Function Norms for Neural Networks[*]

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Abstract

Deep neural networks (DNNs) have become increasingly important due to their excellent empirical performance on a wide range of problems. However, regularization is generally achieved by indirect means, largely due to the complex set of functions defined by a network and the difficulty in measuring function complexity. There exists no method in the literature for additive regularization based on a norm of the function, as is classically considered in statistical learning theory. In this work, we study the tractability of function norms for deep neural networks with ReLU activations. We provide, to the best of our knowledge, the first proof in the literature of the NP-hardness of computing function norms of DNNs of 3 or more layers. We also highlight a fundamental difference between shallow and deep networks. In the light on these results, we propose a new regularization strategy based on approximate function norms, and show its efficiency on a segmentation task with a DNN.

1. Introduction

In the recent years, computer vision has benefited from the growth of neural network applications. Most of the recent results indicate that larger networks provide better performance. Many works link this increase to the expressivity of the function classes encoded by DNNs. [2] and [13] link expressivity to depth, and define a complexity measures (e.g. transitions, activation patterns) that grow exponentially with the number of layers. [12] takes a differential geometry perspective to show that in certain regimes, the global curvature of the neural network function grows exponentially with depth but not width, showing a clear advantage of deep networks over shallow ones.

With the continual increase of the networks size and complexity, it seems natural to look into maximum a posteriori

estimation of the parameters, or equivalently to regularize the training with carefully designed additive measure of the network complexity.

Looking back at classical machine learning algorithms with regularized risk, it appears that direct regularization has often been achieved by penalization of a norm of a function. In the case of linear functions (e.g. Tikhonov regularization [19]), penalizing the parameter vector corresponds to a penalization of a function norm as a straightforward result of the Riesz representation theorem [15]. In the case of reproducing kernel Hilbert space (RKHS) regularization (including splines [21]), penalizing the parameters corresponds by construction to a function norm regularization [20, 16].

In the case of deep neural networks, similar approaches have been applied directly to the parameter vectors, resulting in an approach referred to as weight decay [8]. In contrast to the previously mentioned Hilbert space approaches, this does not directly penalize a measure of function complexity, such as a norm. Indeed, it is straightforward to see that this is not even a function of the mapping encoded by the network, as different weights can result in the same mapping.

In this work, we study the tractability of computing function norms for neural networks. We prove for the first time (to the best of our knowledge) that computing any function norm of a DNN with three or more layers with rectified linear unit (ReLU) activation functions [6] as a function of its parameter values is NP-hard. Moreover, we highlight a fundamental difference between ReLU networks of 2 layers and networks of 3 or more layers by constructing a polynomial-time computable norm for the shallow architectures. This result motivates the use of approximation strategies to be able to use function norm related measures for DNN regularization. We empirically test this new regularization strategy on a segmentation task with a DNN.

2. Function norm based regularization

We consider the supervised training of the weights W of a deep neural network (DNN) given a training set $\mathcal{D} = \{(x_i, y_i)\} \in (\mathcal{X} \times \mathcal{Y})^n$, where $\mathcal{X} \subseteq \mathbb{R}^d$ is the input space

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and $\mathcal{Y} \subseteq \mathbb{R}^s$ the output space. Let $f : \mathcal{X} \rightarrow \tilde{\mathcal{Y}}$ be the function encoded by the neural network. We aim to minimize the risk $\mathcal{R}(f) = \int \ell(f(x), y)\, \mathrm{d}P(x, y)$, where P is the underlying joint distribution of the input-output space. As this distribution is generally inaccessible, empirical risk minimization approximates the risk integral by

$$\hat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i), \qquad (1)$$

where the elements from the dataset $\mathcal{D}$ are supposed to be i.i.d. samples drawn from $P(x, y)$.

When the number of samples n is large, the empirical risk (1) is a good approximation of the risk integral. In the small-sample regime, however, better control of the generalization error can be achieved by adding a regularization term to the objective.

In the statistical learning theory literature, this is most typically achieved through an additive penalty [20, 10]

$$\arg\min_{f} \hat{\mathcal{R}}(f) + \lambda \Omega(f), \qquad (2)$$

where Ω is a measure of function complexity. The regularization biases the objective towards "simpler" candidates in the model space.

In machine learning, using the norm of the learned mapping appears as a natural choice to control its complexity. This choice limits the hypothesis set to a ball in a certain topological set depending on the properties of the problem. In an RKHS, the natural regularizer is a function of the Hilbert space norm: for the space $\mathcal{H}$ induced by a kernel k, $\|f\|_{\mathcal{H}}^2 = \langle f, f \rangle_{\mathcal{H}}$. Several results showed that the use of such a regularizer results in a control of the generalization error [5, 21, 1]. In the context of function estimation, for example using splines, it is customary to use the norm of the approximation function or its derivative in order to obtain a regression that generalizes better [22].

However, for neural networks, defining the best prior for regularization is less obvious. The topology of the function set represented by a neural network is still fairly unknown, which complicates the definition of a proper complexity measure.

Nevertheless, if the activation functions are continuous, any function encoded by a network is in the space of continuous functions. Moreover, supposing the input domain $\mathcal{X}$ is compact, the network function has a finite L_q-norm

$$\|f\|_q = \left(\int \|f(x)\|_q^q \, \mathrm{d}\mu(x) \right)^{\frac{1}{q}}, \qquad (3)$$

where the inner norm represents the q-norm of the output space.

In Sec. 4, we will focus on the special case of L_2. This function space has attractive properties, being a Hilbert space.

However, because of the high dimensionality of neural network function spaces, the optimization of function norms is not an easy task. Indeed, the exact computation of any of these function norms is intractable for networks with ReLU activations, as we show in the following section.

3. Tractability of function norm computation

In this section, we will study separately the networks of 2 or less layers and the networks of 3 or more layers.

3.1. Shallow networks

Definition 1 *Let $\mathcal{H}$ be an RKHS associated with the kernel k over the topological space X. k is **characteristic** [17] if the mapping $P \mapsto \int_X k(., x) dP(x)$ from the set of all Borel probability measures defined on X to $\mathcal{H}$ is injective.*

For example, the Gaussian kernel over $\mathbb{R}^d$ is characteristic.

Proposition 1 *Given a 2-layer neural network f mapping from $\mathbb{R}^d$ to $\mathbb{R}$ with m hidden units, and a kernel k characteristic over $\mathbb{R}^d$, there exists a function norm $\|f\|$ that can be computed in a quadratic time in m and the cost of evaluation of k (assuming we allow a square root operation). For example, for a Gaussian kernel, the cost of the kernel evaluation is linear in d and the function norm can be computed in $\mathcal{O}(m^2 d)$ (assuming that we allow square root and exponential operations).*

We define a norm on two layer ReLU networks by defining an inner product through a RKHS construction based on a characteristic kernel [17] after normalization of the network weights. The kernel must be characteristic to guarantee that the resulting norm is zero iff $f = \mathbf{0}$. The exact construction is provided in [14, Appendix F] due to space constraints here.

3.2. Deep networks

Proposition 2 *For f defined by a deep neural network (of depth greater or equal to 3) with ReLU activation functions, deciding if any function norm $\|f\| = 0$ from the weights of a network is NP-hard.*

To prove this statement, we construct a network of depth 3 for which the Max-Cut problem [7] can be reduced in linear time to deciding if the norm of the function is zero.

Definition 2 (Cut) *Given a graph $G = (V, E)$, a cut is a partition of the vertex set V into two disjoint subsets $S \subseteq V$ and $V \setminus S$. The size of the cut is $|\operatorname{cut}(G, S)| = |\{\{i, j\} \in E, \ i \in S, j \in V \setminus S\}|$.*

Problem 1 (Max-cut decision problem) *Given a graph G and an integer k, decide if there is a cut of at least size k in G. We denote the truth of this statement as $\operatorname{Max-Cut}(G, k)$.*

Given graph G, we define function $f : \mathbb{R}^V \to \mathbb{R}$ as follows:

$$f(x) = h\left(\sum_{(i,j)\in E} f_{ij}(x)\right)$$
$$h(z) = \max(0, z - k + 1)$$
$$f_{ij}(x) = g_1(x_i - x_j) + g_1(x_j - x_i)$$
$$g_1(z) = g_0(z - 1)$$
$$g_0(x) = \varepsilon^{-1}[\max(0, x+\varepsilon) - 2\max(0, x) + \max(0, x-\varepsilon)]$$

where $\varepsilon = \frac{1}{4|V|}$. Note that $g_0(z), g_1(z)$ place some non-zero values in the ε neighborhood of $z = 0$ and $z = 1$, respectively, and zero elsewhere. Furthermore, $g_0(0) = 1$ and $g_1(1) = 1$ (see Figure 1).

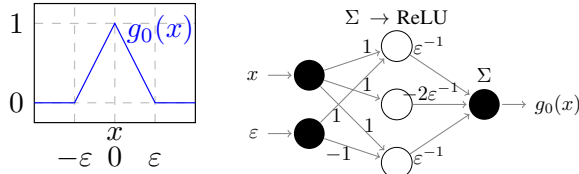Figure 1: Plot of function g_0, and network computing this function.

Lemma 1 *f is continuous by composition of continuous functions.*

Corollary 1 *$\|f\| = 0 \iff f(x) = 0$ everywhere.*

Proposition 3 *$\|f\| \neq 0$ iff Max-Cut$(G, k) = true$.*

Proof: First, suppose that Max-Cut(G, k) is true. Let S define a partition with $|\operatorname{cut}(G, S)| \geq k$. For $i \in S$, set $x_i = 1$. For $j \in V \setminus S$ set $x_j = 0$. We have

$$\sum_{\{i,j\}\in E} f_{ij}(x) = |\operatorname{cut}(G, S)| \geq k. \tag{4}$$

This implies that $f(x) \geq 1$ and thus $\|f\| > 0$ by Corollary 1.

Now suppose that $\|f\| > 0$, then $f(x) > 0$ for some $x \in \mathbb{R}^V$. Define $E' = \{\{i,j\} \in E : f_{ij}(x) > 0\}$, and let $\mathcal{C}$ be the set of connected components of graph (V, E'). For node $i \in C \in \mathcal{C}$ denote $y_i = x_i - \min_{j\in C} x_j$ and $z_i = \operatorname{round}(y_i)$. Let $S = \{i \in V \mid z_i \text{ is even}\}$. We will show next that $|\operatorname{cut}(G, S)| \geq k$, thus proving the claim.

Condition $f(x) > 0$ means that $\sum_{\{i,j\}\in E} f_{ij}(x) > k-1$. Since $f_{ij}(x) \in [0, 1]$ for each $\{i, j\} \in E$, there must be at least k edges in E with $f_{ij}(x) > 0$. Thus, $|E'| \geq k$, and so it suffices to show that $E' \subseteq \operatorname{cut}(G, S)$. By construction,

$$|y_i - y_j| = |x_i - x_j| \in (1-\varepsilon, 1+\varepsilon) \qquad \forall(i, j) \in E'. \tag{5}$$

We claim that $|y_i - z_i| \leq \frac{1}{4}$ for each $i \in V$. Indeed, let $C \in \mathcal{C}$ be the component containing i. Pick $i^* \in \arg\min_{i\in C} x_i$, then $y_{i^*} = 0$. Let P be a path from i^* to i in (V, E'), then $y_i = \sum_{(i',j')\in P}(y_{j'} - y_{i'})$. Eq. (5) now gives $|y_i - \operatorname{round}(y_i)| \leq |P| \cdot \varepsilon \leq |V| \cdot \varepsilon = \frac{1}{4}$, as claimed.

Now consider edge $\{i, j\} \in E'$. Conditions $|y_i - z_i| \leq \frac{1}{4}$, $|y_j - z_j| \leq \frac{1}{4}$ and $|y_j - y_i| \in (\frac{1}{2}, \frac{3}{2})$ imply that $|z_i - z_j| = 1$, and therefore $\{i, j\} \in \operatorname{cut}(G, S)$. $\qquad\square$

Corollary 2 *For a neural network with ReLU activations and three or more layers, deciding whether the function has non-zero norm is NP-hard by polynomial-time reduction from the max-cut decision problem.*

That hardness of a three layer network implies hardness of deeper networks is straightforward as we may implement the identity function by

$$x = \max(0, x) - \max(0, -x). \tag{6}$$

Theorem 1 (Riesz representation theorem [3]) *For $\mathcal{H}$ a Hilbert space an $L : \mathcal{H} \mapsto \mathbb{R}$ or $\mathbb{C}$ a bounded linear functional, there exists a unique vector $h_0 \in \mathcal{H}$ such that:*

$$\forall h \in \mathcal{H}, L(h) = \langle h, h_0 \rangle, \tag{7}$$

and we have $\|L\| = \|h_0\|$.

Proposition 1 and Proposition 2, in combination with the Riesz representation theorem for linear functions (Theorem 1), shows dichotomy in the complexity of norm computation of (deep) neural networks: for two layer networks, we have polynomial time [14] computation, while for networks of depth 3 or higher with ReLU activations, norm computation is NP-hard (Corollary 2).

4. Regularization with approximate norm

In the previous section, we have shown that the exact computation of any function norm for a DNN with ReLU activations is intractable, motivating the need of a stochastic approximation. Assuming the measure μ in the definition of the L_q-norm is a probability measure Q, the function norm can be written as $\|f\|_{2,Q} = \mathbb{E}_{z\sim Q}\left[\|f(z)\|_2^2\right]^{1/2}$. Moreover, assuming we have access to i.i.d samples $z_j \sim Q$, this weighted L_2-function norm can be approximated by

$$\left(\frac{1}{m}\sum_{i=1}^{m} \|f(z_i)\|_2^2\right)^{\frac{1}{2}}. \tag{8}$$

For samples outside the training set, empirical estimates of the squared weighted L_2-function norm are U-statistics of order 1, and have an asymptotic Gaussian distribution to which finite sample estimates converge quickly as $\mathcal{O}(m^{-1/2})$ [9]. In the next experiments, we show the efficiency of such a regularization strategy in a semantic image segmentation task with DNNs.

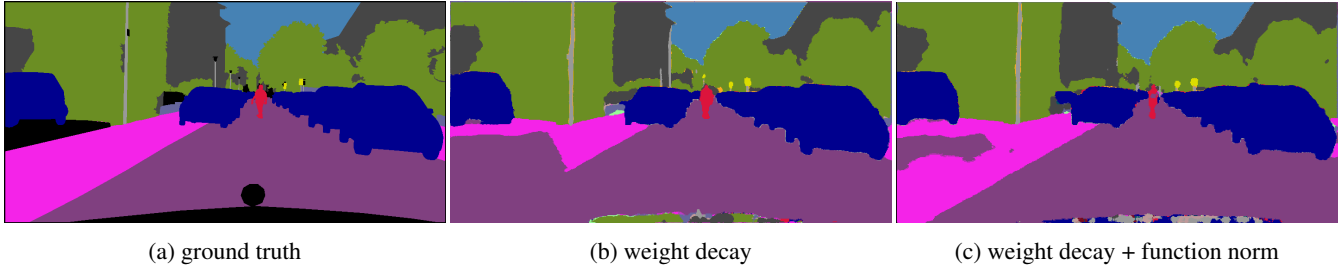| (a) ground truth | (b) weight decay | (c) weight decay + function norm |

Figure 2: ENet outputs, after training on 500 samples of Cityscapes, without (b) and with (c) weighted function norm regularization (standard Cityscape color palette – black regions are *unlabelled* and not discounted in the evaluation.
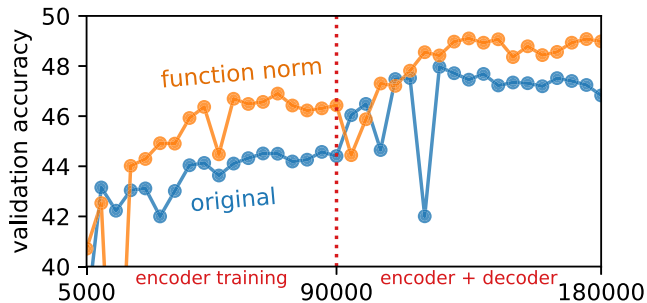

Figure 3: Evolution of the validation accuracy of ENet during training with the network's original regularization settings, and with added weighted function norm regularization.

Regularized training of ENet: We consider the training of ENet [11], a network architecture designed for fast image segmentation, on the Cityscapes dataset [4]. As regularization plays a more significant role in the low-data regime, we consider a fixed random subset of $n = 500$ images of the training set of Cityscapes as an alternative to the full 2975 training images. We compare training ENet similarly to the author's original optimization settings, in a two-stage training of the encoder and the encoder + decoder part of the architecture, using weighted cross-entropy loss. We use Adam with a base learning rate of $2.5 \cdot 10^{-4}$ with a polynomially decaying learning rate schedule and 90000 batches of size 10 for both training stages. We found the validation performance of the model trained under these settings with all images to be 60.77% mean IoU; this performance is reduced to 47.15% when training only on the subset.

We use our proposed approximate function norm regularization using unlabeled samples taken from the 20000 images of the "coarse" training set of Cityscapes, disjoint from the training set. Figure 3 shows the evolution of the validation accuracy during training. We see that the added regularization leads to a higher performance on the validation set. Figure 2 shows a segmentation output with higher performance after adding the regularization.

Results: In our experiments, we were not able to observe an improvement over the baseline in the same setting with a state-of-the-art semi-supervised method, mean-teacher [18]. We therefore believe the observed effect to be attributed to the effect of the regularization. The impact of semi-supervision in the regime of such high resolution images for segmentation is however largely unknown and it is possible that a more thorough exploration of unsupervised methods would lead to a better usage of the unlabeled data.

5. Discussion and Conclusions

While function norms played a central role in regularization for classical machine learning algorithms, regularized training of neural networks has focused mainly on indirect control of complexity. We have shown here for the first time that norm computation in a low fixed depth neural network with ReLU activations is NP-hard, elucidating some of the challenges of working with DNN function classes. This result constitutes a fundamental difference with shallower networks, for which we can construct a polynomial time norm based on the weights. This result motivates the use of stochastic approximations to weighted norm, which is readily compatible with stochastic gradient descent optimization strategies. We empirically validated the expected effect of the employed regularizer with experiments on the training of ENet on Cityscapes.

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