Generalization Theory for Deep Learning

Basic version: finite hypothesis class

Finite hypothesis class: with probability $1-\delta$ over the choice of a training set of size n, for a bounded loss ℓ, we have

$$\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i),y_i)-\mathbb{E}_{(x,y)\sim D}\left[\ell(f(x),y)\right]\right|=O\left(\sqrt{\frac{\log|\mathcal{F}|+\log 1/\delta}{n}}\right)$$

VC-Dimension

Motivation: Do we need to consider **every** classifier in $\mathcal{F}$?

Intuitively, **pattern of classifications** on the training set should suffice. (Two predictors that predict identically on the training set should generalize similarly).

Let $\mathcal{F} = \{f : \mathbb{R}^d \to \{+1, -1\}\}$ be a class of binary classifiers.

The growth function $\Pi_{\mathcal{F}} : \mathbb{N} \to \mathbb{F}$ is defined as:

$$\Pi_{\mathcal{F}}(m) = \max_{(x_1, x_2, \ldots, x_m)} \left| \left\{ (f(x_1), f(x_2), \ldots, f(x_m)) \mid f \in \mathcal{F} \right\} \right| .$$

The VC dimension of $\mathcal{F}$ is defined as:

$$\text{VCdim}(\mathcal{F}) = \max\{m : \Pi_{\mathcal{F}}(m) = 2^m\} .$$

VC-dimension Generalization bound

Theorem (Vapnik-Chervonenkis): with probability $1-\delta$ over the choice of a training set, for a bounded loss ℓ, we have

$$\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i),y_i)-\mathbb{E}_{(x,y)\sim D}\left[\ell(f(x),y)\right]\right| = O\left(\sqrt{\frac{\text{VCdim}(\mathcal{F})\log n+\log 1/\delta}{n}}\right)$$

Examples:

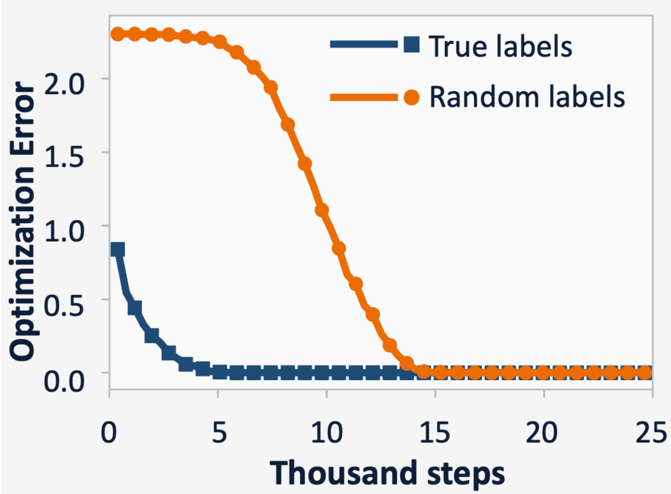
- Linear functions: VC-dim = O(dimension)
- Neural network: VC-dimension of fully-connected net with width W and H layers is $\widetilde{\Theta}(WH)$ (Bartlett et al., '17).

Problems with VC-dimension bound

1. In over-parameterized regime, bound >> 1.
2. Cannot explain the random noise phenomenon:
   - Neural networks that fit random labels and that fit true labels have the same VC-dimension.

Practice: gradient descent

$$\theta(t+1) \leftarrow \theta(t) - \eta \frac{\partial L(\theta(t))}{\partial \theta(t)}$$



Optimization error **-> 0** for both ***true labels*** and ***random labels*** !

Zhang Bengio Hardt Recht Vinyals 2017
Understanding DL Requires Rethinking Generalization

PAC Bayesian Generalization Bounds

Setup: Let P be a prior over function in class $\mathcal{F}$, let Q be the posterior (after algorithm's training).

Theorem: with probability $1 - \delta$ over the choice of a training set, for a bounded loss ℓ, we have

$$\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y)\sim D} \left[\ell(f(x), y) \right] \right| = O\left(\sqrt{\frac{KL(Q\,||\,P) + \log 1/\delta}{n}} \right)$$

Rademacher Complexity

Intuition: how well can a classifier class **fit random noise?**

(Empirical) **Rademacher complexity:** For a training set $S = \{x_1, x_2, \ldots, x_n\}$, and a class $\mathcal{F}$, denote:

$$\hat{R}_n(S) = \mathbb{E}_\sigma \sup_{f \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i f(x_i) \; .$$

where $\sigma_i \sim$ Unif$\{+1, -1\}$ (Rademacher R.V.).

(Population) **Rademacher complexity:**

$$R_n = \mathbb{E}_S \left[\hat{R}_n(s) \right].$$

Rademacher Complexity Generalization Bound

Theorem: with probability $1-\delta$ over the choice of a training set, for a bounded loss ℓ, we have

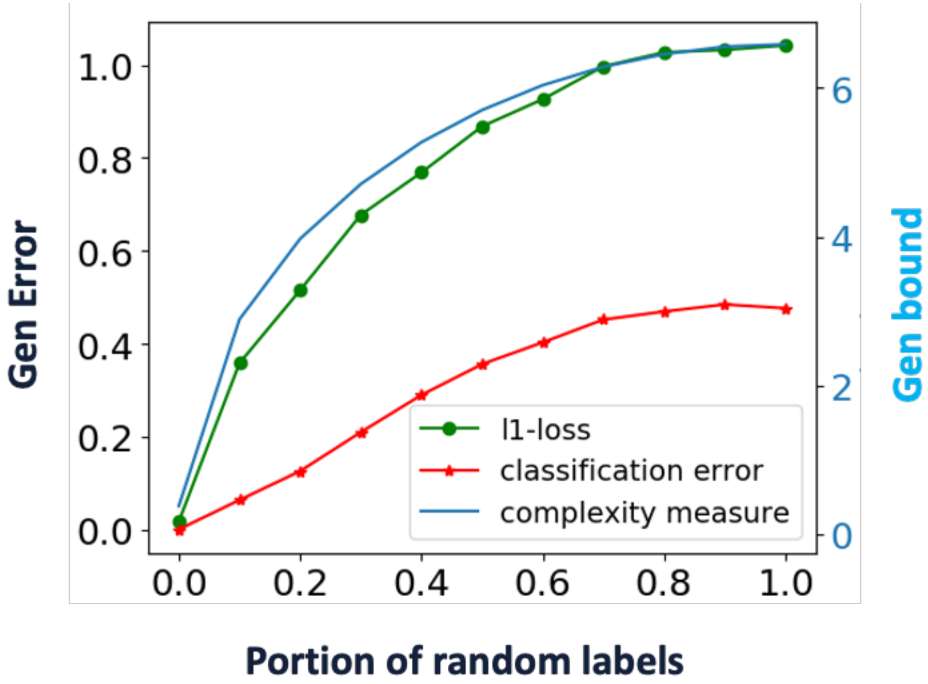
$$\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i),y_i)-\mathbb{E}_{(x,y)\sim D}\left[\ell(f(x),y)\right]\right| = O\left(\frac{\hat{R}_n}{n}+\sqrt{\frac{\log 1/\delta}{n}}\right)$$

and

$$\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i),y_i)-\mathbb{E}_{(x,y)\sim D}\left[\ell(f(x),y)\right]\right| = O\left(\frac{R_n}{n}+\sqrt{\frac{\log 1/\delta}{n}}\right)$$

Kernel generalization bound

Use Rademacher complexity theory, we can obtain a generalization bound $O(\sqrt{y^\top (H^*)^{-1} y/n})$ where $y \in \mathbb{R}^n$ are n labels, and $H^* \in \mathbb{R}^{n\times n}$ is the kernel (e.g., NTK) matrix.



Norm-based Rademacher complexity bound

Theorem: If the activation function is σ is ρ-Lipschitz. Let
$\mathcal{F} = \{x \mapsto W_{H+1}\sigma(W_h\sigma(\cdots\sigma(W_1x)\cdots)), \|W_h^T\|_{1,\infty} \leq B \forall h \in [H]\}$
then $R_n(\mathcal{S}) \leq \|X^\top\|_{2,\infty}(2\rho B)^{H+1}\sqrt{2\ln d}$ where
$X = [x_1, \ldots, x_n] \in \mathbb{R}^{d\times n}$ is the input data matrix.

Comments on generalization bounds

- When plugged in real values, the bounds are rarely non-trivial (i.e., smaller than 1)
- "*Fantastic Generalization Measures and Where to Find them*" by Jiang et al. '19 : large-scale investigation of the correlation of extant generalization measures with true generalization.

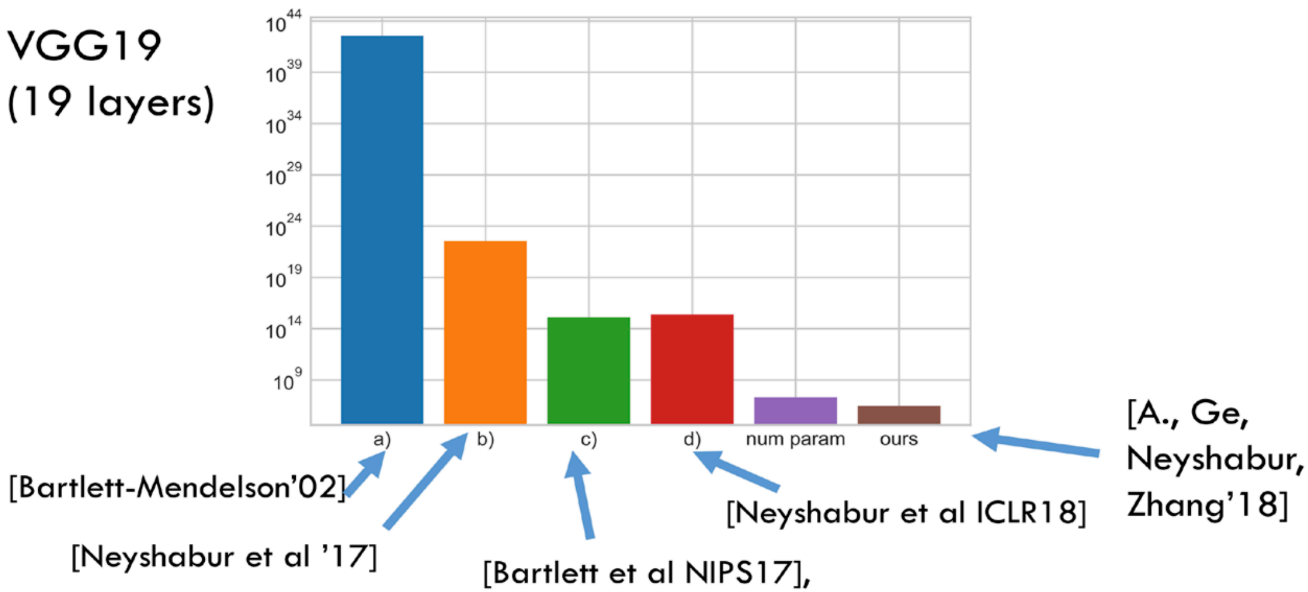


Image credits to Andrej Risteski

Comments on generalization bounds

- Uniform convergence may be unable to explain generalization of deep learning [Nagarajan and Kolter, '19]
  - Uniform convergence: a bound for all $f \in \mathcal{F}$
  - Exists example that 1) can generalize, 2) uniform convergence fails.

- Rates:
  - Most bounds: $1/\sqrt{n}$.
  - Local Rademacher complexity: $1/n$.

Separation between NN and kernel

- For approximation and optimization, neural network has no advantage over kernel. Why NN gives better performance: generalization.

- [Allen-Zhu and Li ’20] Construct a class of functions $\mathscr{F}$ such that $y = f(x)$ for some $f \in \mathscr{F}$:
  - no kernel is sample-efficient;
  - Exists a neural network that is sample-efficient.

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