training set. We see that the network end up severely under-fitting for small values of $L$. Not because the optimal classifier is not part of the hypothesis space, but rather because the minimizer of binary cross entropy is not necessarily the minimizer of the error. As $L$ grows, we close to up to the maximum accuracy. The loss itself is responsible for the poor score, and not by any means the hypothesis space. Bigger Lipschitz constant might ultimately lead to overfitting, playing the same role as the (usually omitted) temperature scaling parameter $T \in \mathbb{R}_+$:

$$\mathcal{L}_T(f(x), y) = -\log \sigma(y T f(x)).$$

Nonetheless, the class of Lipschitz classifiers enjoys another remarkable property since it is a Glivenko-Cantelli class: BCE is a consistent estimator, as well as other Lipschitz losses like Hinge or Huber. Said otherwise, as the size of the training set increases the training loss becomes a proxy for the test loss: 1-Lipschitz neural networks will not overfit in the limit of (very) large sample size.

**Proposition 5** (Train Loss is a proxy of Test Loss). Let $P_{XY}$ a probability measure on $\mathcal{X} \times \mathcal{Y}$ where $\mathcal{X} \subset \mathbb{R}^n$ is a bounded set. Let $(x_i, y_i)_{1 \leq i \leq p}$ be a sample of $p$ iid random variables with law $P_{XY}$.
Table 1: Summary of different candidate losses, and influence of the Lipschitz constraint on the minimum. BCE minimization is ill-posed for unconstrained NN, but because of Vanishing Gradient the algorithm converges nonetheless. For margin $m$ small enough, if the classes are separable, 0% training error is achievable by hinge.

Let:

$$E_p(f) = \frac{1}{p} \sum_{i=1}^{p} L_T(f(x_i), y_i) \text{ and } E_\infty(f) = \mathbb{E}_{(x,y) \sim \mathcal{P}_{XY}}[L_T(f(x), y)]$$

Then we have (taking the limit $p \to \infty$):

$$\min_{f \in L_{1}(\mathbb{R})} E_p(f) \xrightarrow{a.s.} \min_{f \in L_{1}(\mathbb{R})} E_\infty(f)$$

It is an other flavor of the bias-variance trade-off. We know thanks to Corollary 2 that the class of Lipschitz function does not suffer any bias when it comes to classification. With Proposition 5 we also know that the variance can be made as small as we want by increasing the size of the training set. While this statement seems rather trivial, we emphasize that is not a property shared by unconstrained neural networks: increasing the size of the training set does not give any formal guarantee to generalization capabilities. Adversarial examples are an example of such failure to reduce variance.

5 Alternative losses and link with Optimal Transport

We see that BCE is not necessarily the most suitable loss for 1-Lip learning due to its dependence in the Lipschitz constant. According to Section 3.2 under 1-Lipschitz constraints maximizing the robustness is equivalent to maximize the logits $|f(x)|$, so the loss $L_W(f(x), y) = -y f(x)$ might seem to be a good pick at first sight. Unfortunately its minimum is the Wasserstein distance between $P$ and $Q$ according to the Kantorovich-Rubinstein (KR) duality:

$$\min_{f \in L_{1}(\mathbb{R}^n, \mathbb{R})} \mathbb{E}_{P_X}[L_W(f(x), y)] = \mathcal{W}(P, Q)$$

The minimizer of is known to be a weak classifier, as demonstrated empirically in [32]. We precise their observations in Proposition 6.

Proposition 6 (KR minimizer is a weak classifier). For every $\epsilon > 0$ there exists distributions $P$ and $Q$ with disjoint supports in $\mathbb{R}$ such that for any minimizer $f$ of equation 6 the error of classifier $\text{sign} \circ f$ is superior to $\frac{1}{2} - \epsilon$.

Hinge loss $L_m(f(x), y) = \max(0, m - y f(x))$ allows, in principle, to reach maximum accuracy, as used in [2]. The combination $L_\lambda(f(x), y) = L_W(f(x), y) + \lambda L_m(f(x), y)$ is still a regularized OT problem [32]. BCE minimization can also be seen through the lens of OT (Appendix E). Results are
summarized in Table 1. Most losses that are Lipschitz continuous revealed to be consistent estimators with Lipschitz neural networks.

With margin $m > 0$ we can bound the VC dimension $\|f(x)\|$ of hypothesis class. The value $|f(x)|$ can be understood as confidence. Hence, we may be interested in a classifier that takes decision only if the logit is above some threshold $m > 0$, while $|f(x)| < m$ can be understood as examples $x$ for which the classifier is unsure: the label may be flipped using attacks of norm $\|\delta\| \leq m$. In this setting, we fall back to PAC learnability [42].

**Proposition 7** (1-Lipschitz Functions with margin are PAC learnable). Consider a binary classification task with bounded support $\mathcal{X}$. Let $m > 0$ the margin. Let $\mathcal{C}^m(\mathcal{X}) = \{c^m_j : \mathcal{X} \rightarrow \{-1, 1\}, f \in \text{Lip}(\mathcal{X}, \mathbb{R}) \}$ the hypothesis class defined as follow.

$$c^m_j(x) = \begin{cases} +1 & \text{if } f(x) \geq m \\ -1 & \text{if } f(x) \leq -m \\ \bot & \text{otherwise} \end{cases}$$  \hspace{1cm} (7)

Then the VC dimension of $\mathcal{C}^m$ is finite:

$$\left(\frac{1}{m}\right)^n A \leq VC_{\text{dim}}(\mathcal{C}^m(\mathcal{X})) \leq \left(\frac{2}{m}\right)^n B$$ \hspace{1cm} (8)

with $A = \frac{\text{vol}(\mathcal{X})}{\text{vol}(B(1, 1))}$ and $B = \frac{\text{vol}(\mathcal{X} + \frac{m}{2}B(1, 1))}{\text{vol}(B(1, 1))}$. $B(\cdot, 1)$ is the unit ball, and $\mathcal{X} + \frac{m}{2}B(\cdot, 1)$ must be understood as Minkovski sum [43].

Here $\bot$ is a dummy symbol that the classifier may use to say “I don’t feel confident”; using it is not allowed to shatter a set. Interestingly if the classes are $\epsilon$ separable ($\epsilon > 0$), choosing $m = \epsilon$ guarantees that maximal accuracy is reachable. Prior over the separability of the input space is turned into VC bounds over the space of hypothesis. This approach with margins $m$ yields objects known in literature as $m$-fat shattering sets [34].

When $m = 0$ the VC dimension of space $\mathcal{C}^m(\mathcal{X})$ becomes infinite and the class in not PAC learnable anymore: the training error will not converge to test error in general, regardless of the size of the training set. It might seem like a contradiction with Proposition 5 but it is not: error $E(c^m_j(x))$ lacks continuity w.r.t $f(x)$ which prevents it to be a consistent estimator. Practically, it means that even when a Lipschitz classifier badly overfit, we might detect it since BCE can remain high: $L_T(m, y) = \ln(2) - \frac{T_m}{2} + o(m^2)$.

We can give an other bound corresponding to a practical implementation of Lipschitz networks. With GroupSort2 activation functions (as in the work of [17]) we get the following rough upper bound:

**Proposition 8** (VC dimension of 1-Lipschitz neural network with Sorting). Let $f_\theta : \mathbb{R}^n \rightarrow \mathbb{R}$ a 1-Lipschitz neural network with parameters $\theta \in \Theta$, with GroupSort2 activation functions, and a total of $W$ neurons. Let $\mathcal{H} = \{\text{sign}f_\theta | \theta \in \Theta \}$ the hypothesis class spanned by this architecture. Then:

$$VC_{\text{dim}}(\mathcal{H}) = O \left((n + 1)2^W\right)$$ \hspace{1cm} (9)

From Proposition 8 we can derive generalization bounds using PAC theory. Note that most results on VC dimension of neural network uses the hypothesis that the activation function is applied element-wise (such as in [44]) and get asymptotically tighter lower bounds for ReLU case. Such hypothesis does not apply anymore here, however we believe that the preliminary result can be strengthened. Our result is actually a bit more general and apply more broadly to activation functions that piece-wise linear and partition the input space into convex sets (see Lemma 1 in Appendix).

6 Conclusion

In this paper, our goal was to challenge the common belief that constraining Lipschitz constant degrades the classification performances of neural networks. We proved that 1-Lip NN exhibit numerous attractive properties: they provide robustness radius certificates by definition and do not restrict the expressive power. We show and illustrate that with Lipschitz constraints the optimization problem is not longer ill-posed and yields to generalization guarantees.

However the loss function must be chosen accordingly: we pointed out that Cross Entropy is not necessarily the best choice, margin based losses, such as hinge or its variants, have appealing
properties (see Table 1). Last we point out that classification with 1-Lip NN is related to optimal transport.

Their training remains a challenge. The solutions of the optimization problem in equation 4 still need to be characterized and understood. In particular, what is the bias induced by the minimizer of the loss on this particular space of functions?

If future works can overcome these challenges, it open the path to neural networks that are both effective and provably robust. For these reasons we believe they are a promising direction of further research for the community.

Acknowledgments and Disclosure of Funding

This work received funding from the French Investing for the Future PIA3 program within the Artificial and Natural Intelligence Toulouse Institute (ANITI). A special thanks to Thibaut Boissin for the support with Deel-Lip library. We also thank Sébastien Gerchinovitz for critical proof checking, Jean-Michel Loubes for useful discussions, and Etienne de Montbrun for read-checking.

References

[1] Christian Szegedy, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian Goodfellow, and Rob Fergus. Intriguing properties of neural networks. In International Conference on Learning Representations, 2014.

[2] Qiyang Li, Saminul Haque, Cem Anil, James Lucas, Roger B Grosse, and Jörn-Henrik Jacobsen. Preventing gradient attenuation in lipschitz constrained convolutional networks. In Advances in Neural Information Processing Systems (NeurIPS), volume 32, Cambridge, MA, 2019. MIT Press.

[3] J. Sokolic, R. Giryes, G. Sapiro, and M. R. D. Rodrigues. Robust large margin deep neural networks. IEEE Transactions on Signal Processing, 65(16):4265–4280, 2017.

[4] Dimitris Tspiras, Shibani Santurkar, Logan Engstrom, Alexander Turner, and Aleksander Madry. Robustness may be at odds with accuracy. In International Conference on Learning Representations, 2019.

[5] Martin Arjovsky, Soumith Chintala, and Léon Bottou. Wasserstein generative adversarial networks. In International conference on machine learning, pages 214–223. PMLR, 2017.

[6] Ishaan Gulrajani, Faruk Ahmed, Martin Arjovsky, Vincent Dumoulin, and Aaron C Courville. Improved training of wasserstein gans. In Advances in Neural Information Processing Systems, volume 30, pages 5767–5777. Curran Associates, Inc., 2017.

[7] Yuichi Yoshida and Takeru Miyato. Spectral norm regularization for improving the generalizability of deep learning. arXiv preprint arXiv:1705.10941, 2017.

[8] Cem Anil, James Lucas, and Roger Grosse. Sorting out lipschitz function approximation. In International Conference on Machine Learning, pages 291–301. PMLR, 2019.

[9] Yao-Yuan Yang, Cyrus Rashtchian, Hongyang Zhang, Russ R Salakhutdinov, and Kamalika Chaudhuri. A closer look at accuracy vs. robustness. Advances in Neural Information Processing Systems, 33, 2020.

[10] Kevin Scaman and Aladin Virmaux. Lipschitz regularity of deep neural networks: analysis and efficient estimation. In Proceedings of the 32nd International Conference on Neural Information Processing Systems, pages 3839–3848, 2018.

[11] Aladin Virmaux and Kevin Scaman. Lipschitz regularity of deep neural networks: analysis and efficient estimation. Advances in Neural Information Processing Systems, 31:3835–3844, 2018.

[12] Tim Salimans and Diederik P Kingma. Weight normalization: A simple reparameterization to accelerate training of deep neural networks. In NIPS, 2016.

[13] Takeru Miyato, Toshiki Kataoka, Masanori Koyama, and Yuichi Yoshida. Spectral normalization for generative adversarial networks. In International Conference on Learning Representations, 2018.

[14] Hyunjik Kim, George Papamakarios, and Andriy Mnih. The lipschitz constant of self-attention. arXiv preprint arXiv:2006.04710, 2020.

[15] N. Benjamin Erickson, Omri Azencot, Alejandro Queiruga, Liam Hodgkinson, and Michael W. Mahoney. Lipschitz recurrent neural networks. In International Conference on Learning Representations, 2021.

[16] Åke Björck and Clazett Bowie. An iterative algorithm for computing the best estimate of an orthogonal matrix. SIAM Journal on Numerical Analysis, 8(2):358–364, 1971.
[17] Ugo Tanielian and Gerard Biau. Approximating lipschitz continuous functions with groupsort neural networks. In *International Conference on Artificial Intelligence and Statistics*, pages 442–450. PMLR, 2021.

[18] Jiayun Wang, Yubei Chen, Rudrasis Chakraborty, and Stella X Yu. Orthogonal convolutional neural networks. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 11505–11515, 2020.

[19] Sheng Liu, Xiao Li, Yuexiang Zhai, Chong You, Zhihui Zhu, Carlos Fernandez-Granda, and Qing Qu. Convolutional normalization: Improving deep convolutional network robustness and training. *arXiv preprint arXiv:2103.00673*, 2021.

[20] Asher Trockman and J Zico Kolter. Orthogonalizing convolutional layers with the cayley transform. In *International Conference on Learning Representations*, 2021.

[21] Leonard Hasenclever, Jakub M Tomczak, Rianne van den Berg, and Max Welling. Variational inference with orthogonal normalizing flows. In *Bayesian Deep Learning, NIPS 2017 workshop*, 2017.

[22] P-A Absil, Robert Mahony, and Rodolphe Sepulchre. *Optimization algorithms on matrix manifolds*. Princeton University Press, 2009.

[23] Mario Lezcano-Casado and David Martinez-Rubio. Cheap orthogonal constraints in neural networks: A simple parametrization of the orthogonal and unitary group. In *International Conference on Machine Learning*, pages 3794–3803. PMLR, 2019.

[24] Lei Huang, Xianglong Liu, Bo Lang, Adams Yu, Yongliang Wang, and Bo Li. Orthogonal weight normalization: Solution to optimization over multiple dependent stiefel manifolds in deep neural networks. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32, 2018.

[25] Krzysztof Choromanski, David Cheikhi, Jared Davis, Valerii Likhosherstov, Achille Nazaret, Acharf Bahamou, Xingyou Song, Mrugank Akarte, Jack Parker-Holder, Jacob Bergquist, et al. Stochastic flows and geometric optimization on the orthogonal group. In *International Conference on Machine Learning*, pages 1918–1928. PMLR, 2020.

[26] Xiaoyong Yuan, Pan He, Qile Zhu, and Xiaolin Li. Adversarial examples: Attacks and defenses for deep learning. *IEEE transactions on neural networks and learning systems*, 30(9):2805–2824, 2019.

[27] Tsui-Wei Weng, Huan Zhang, Pin-Yu Chen, Jinfeng Yi, Dong Su, Yupeng Gao, Cho-Jui Hsieh, and Luca Daniel. Evaluating the robustness of neural networks: An extreme value theory approach. In *International Conference on Learning Representations*, 2018.

[28] Lily Weng, Huan Zhang, Hongge Chen, Zhao Song, Cho-Jui Hsieh, Luca Daniel, Duane Boning, and Inderjit Dhillon. Towards fast computation of certified robustness for relu networks. In *International Conference on Machine Learning*, pages 5276–5285. PMLR, 2018.

[29] Fabian Latorre, Paul Rolland, and Volkan Cevher. Lipschitz constant estimation of neural networks via sparse polynomial optimization. In *International Conference on Learning Representations*, 2019.

[30] Yusuke Tsuzuku, Issei Sato, and Masashi Sugiyama. Lipschitz-margin training: Scalable certification of perturbation invariance for deep neural networks. In *Advances in Neural Information Processing Systems*, volume 31, pages 6541–6550. Curran Associates, Inc., 2018.

[31] Mathieu Serrurier, Franck Mamalet, Alberto Gonzalez-Sanz, Thibaut Boissin, Jean-Michel Loubes, and Eustasio del Barrio. Achieving robustness in classification using optimal transport with hinge regularization. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, 2021.

[32] Ulrike von Luxburg and Olivier Bousquet. Distance-based classification with lipschitz functions. *J. Mach. Learn. Res.*, 5:669–695, 2004.

[33] Lee-Ad Gottlieb, Aryeh Kontorovich, and Robert Krauthgamer. Efficient classification for metric data. *IEEE Transactions on Information Theory*, 60(9):5750–5759, 2014.

[34] Peter L Bartlett, Dylan J Foster, and Matus Telgarsky. Spectrally-normalized margin bounds for neural networks. In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, pages 6241–6250, 2017.

[35] Fartash Faghri, Cristina Vasconcelos, David J. Fleet, Fabian Pedregosa, and Nicolas Le Roux. Bridging the gap between adversarial robustness and optimization bias, 2021.

[36] Jeremy Cohen, Elan Rosenfeld, and Zico Kolter. Certified adversarial robustness via randomized smoothing. In *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 1310–1320. PMLR, 2019.
[38] Alex Krizhevsky. Learning multiple layers of features from tiny images. Technical report, cs.toronto.edu, 2009.

[39] Christopher M Bishop. Pattern recognition and machine learning. Springer, 2006.

[40] Cédric Villani. Optimal transport: old and new, volume 338. Springer Science & Business Media, 2008.

[41] VN Vapnik and A Ya Chervonenkis. On the uniform convergence of relative frequencies of events to their probabilities. Theory of Probability & Its Applications, 16(2):264–280, 1971.

[42] Leslie G Valiant. A theory of the learnable. Communications of the ACM, 27(11):1134–1142, 1984.

[43] Stanislaw J Szarek. Metric entropy of homogeneous spaces. Banach Center Publications, 43(1):395–410, 1998.

[44] Peter L. Bartlett, Nick Harvey, Christopher Liaw, and Abbas Mehrabian. Nearly-tight vc-dimension and pseudodimension bounds for piecewise linear neural networks. Journal of Machine Learning Research, 20:63–1, 2019.

[45] Jon Wellner A.W. van der vaart. Weak Convergence and Empirical Processes. Springer-Verlag New York, 1996.

[46] Anselm Blumer, Andrzej Ehrenfeucht, David Haussler, and Manfred K Warmuth. Learnability and the vapnik-chervonenkis dimension. Journal of the ACM (JACM), 36(4):929–965, 1989.

[47] Vladimir Vapnik. The nature of statistical learning theory. Springer science & business media, 2013.

[48] Emerson León and Günter M Ziegler. Spaces of convex n-partitions. In New Trends in Intuitive Geometry, pages 279–306. Springer, 2018.

[49] Felix A Gers, Jürgen Schmidhuber, and Fred Cummins. Learning to forget: Continual prediction with lstm. In Ninth International Conference on Artificial Neural Networks ICANN 99. IET, 1999.

[50] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 770–778, 2016.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope? [Yes] since abstract and introduction contains a summary of paper content.
   (b) Did you describe the limitations of your work? [Yes] since our work is mainly theoretical, but mentions of difficulties of training 1-Lip NN in practice can be found in Related Work or Conclusion.
   (c) Did you discuss any potential negative societal impacts of your work? [No] since we do not see any straightforward practical application of our work leading to negative societal impact.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] assumptions are clearly stated in each theorem, and Section 2.1 ensures that every object is well defined.
   (b) Did you include complete proofs of all theoretical results? [Yes], mainly in Appendix due to space constraints.

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] in supplementary material.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] for each experiment.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [No] most experiments were only run once.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] in Appendix C.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   
   (a) If your work uses existing assets, did you cite the creators? [Yes] because we are using CIFAR10 dataset
   
   (b) Did you mention the license of the assets? [No]
   
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes]
       our code is in supplementary material.
   
   (d) Did you discuss whether and how consent was obtained from people whose data you’re using/curating? [N/A] since we are working on CIFAR10 only.
   
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A] since we are working on CIFAR10 only.

5. If you used crowdsourcing or conducted research with human subjects...

   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]
A Proofs of Section 3

The proof of Proposition 1 is constructive, we need to introduce the Highest Mountain Function first.

Definition 3 (Highest Mountain Function)
Let \( c : X \to \{ -1, +1 \} \) be any classifier with closed pre-images. Let \( \hat{A} = \{ x \in \mathbb{R}^n | c(x) = +1 \} \) and \( \hat{B} = \{ x \in \mathbb{R}^n | c(x) = -1 \} = X \setminus \hat{A} \). Let \( d(x, y) = \| x - y \| \) and \( d(x, S) = \min_{y \in S} d(x, y) \) the distance to a closed set \( S \). Let \( \partial = \{ x \in \mathbb{R}^n | d(x, \hat{A}) = d(x, \hat{B}) \} \). We define \( f : \mathbb{R}^n \to \mathbb{R} \) as follow:

\[
f(x) = \begin{cases} d(x, \partial) & \text{if } d(x, \hat{B}) \geq d(x, \hat{A}) \\ -d(x, \partial) & \text{if } d(x, \hat{B}) < d(x, \hat{A}) \end{cases}
\]  

(10)

Now we can prove that the function \( f \) previously defined verifies all the properties.

Proof. We start by proving that \( f \) is 1-Lipschitz. The reasoning applies more broadly to arbitrary Banach space (topological normed vector space), not only \((\mathbb{R}^n, \| \cdot \|_2)\).

First, consider the case \( d(x, \hat{B}) \geq d(x, \hat{A}) \) and \( d(y, \hat{B}) \geq d(y, \hat{A}) \). Then \(| f(x) - f(y) | = | d(x, \partial) - d(y, \partial) | \). Assume without loss of generality that \( d(x, \partial) \geq d(y, \partial) \). Let \( z \in \partial \) such that \( d(y, \partial) = d(y, z) \) (guaranteed to exist since \( \partial \) is closed). Then by definition of \( d(x, \partial) \) we have \( d(x, z) \geq d(x, \partial) \). So:

\[
| f(x) - f(y) | = | d(x, \partial) - d(y, \partial) | \leq d(x, z) - d(y, z) \leq d(x, y)
\]  

(11)

The case \( d(x, \hat{B}) < d(x, \hat{A}) \) and \( d(y, \hat{B}) < d(y, \hat{A}) \) is identical. Now consider the case \( d(x, \hat{B}) < d(x, \hat{A}) \) and \( d(y, \hat{B}) \geq d(y, \hat{A}) \). We have \(| f(x) - f(y) | = d(x, \partial) + d(y, \partial) \). We will proceed by contradiction. Such complicated reasoning is superfluous for \((\mathbb{R}^n, \| \cdot \|_2)\), but has the appealing property to generalize to any Banach space. Assume that \( d(x, \partial) + d(y, \partial) > d(x, y) \). Let \( R > 0 \) such that \( R < d(x, \partial) \) and \( R + d(y, \partial) > d(x, y) \). Let:

\[
z = x + \frac{R}{d(x, y)} (x - y)
\]

Then \( d(x, z) = \| \frac{R}{d(x, y)} (x - y) \| = \frac{R}{d(x, y)} d(x, y) = R < d(x, \partial) \). So by definition of \( \partial \) we have \( d(z, \hat{B}) < d(z, \hat{A}) \). But we also have:

\[
d(y, z) = \| (x - y) + \frac{R}{d(x, y)} (x - y) \| = | 1 - \frac{R}{d(x, y)} | \times \| x - y \|
\]

\[
= | d(x, y) - R | < | d(y, \partial) | \text{ using the hypothesis on } R
\]

(12)

So we have \( d(z, \hat{B}) \geq d(z, \hat{A}) \) which is a contradiction. Consequently, we must have \( d(x, \partial) + d(y, \partial) \leq d(x, y) \). The function \( f \) is indeed 1-Lipschitz.

Now, we will prove that \( \| \nabla_x f \| = 1 \) everywhere it is defined. Let \( x \) be such that \( y \in \arg \min_{y \in \hat{B}} d(x, y) \) is unique. Consider \( h = \epsilon (\frac{y - x}{\| y - x \|}) \) with \( 1 \geq \epsilon > 0 \) a small positive real. We have \( d(x, x + h) = \epsilon \), it follows by triangular inequality that \( d(x + h, \partial) = d(x, \partial) - \epsilon \). We see that:

\[
\lim_{\epsilon \to +\infty} \frac{f(x + h) - f(x)}{\| h \|} = -1
\]

The vector \( u = -\nabla_x f \) is the (unique) vector for which \( \langle u, \frac{f(x + h) - f(x)}{\| h \|} \rangle \) is minimal. Knowing that \( f \) is 1-Lipschitz yields that \( \| \nabla_x f \| = 1 \). For points \( x \) for which \( \arg \min_{y \in \hat{B}} d(x, y) \) is not unique, the gradient is not defined because different directions minimize \( \langle u, \frac{f(x + h) - f(x)}{\| h \|} \rangle \) which contradicts the uniqueness of gradient vector. The number of points for which \( y \in \arg \min_{y \in \hat{B}} d(x, y) \) is not unique must have null measure, since Lipschitz functions are almost everywhere differentiable (textbook result).

Finally, note that \( \text{sign} f(x) = c(x) \) on \( \hat{A} \) and \( \hat{B} \). Indeed, in this case either \( d(x, \hat{B}) < d(x, \hat{A}) \) either \( d(x, \hat{B}) > d(x, \hat{A}) \) and the result is straightforward.

☐

For the case \( K > 2 \) we must slightly change the definition to prove Proposition 2.
We need to prove that with same classification power, and finally approximate those functions (in the sense of uniform convergence) with 1-Lip NN.

The proof of Definition 4

Proof. We start by proving that $f$ is 1-Lipschitz.

We need to prove that $\|f(x) - f(y)\|_p \leq \|x - y\|$ for any $p$-norm on $\mathbb{R}^K$ with $p \geq 1$. First, consider the case $f_k(x) = f_k(y) \neq 0$. Then $\|f(x) - f(y)\|_p = |f_k(x) - f_k(y)| = |d(x, \partial) - d(y, \partial)| \leq \|x - y\|$ using the proof of Proposition 1. Now, consider the case $f_k(x) > 0$, $f_k(y) > 0$ and $k \neq l$. Then:

$$\|f(x) - f(y)\|_p = \sqrt{f_k^2(x) + f_l^2(y)} \leq |f_k(x)| + |f_l(y)| = d(x, \partial) + d(y, \partial)$$

Using the same technique as in the previous proof, if we assume $d(x, \partial) + d(y, \partial) > d(x, y)$ then we can construct $z$ verifying both $f_k(z) < f_l(z)$ and $f_l(z) < f_k(z)$ which is a contradiction. Consequently $d(x, \partial) + d(y, \partial) \leq d(x, y)$.

Each row of $J_x f$ is either full of zeros, either the gradient of some $f_k$ on which the reasoning of the case $K = 2$ applies (like in previous proof). In this case, the spectral norm $J_x f$ is equal to the norm of the gradient of the non zero row. We conclude similarly that $\|J_x f\| = 1$ everywhere it is defined.

Finally, note that $\arg\max_k f_k(x)$ is equal to $c(x)$ everywhere $c$ is defined, which concludes the proof. 

Proof of Corollary 1. The proof sketched is enough to show that 1-Lip NN and unconstrained ones have same decision frontiers. We could have also taken a more convoluted path: take the classifier $c$ associated to an unconstrained NN, consider the restriction to a subset $\mathcal{X}$ of the input space making the pre-images separated. Then we can apply Proposition 1 to get 1-Lip functions with same classification power, and finally approximate those functions (in the sense of uniform convergence) with 1-Lip NN.

Proof of Corollary 2. If classes are separable the optimal Bayes classifier $b$ achieves zero error. Moreover, the topological closure $\overline{b^{-1}(\{y\})}, y \in \mathcal{Y}$ yields a set of closed sets that are all disjoints (since $\epsilon > 0$) and on which Proposition 2 can be applied, yielding a 1-Lipschitz neural network with the wanted properties.

Proof of Corollary 3. Those properties hold by construction. The risk $\mathcal{R}(\text{sign}(f))$ is minimal since $f$ is build from the optimal Bayes classifier. Note that, in general, for any classifier $c : \mathcal{X} \to \mathcal{Y}$ the bound of Property 1 is tight by construction for HMF(c). Indeed $f(x)$ is the distance to the frontier, and the direction is given by $\nabla_x f(x)$.

B Proofs of Section 4

The proof of Proposition 3 only requires to take a look at the logits of two examples having different labels.

Proof. Let $t \in \mathbb{N}$. For the pair $i, j$, as $y_i \neq y_j$, by positivity of $\mathcal{L}$ we must have:

$$0 \leq \mathcal{L}(f_t(x_i), +1) + \mathcal{L}(f_t(x_j), -1) \leq \mathcal{E}(f_t, X)$$

As the right hand side has limit zero, we have:

$$\lim_{t \to \infty} \mathcal{L}(f_t(x_i), +1) = \lim_{t \to \infty} \mathcal{L}(f_t(x_j), -1) = 0$$

$$\implies \lim_{t \to \infty} f_t(x_i) = \lim_{t \to \infty} f_t(x_j) = -\infty$$

Consequently $\lim_{t \to \infty} |f_t(x_i) - f_t(x_j)| = +\infty$. By definition $L_t \geq \frac{|f_t(x_i) - f_t(x_j)|}{\|x_i - x_j\|}$ so $\lim_{t \to \infty} L_t = +\infty$. 


The solutions of the problems are invariant by translations: if \( f(x) \) is a solution, then \( f(x + c) \) is also a solution. Let's take a look at classifier \( f \) and \( g \). Consider a sequence of functions \( f^t \) in \( \text{Lip}_L(\mathcal{X}, \mathbb{R}) \) such that \( \lim_{t \to \infty} \mathcal{E}(f^t) = \inf_{f \in \text{Lip}_L(\mathcal{X}, \mathbb{R})} \mathcal{E}(f) = E^* \).

Consider the sequence \( u_t = \|f_t\|_\infty \). We want to prove that \( \{u_t\}_{t \in \mathbb{N}} \) is bounded. Proceed by contradiction and observe that if \( \lim_{t \to \infty} u_t = +\infty \) then \( \lim_{t \to \infty} \mathcal{E}(f_t) = +\infty \). Indeed, for \( \|f_t\|_\infty \geq 2L \text{diam } \mathcal{X} \) we can guarantee that \( \text{sign } f_t \) is constant over \( \mathcal{X} \) and in this case one of the two classes \( y \) is misclassified, knowing that \( \lim_{t \to \infty} \mathcal{L}_{-y f(x), y} = O(\mathcal{L}(f(x))) \to +\infty \) yields the desired result.

But if \( \lim_{t \to \infty} \mathcal{E}(f_t) = +\infty \), then \( \mathcal{E}(f_t) \) cannot converges to \( E^* \). Consequently, \( u_t \) must be upper bounded by some \( M \).

Hence the sequence \( f_t \) is uniformly bounded. Moreover each function \( f_t \) is \( L \)-Lipschitz so the sequence \( f_t \) is uniformly equicontinuous. By applying Arzelà–Ascoli theorem we deduce that it exists a subsequence \( f_{\phi(t)} \) (where \( \phi : \mathbb{N} \to \mathbb{N} \) is strictly increasing) that converges uniformly to some \( f^* \), and \( f^* \in \text{Lip}_L(\mathcal{X}, \mathbb{R}) \). As \( \mathcal{E}(f^*) = E^* \), the infimum is indeed a minimum.

**Proof of Theorem** is an application of Glivenko-Cantelli theorem.

We proved in Proposition 4 that the minimum of equation 4 is attained, so we replace inf by min. We restrict ourselves to a subset of \( \text{Lip}_L(\mathcal{X}, \mathbb{R}) \) on which \( \|f\|_\infty \leq 2L \text{diam } \mathcal{X} \) because the minimum lies in this subspace. We have:

\[
|\min_f \mathcal{E}_p(f) - \min_f \mathcal{E}_\infty(f)| \leq \max_f |\mathcal{E}_p(f) - \mathcal{E}_\infty(f)|
\]

Let \( g_y(x) = \mathcal{L}(f(x), y) = -\log (1 + \exp -y f(x)) \). Note that \( g \) is also Lipschitz and bounded on \( \mathcal{X} \). The entropy with bracket (see [45], Chapter 2.1) of the class of functions \( \mathcal{G} = \{g_y = \mathcal{L} \circ f | f \in \text{Lip}_L(\mathcal{X}, \mathbb{R}), y \in \mathcal{Y}, \mathcal{X} \text{ bounded and } \|f\|_\infty \leq 2L \text{diam } \mathcal{X} \} \) is finite (see [45], Chapter 3.2). Consequently \( \mathcal{G} \) is Glivenko-Cantelli. Finally \( \max_f |\mathcal{E}_p(f) - \mathcal{E}_\infty(f)| \overset{a.s.}{\to} 0 \) which concludes the proof.

Results of Table 1. We can apply the same reasoning as in the proof of Proposition 5. If we replace BCE with hinge, the resulting class is still Glivenko-Cantelli, so the theorem apply. Hence, hinge is a consistent estimator in the space of 1-Lipschitz functions. The result is also straightforward for \( L_W \): consistency of Wasserstein distance is a textbook result. Loss \( L_\lambda \) still belong to Glivenko-Cantelli classes as sum of functions from Glivenko-Cantelli classes (on same distribution \( \mathbb{P}_X \)).

**C Proofs of Section 5**

**Proof of Proposition 6**

We will build \( P \) and \( Q \) as a finite collection of Diracs. Let \( P = \frac{1}{n} \sum_{i=1}^{n} \delta_{4i-1} \) and \( Q = \frac{1}{n} \sum_{i=1}^{n} \delta_{4i-1} \) for some \( n \in \mathbb{N} \), where \( \delta_x \) denotes the Dirac distribution in \( x \in \mathbb{R} \). A example is depicted in Figure 1 for \( n = 20 \). In dimension one, the optimal transportation plan is easy to compute: each atom of mass from \( P \) at position \( i \) is matched with the corresponding one in \( Q \) to its immediate right. Consequently we must have \( f(4i-1) = f(4(i-1)) + 3 \). The function \( f \) is not uniquely defined on segments \( [4i-1, 4i] \) but it does not matter: since \( f \) is 1-Lipschitz we must have \( |f(4i-1) - f(4i)| \leq 1 \). Consequently in every case for \( i < j \) we must have \( f(4(i-1)) < f(4(j-1)) \) and \( f(4i-1) < f(4j-1) \). Said otherwise, \( f \) is strictly increasing on supp \( P \) and supp \( Q \).

The solutions of the problems are invariant by translations: if \( f \) is solution, then \( f - T \) with \( T \in \mathbb{R} \) is also a solution. Let's take a look at classifier \( c(x) = \text{sign}(f(x) - T) \). If \( T \) is chosen such that \( f(4(i-1)) - T < 0 \) and \( f(4i-1) - T > 0 \) for some \( 1 \leq i \leq n \) then \( (n+1) + 2 = n + 1 \) points are correctly classified on a total of \( 2n \) points. It corresponds to an error of \( \frac{n-1}{2n} = \frac{1}{2} - \frac{1}{2n} \). Take \( n = \lceil \frac{1}{2r} \rceil \) to conclude.
Proof of Proposition 7.

Proof. The implication “finite VC dimension” $\implies$ “PAC learnable” is a classical result from [46].

The VC dimension of $C_m(X)$ is the maximum size of a set shattered by $C_m(X)$. As the functions $f$ are 1-Lipschitz, if $c^m_f(x) = -c^m_f(y)$ then $f(x) \geq m$, $f(y) \leq m$ and $\|x - y\| \geq 2m$. Consequently, a finite set $X \subseteq X^n$ is shattered by $C_m(X)$ if and only if for all $x, y \in X$ we have $B(x, m) \cap B(y, m) = \emptyset$ where $B(x, m)$ is the open ball of center $x$ and radius $m$.

The maximum number of disjoint balls of radius $m$ that fit inside $X$ is known as the packing number of $X$ with radius $m$. $X$ is bounded, hence its packing number is finite.

The bounds on the packing number are a direct application of [43] (Lemma 1).

The proof of Proposition 8 uses the number of affine pieces generated by GroupSort2 activation function.

Proof. We first prove that that $f$ is piecewise affine and the number of such pieces is not greater than $\prod_{i=1}^{K} 2^{w_i^2} = \sqrt{2^W}$, where $w_i$ is the number of neurons in layer $i$. We proceed by induction on the depth of the neural network. For depth $K = 0$ we have an affine function $\mathbb{R}^n \rightarrow \mathbb{R}$ which contain only one affine piece by definition (the whole domain), so the result is true.

Now assume that a neural network $\mathbb{R}^{w_1} \rightarrow \mathbb{R}$ of depth $K$ with widths $w_2 w_3 \ldots w_k$ has $S_k$ affine pieces. The enumeration starting at $w_2$ is not a mistake: we pursue the induction for a neural network $\mathbb{R}^n \rightarrow \mathbb{R}$ of depth $K + 1$ and widths $w_1 w_2 \ldots w_k$. The composition of affine function is affine, hence applying an affine transformation $\mathbb{R}^n \rightarrow \mathbb{R}^{w_1}$ preserves the number of pieces. The analysis fall back to the number of distinct affine pieces created by GroupSort2 activation function. If such activation function creates $S$ pieces then we have the immediate bound $S_{K+1} \leq SS_k$.

Let $(Jf)(x) \in \mathbb{R}^{w_1 \times w_1}$ be the Jacobian of the GroupSort2 operation evaluated in $x$. The cardinal $|\{(Jf)(x), x \in \mathbb{R}^{w_1}\}|$ is the number of distinct affine pieces. For GroupSort2 we have a combinations of $\frac{w}{2}$ MinMax gates. Each MinMax gate is defined on $\mathbb{R}^2$ and contains two pieces: one on which the gate behaves like identity and the other one on which the gate behaves like a transposition. Consequently we have $S_{k+1} \leq 2^{\frac{w}{2}} S_k$ and unrolling the recurrence yields the desired result.

Now, we just need to apply the Lemma 1 with $B = \sqrt{2^W}$.

Lemma 1 (Piecewise affine function). Let $\mathcal{H}$ a class of classifiers that are piecewise affine, such that the pieces form a convex partition of $\mathbb{R}^n$ with $B$ pieces (each piece of the partition is a convex set). Then we have:

$$VC_{dim}(\mathcal{H}) = O\left((n + 1)B^2\right)$$

The proof of Lemma 1 is detailed below.
Let $G(N)$ the growth function \[47\] of $\mathcal{H}$. According to Sauer’s lemma \[47\] if it grows polynomially with the number of points, then the degree of the polynomial is an upper bound on the VC dimension. We will show that is indeed the case by computing a crude upper bound of the degree. Assume that we are given $N$ points, and $N$ big enough such that Sauer’s lemma can be applied.

Assume that we can choose freely the convex partition, and then only the affine classifier inside each piece. In general for neural networks that might not be the case (the boundary between partitions depends of the affine functions inside it, since neural networks are continuous); however we are only interested in an upper bound so we can consider this generalization.

Each piece of the partition is a polytope \[48\]. Each polytope is characterized by a set of exactly $B − 1$ affine inequalities, since each polytope is the intersection of $B − 1$ halfspaces \[48\]. The latter is usually avoided by regularizing the weights of the networks and using bounded losses.

To prove Proposition 9 yields the desired result. Finally, for $h^i(H^{i-1}(x)) = W^i H^{i-1}(x) + B^i$ we replace $\theta$ by the appropriate parameter which yields the desired result. \[\square\]

## D Gradient Preserving layers

Vanishing and Exploding gradients have been a long time issue in the training of neural networks. The latter is usually avoided by regularizing the weights of the networks and using bounded losses, while the former can be avoided using residual connections (such ideas can found on LSTM \[49\] or ResNet \[50\]). On 1-Lipschitz neural networks we can guarantee the absence of exploding gradient.

**Proposition 9** (No exploding gradients \[2\]). Assume that $f = h^M \circ h^{M-1} \circ \ldots \circ h^2 \circ h^1$ is a feed forward neural network and that each layer $h^i$ is 1-Lipschitz, where $h^i$ is either a 1-Lipschitz affine transformation $h^i(x) = W^i x + B^i$ either a 1-Lipschitz activation function. Let $L : \mathbb{R}^k \times \mathcal{Y} \to \mathbb{R}$ the loss function. Let $\tilde{y} = f(x)$, $H^i = h^i \circ h^{i-1} \circ \ldots \circ h^2 \circ h^1$ and $H^0(x) = x$. Then:

\[
\|\nabla_{W^i}L(\tilde{y},y)\| \leq \|\nabla_{\tilde{y}}L(\tilde{y},y)\|\|H^{i-1}(x)\| \quad (17)
\]

\[
\|\nabla_{B^i}L(\tilde{y},y)\| \leq \|\nabla_{\tilde{y}}L(\tilde{y},y)\| \quad (18)
\]

To prove Proposition 9 we just need to write the chain rule.

**Proof.** The gradient is computed using chain rule. Let $\theta$ be any parameter of layer $h^i$. Let $h_{\tilde{y}}^i$ be a dummy variable corresponding to the input of layer $h^i$, which is also the output of layer $h^{i-1}$. Then:

\[
\nabla_{\theta}L(\tilde{y},y) = \nabla_{\tilde{y}}L(\tilde{y},y) M(\theta h^i(H^{i-1}(x)))
\]

with $M = \left( \prod_{j=M}^{i+1} \int_{h^j} h^j(H^{j-1}(x)) \right)$. As the layers of the neural network are all 1-Lipschitz, then:

\[
\|J_{h^j} h^j(H^{j-1}(x))\| \leq 1
\]

Hence:

\[
\|\nabla_{\theta}L(\tilde{y},y)\| \leq \|\nabla_{\tilde{y}}L(\tilde{y},y)\|\|J_{\theta} h^i(H^{i-1}(x))\| \quad (19)
\]

Finally, for $h^i(H^{i-1}(x)) = W^i H^{i-1}(x) + B^i$ we replace $\theta$ by the appropriate parameter which yields the desired result. \[\square\]
There is still a risk of vanishing gradient, which strongly depends of the loss $\mathcal{L}$. For Lipschitz neural networks, BCE $\mathcal{L}_T$ does not suffer of vanishing gradient.

**Proposition 10** (No vanishing BCE gradients). Let $(x_i, y_i)_{1 \leq i \leq n}$ be a non trivial training set (i.e. with more than one class) such that $x_i \in \mathcal{X}$, $\mathcal{X}$ a bounded subset of $\mathbb{R}^n$. Then there exists a constant $K > 0$ such that, for every minimizer $f_L^*$ of BCE (known to exists thanks to Proposition 4):

$$f_L^* \in \arg\min_{f \in \mathcal{P}_{\mathcal{L}_i}(\mathcal{X}, \mathbb{R})} \mathbb{E}_{(x,y) \sim P_X \times Y} [\mathcal{L}_T(f(x), y)]$$

And such that for every $1 \leq i \leq p$ we have the following:

$$\left| \frac{\partial f_L^*}{\partial y} \mathcal{L}_T(\hat{y} = f_L^*(x_i), y_i) \right| \geq K$$

Note that $K$ only depends of the training set, not $f_L^*$.

**Proof.** Note that it exists $K' > 0$ such that $|f_L^*(x_i)| \leq K'$ for all $x_i$ and all minimizers $f_L^*$, just like in the proof of Proposition 4 because otherwise we could exhibit a sequence of minimizers $(f_L^*)_i$ not uniformly bounded, which is a contradiction.

Consequently $\left| \frac{\partial f_L^*}{\partial y} \mathcal{L}_T(\hat{y} = f(x_i), y_i) \right| \geq \frac{1}{1+\exp |f(x_i)|} \geq \frac{1}{1+\exp(K')} = K$.

It means that a non null gradient will remain for each training example taken independently, but their sum after convergence will be the null vector. Consequently we must expect high variance in gradients and oscillations when we get closer to the minimum.

**Remark** (Residual connections). If $f$ verifies $\|\nabla_x f(x)\| = 1$ almost everywhere, and if $g$ verifies $\|\nabla_x g(x)\| = 1$ almost everywhere, then $\|\nabla_x (f^2 f(x) + 1/2 g(x))\| < 1$ in general, unless $\nabla_x f(x) = \nabla_x g(x)$. Taking $f(x) = x$ we end up with residual connections, for which ensuring $\|\nabla_x (f^2 f(x) + 1/2 g(x))\| = 1$ almost everywhere is not trivial.

## E BCE through the lens of OT

In the following we try to draw links between BCE minimization and optimal transport. Since the objective function is optimized with gradient descent, the gradients of the loss is the object of interest. We re-introduce $f_\theta$ as a function parameterized by $\theta$, mapping the input to the logits. Let $g_\theta^0(x) = \sigma(f_\theta(x))$ and $g_\theta^1(x) = 1 - \sigma(f_\theta(x))$. $g_\theta^0(x)$ (resp. $g_\theta^1(x)$) are the predicted probabilities of class $+1$ (resp. $-1$).

Now define $\mathcal{Z}_\theta^0 = \mathbb{E}_{x \sim P}[g_\theta^0(x)]$ and $\mathcal{Z}_\theta^1 = \mathbb{E}_{x \sim Q}[g_\theta^1(x)]$. $\mathcal{Z}_\theta^0$ can be seen as the weighted rate of false negatives. That is, the average mass of probability given to class $-1$ by $f_\theta$ when examples are sampled from class $+1$. Similarly, $\mathcal{Z}_\theta^1$ can be seen as the rate of false positives. Let:

$$dP_\theta(x) = \frac{1}{2\mathcal{Z}_\theta^0} g_\theta^0(x) dP(x) \text{ and } dQ_\theta(x) = \frac{1}{2\mathcal{Z}_\theta^1} g_\theta^1(x) dQ(x)$$

Consequently, $P_\theta$ (resp. $Q_\theta$) is a valid probability distribution on $\mathbb{R}^n$ corresponding to the probability of an example $x$ to be incorrectly classified in class $-1$ (resp. $+1$). With these notations the full expression of the gradient takes a simple form. Behold the minus sign: it is a gradient descent and not a gradient ascent.

$$-\nabla_\theta \left( \mathbb{E}_{x \sim P}[\mathcal{L}(f_\theta(x), +1)] + \mathbb{E}_{x \sim Q}[\mathcal{L}(f_\theta(x), -1)] \right) = \mathcal{Z}_\theta^0 \mathbb{E}_{x \sim P}[\nabla_\theta f_\theta(x)] - \mathcal{Z}_\theta^1 \mathbb{E}_{x \sim Q}[\nabla_\theta f_\theta(x)]$$

We apply a bias term $T \in \mathbb{R}$ to classify with $f_\theta - T$ instead. For a well chosen $T$ we can enforce $\mathcal{Z}_\theta^0 = \mathcal{Z}_\theta^1$ and such $T$ can be find using bisection method. The optimization is performed over the set of 1-Lipschitz functions. We end up with:

$$\mathcal{Z}_\theta^0 (\mathbb{E}_{x \sim P}[\nabla_\theta f_\theta(x)]) - \mathbb{E}_{x \sim Q}[\nabla_\theta f_\theta(x)]$$

This is the gradient for the computation of Wasserstein metric $\mathcal{W}$ between $P_\theta$ and $Q_\theta$, using Rubinstein-Kantorovich dual formulation. Hence, binary cross-entropy minimization is similar to the computation of a transportation plan between $P_\theta$ and $Q_\theta$. Note that $P_\theta$ and $Q_\theta$ depend of the current classifier $f_\theta - T$, so the problem is not stationary.
F Alternative formulation

The dual problem can be reformulated by swapping the objective and the constraint.

$$\min_{P f - Q f \geq \epsilon W(P, Q)} \text{Lip}(f) = \epsilon \min_{P f - Q f \geq \epsilon W(P, Q)} \text{Lip}(f)$$

$$= \epsilon \max_{\text{Lip}(f)=1} P f - Q f$$

$$= \arg \max_{\text{Lip}(f)=\epsilon} P f - Q f \tag{26}$$

$\epsilon$ can be seen as re-scaling (change of units in physicist vocabulary). This make more clear the fact that changing the Lipschitz constant is just changing the units used to measure distance.

G HKR, Unconstrained networks, experimental setting

All experiments in the paper were run on a personal workstation with NVIDIA Geforce 1080 GTX and 8GB VRAM, 16 cores Xeon and 32GB RAM, in less than an hour, using Tensorflow framework.

The experiments of Figure 3 can be reproduced with unconstrained neural network, in Figure 5.

The experiments of Figure 6 can be done with HKR loss as well, in Figure 5.
Figure 6: Training Loss and Training Error as function of epoch, on Cifar10 dataset ("dogs" versus "cats"). HKR loss with $\lambda = 100$ and various values for $m$. Metrics on the test set are not displayed on purpose, since our goal is to understand the optimization problem and not evaluate generalization capabilities. Log scale on y-axis loss.