Intrinsic dimensionality and generalization properties of the $\mathcal{R}$-norm inductive bias

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Abstract

Our Problem: We study **statistical** and **approximation** properties of **interpolating** two layer ReLU networks with small **variational norm** ($\mathcal{R}$-norm).

- This norm captures the functional effect of **controlling the size of network weights**.
- This allows the network width to be **unbounded**.
- Practically motivated:
  - Correspond to **weight decay** regularization in neural network training.
  - It has connections to **implicit bias of GD** in the feature learning regime.
- It is known that neural networks trained with **optimal weight decay regulartization** can be **adaptive to low dimesnional structure.**

Our Findings: For **certain target distributions**, minimum $\mathcal{R}$-norm interpolants are:

1. **Intrinsically multivariate functions** (vary in many directions), even when there are ridge functions (vary in only one direction) that fit the data.
2. **Statistically sub-optimal** in terms of generalization.

Bounded Norm Neural Networks

Model: Suppose the data consist of n samples $(\mathbf{x}_i, \mathbf{y}_i)_{i\leq n} \sim \nu \in \mathcal{P}(\Omega \times \mathbb{R})$, where $\Omega \subseteq \mathbb{R}^d$ is a spherically symmetric bounded domain. Let $\boldsymbol{\nu}_n$ denote the empirical data distribution.

Euclidean Formulation: Consider two layer **ReLU** neural networks, with width m, a skip connection, and parameters $\theta = (a_i, b_i, c_i)_{i\leq m} \in (\mathbb{R} \times \mathbb{R}^d \times \mathbb{R})^m$,

$$f_\theta : \Omega \to \mathbb{R} : x \mapsto \sum_{i=1}^{m} a_i \left(b_i^\intercal x + c_i\right)_+ + a_0 \left(b_0^\intercal x + c_0\right).$$

The $\mathcal{R}$-norm of a function $f : \Omega \to \mathbb{R}$ is the **minimum cost** of approximating it arbitrary well by two layer ReLU networks,

$$\|f\|_{\mathcal{R}} := \lim_{\epsilon\to 0} \inf_{m,\,\theta} C(\theta) := \frac{1}{2}\sum_{i=1}^{m} |a_i|^2 + \|b_i\|_2^2 \quad \text{s.t.} \quad \|f - f_\theta\|_{\mathbb{L}^\infty(\Omega)} \leq \epsilon$$

Note that the infimum is over both width, and network parameters.

Problem: What are properties of $\mathcal{R}$-norm inductive bias for certain target distributions?

$$\inf_{f:\Omega\to\mathbb{R}} \|f\|_{\mathcal{R}} \quad \text{s.t.} \quad f(x) = y \quad \nu\text{-almost everywhere} \tag{1}$$

- **Statistical:** What is the required sample complexity (if we replace ν with $\boldsymbol{\nu}_n$)?
- **Approximation:** What do solutions to (1) look like?

Properties of $\mathcal{R}$-norm

Representer Theorem: Though $\mathcal{R}$-norm is **not a RKHS norm**, [7] showed **a minimizer** of the variational problem exists with width $m \leq n$,

$$\forall \epsilon \geq 0 \quad f_{\hat{\theta}_\epsilon} \in \arg\min_{f:\Omega\to\mathbb{R}} \|f\|_{\mathcal{R}} \quad \text{s.t.} \quad \|y - f(x)\|_{\mathbb{L}^2(\boldsymbol{\nu}_n)} \leq \epsilon \tag{2}$$

Characterizing the Norm and Variational Problem: Though $\mathcal{R}$-norm is a variational norm, it can be explicitly characterized in terms of the functions itself under mild assumptions:

1. **Univariate Functions:**
   - For $d = 1$, [9] showed $\|f\|_{\mathcal{R}} = \|f''\|_{\mathbb{L}^1(\Omega)} = \int_\Omega |f''(x)|\, dx$.
   - [4, ?] characterized all the solutions to the variational problem (1).
2. **Multivatiate Functions:**
   - In general [6] showed that $\mathcal{R}$-norm is related to Radon Transform of **higher order derivatives** of the function.
   - Characterizing even a solution to the variational problem in general is difficult.
   - Recent work [5] do so for rank-one datasets using convex duality.
3. Ridge Functions:
   - For functions that only vary in one direction, it reduces to the univariate case,

$$\exists\, w \in \mathbb{S}^{d-1} \;\; \forall\, x \in \Omega \quad f(x) = g(w^\intercal x) \Rightarrow \|f\|_{\mathcal{R}} = \|g\|_{\mathcal{R}}\,.$$

Adaptivity

Curse of dimensionality

- Without any assumption on the data we are doomed to require $n = e^{\Omega(d)}$ number of samples in the in the worst case.
- Inductive biases based on certain variational norms, such as the $\mathcal{R}$-norm, are believed to offer a way around the curse of dimensionality **suffered by kernel methods** [1].
- For optimally chosen ϵ, solutions to (2) can be **adaptive to low dimensional structure** and have sample complexity bounds whose exponent depends on the **intrinsic dimension** [1, 8].
- But how? One may believe that $\mathcal{R}$-norm inductive bias achieves this adaptivity by **favoring functions with low dimensional structure**.
- Empirical/theoretical evidence that neural networks with weight decay regularization can **identify** the low dimensional architecture for certain learning tasks.

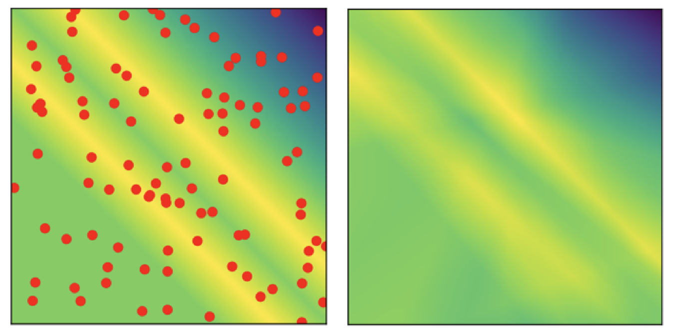


Figure 1. Image from [8]

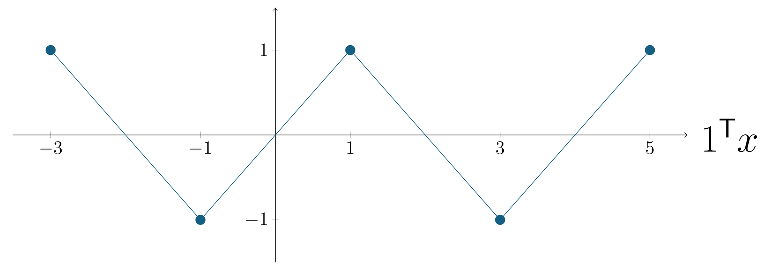
Question: Do minimum $\mathcal{R}$-norm interpolants have a low dimensional structure when such structure is present in the target distribution?

Main Results (Simplified)

Parity Distribution: Consider the target distribution $(\mathbf{x}, \mathbf{y}) \sim \nu \in \mathcal{P}(\{\pm 1\}^d \times \{\pm 1\})$ where $\mathbf{x} \sim \text{Uniform}\{\pm 1\}^d$ is uniformly sampled from **hypercube** and labeled $\mathbf{y} = \chi(\mathbf{x}) = \Pi_{j=1}^{d} \mathbf{x}_j$.

- Parity can be represented by **ridge functions**,

$$\forall x \in \{\pm 1\}^d \quad \chi(x) = g(1^\intercal x).$$



Approximation

Theorem: For parity distribution $\nu \in \mathcal{P}(\{\pm 1\}^d \times \{\pm 1\})$,

- **Ridge function** approximators suffer **high variational norms**,

$$\inf\{\|f\|_{\mathcal{R}} : f \in \text{Ridge}_d,\ \|\chi - f\|_{\mathbb{L}^\infty(\nu)} \leq \frac{1}{2}\} = \Theta(d^{\frac{3}{2}})$$

- **Multidirectional functions** can interpolate more efficiently,

$$\inf\left\{\|f\|_{\mathcal{R}} : \|\chi - f\|_{\mathbb{L}^\infty(\nu)} = 0\right\} = \Theta(d)$$

- No solution to the variational problem with low-dimensional structure is guaranteed to exist, even when the data distribution has low-dimensional structure.
- Results can be extended to distributions other than parity (see paper).

Generalization

Theorem: Given n samples from parity distribution $\nu \in \mathcal{P}(\{\pm 1\}^d \times \{\pm 1\})$,

$$\hat{\mathcal{F}} = \arg\min_{f:\Omega\to\mathbb{R}} \|f\|_{\mathcal{R}} \quad \text{s.t.} \quad f(\mathbf{x}_i) = \mathbf{y}_i.$$

- **(Upper Bound)** When $n = \tilde{\omega}(d^3)$ all minima **approximates parity well** with high probability.

$$\forall \hat{f} \in \hat{\mathcal{F}} \quad \left\|\chi - \text{clip} \circ \hat{f}\right\|_{\mathbb{L}^2(\nu)} = o(1)$$

- **(Lower Bound)** When $n = \tilde{o}(d^2)$ all minima are **far from parity** with high probability.

$$\forall \hat{f} \in \hat{\mathcal{F}} \quad \left\|\chi - \text{clip} \circ \hat{f}\right\|_{\mathbb{L}^2(\nu)} = 1 - o(1)$$

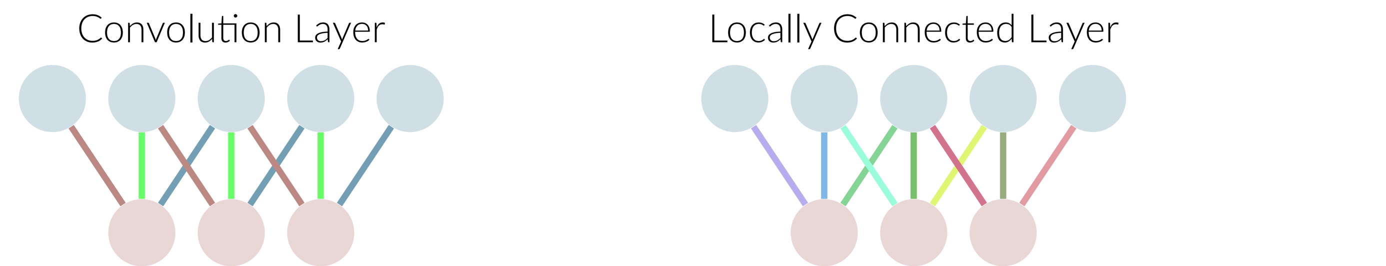
- Information theoretically $n = \Omega(d)$ is sufficient to learn parity (gaussian elimination).
- $\mathcal{R}$-norm inductive bias is not sufficient to achieve statistically optimal sample complexity for learning parity functions.

Proof Ideas (Informal)

1. Approximation:
   - Any ridge function that approximates parity must alternates between slopes of $\pm\Theta(\sqrt{d})$ at least d times. This implies a lower bound on R-norm.
   - We employ an **averaging strategy** that combines a collection of distinct ridge functions, each of which has **few alternations**, and perfectly **fits a fraction** of the parity dataset.
2. Generalization:
   - We use standard **Rademacher complexity** bounds for **bounded $\mathcal{R}$-norm function class**.
   - Using "cap construction" from [2] we produce a robust network with **small Lipschitz** $\tilde{O}(\frac{n}{d})$.

Experiments

Question: Do large neural networks trained on real-world datasets also attain smaller variational norms when they aren't restricted to low-dimensional structures?



- Convolutional architecture (CNN) can be thought of as a function with **low dimenional structure** due to **weight sharing**.
- Inspired by [3], we **decouple the weights** throughout different stages of training a CNN, embed the network into a locally connected network (eLCN), and **continue training** the eLCN.
- Decoupling increases the parameter count and permits the model to have different convolutional kernels in different regions, increasing the intrinsic dimensionality of the model.

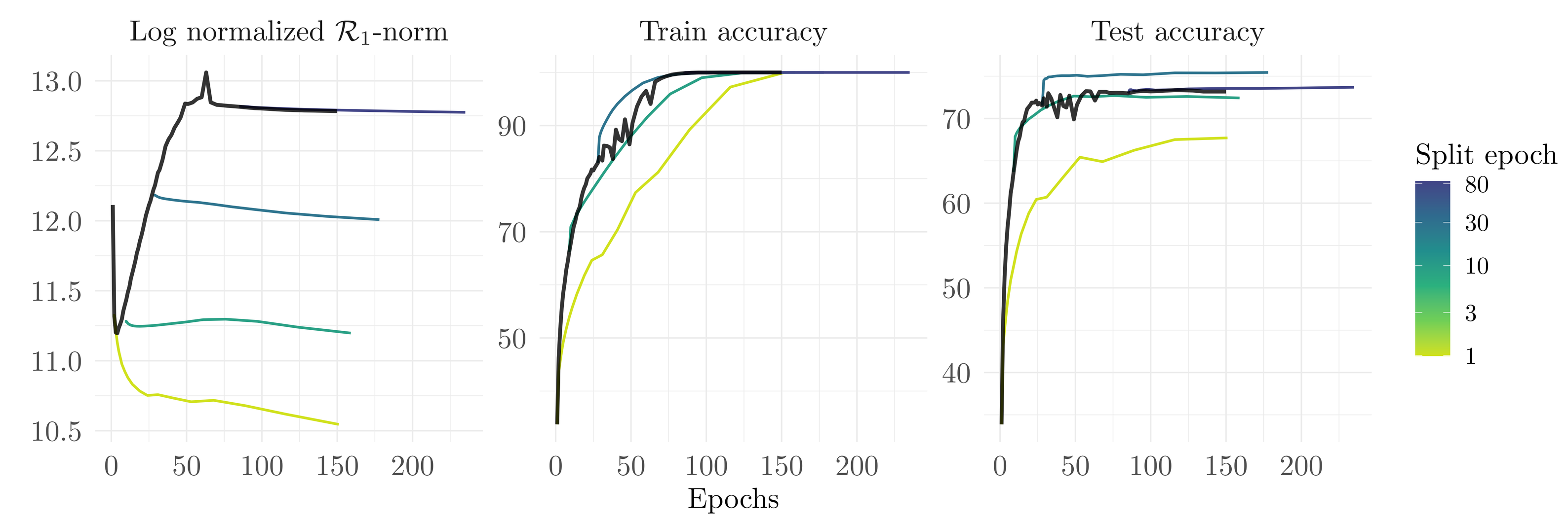


Figure 2. Black line represents the CNN performance.

- Standard training is **biased in favor of networks with low variational norms**.
- Lower variational norms are achieved by eLCNs (high dimensional functions) as compared to the original CNNs (low dimensional functions).

References

[1] Francis Bach. Breaking the curse of dimensionality with convex neural networks. *Journal of Machine Learning Research*, 18(1):629–681, 2017.

[2] Sébastien Bubeck, Yuanzhi Li, and Dheeraj M Nagaraj. A law of robustness for two-layers neural networks. In *Conference on Learning Theory*, 2021.

[3] Stéphane d'Ascoli, Levent Sagun, Giulio Biroli, and Joan Bruna. Finding the needle in the haystack with convolutions: On the benefits of architectural bias. In *Advances in Neural Information Processing Systems 32*, 2019.

[4] Thomas Debarre, Quentin Denoyelle, Michael Unser, and Julien Fageot. Sparsest piecewise-linear regression of one-dimensional data. *Journal of Computational and Applied Mathematics*, 406:114044, 2022.

[5] Tolga Ergen and Mert Pilanci. Convex geometry and duality of over-parameterized neural networks. *Journal of Machine Learning Research*, 22(212):1–63, 2021.

[6] Greg Ongie, Rebecca Willett, Daniel Soudry, and Nathan Srebro. A function space view of bounded norm infinite width ReLU nets: The multivariate case. In *International Conference on Learning Representations*, 2019.

[7] Rahul Parhi and Robert D Nowak. Banach space representer theorems for neural networks and ridge splines. *Journal of Machine Learning Research*, 22(43):1–40, 2021.

[8] Rahul Parhi and Robert D Nowak. Near-minimax optimal estimation with shallow ReLU neural networks. *arXiv preprint arXiv:2109.08844*, 2021.

[9] Pedro Savarese, Itay Evron, Daniel Soudry, and Nathan Srebro. How do infinite width bounded norm networks look in function space? In *Conference on Learning Theory*, 2019.

https://arxiv.org/pdf/2206.05317.pdf

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