Recent Generalization Bound for DNNs

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Outline

- Why leanring with DNNs is surprizing?
- Basic concepts (lots of maths 7-10)
- Some of the recent bounds on generalization of DNNs
- Deriving bound using uniform convergence is hard (Nagarajan '19)

Problem Setting

- Dataset $(\mathbf{x}_i, y_i)_{i=1}^n \sim \mathcal{D}^n$
- Function class $\mathcal{F}_\Theta = \{f_\theta : \mathcal{X} \to \mathcal{Y} | \theta \in \Theta\}$
- Loss function $\mathcal{L}(\hat{y}, y)$

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- **Excess Risk**

$$\mathcal{E}(f_{\hat{\theta}}) := \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}[\mathcal{L}(f_{\hat{\theta}}(\mathbf{x}), y) - \mathcal{L}(f_{\theta^*}(\mathbf{x}), y)]$$

- Generalization $\mathcal{E}(f_{\hat{\theta}}) \xrightarrow{n\to\infty} 0$

Optimization Landscape

- Highly non-convex loss function
- Possibly lots of saddle points and local optimas

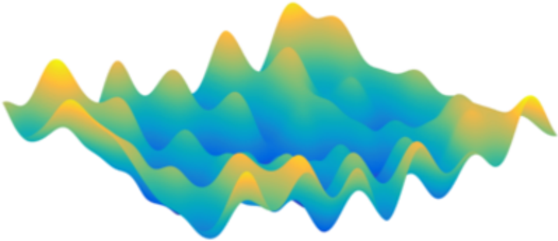

Figure 1: Loss Landscape

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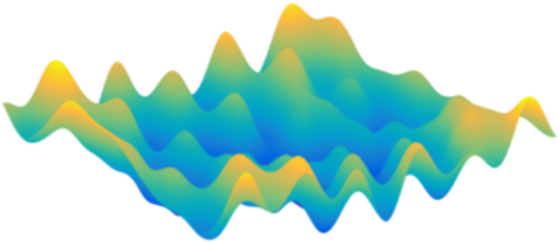
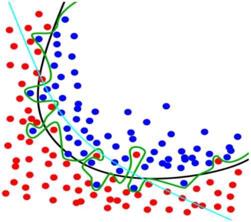


Figure 1: Loss Landscape

- Yet, SGD finds a solution with **low empirical risk**

Underfitting and Overfitting



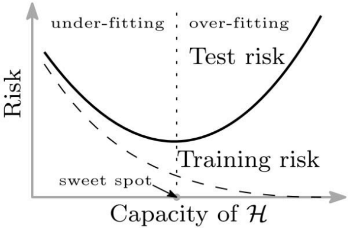


Figure 2: (cyan) Very small and (green) very large number of params (right) overfitting with higher capacity

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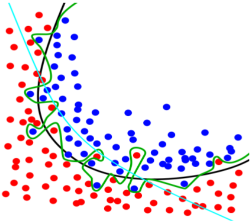


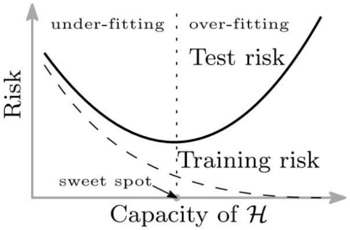


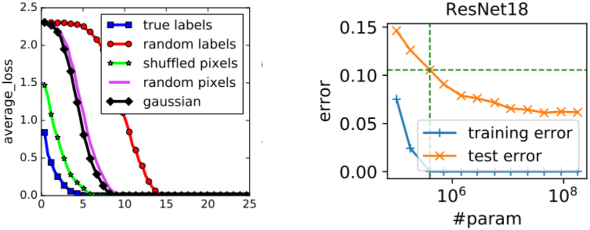
Figure 2: (cyan) Very small and (green) very large number of params (right) overfitting with higher capacity

- Traditionally handled with regularization

$$f_{\hat{\theta}} := \underset{\theta \in \Theta}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(f_\theta(\mathbf{x}_i), y_i) + \lambda \|\theta\|$$

Observations Contradict Traditional Beliefs in ML

- DNNs' capacity is enough to memorize random data (Zhang '18)



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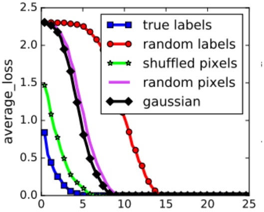

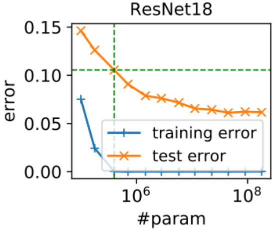

Figure 3: (left) Training classification loss on CIFAR10 (right) better generalization with more params

- Yet, SGD finds a solution that Generalizes to unseen data

Training NN with SGD on **real data** induces regularization

Generalization Gap and Uniform Bound

$$\mathcal{E}(f_{\hat{\theta}}) := \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}[\mathcal{L}(f_{\hat{\theta}}(\mathbf{x}), y) - \mathcal{L}(f_{\theta^*}(\mathbf{x}), y)]$$
$$\leq \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}[\mathcal{L}(f_{\hat{\theta}}(\mathbf{x}), y)] - \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}(f_{\hat{\theta}}(\mathbf{x}_i), y_i) + \epsilon$$

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When $n \to \infty$

- ϵ converges with central limit theorem
- Excess risk converges with the same rate as Generalization Gap
- Not i.i.d samples

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Uniform bound

Orange term $\leq \sup_{\theta\in\Theta}\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}[\mathcal{L}(f_{\theta}(\mathbf{x}),y)] - \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}(f_{\theta}(\mathbf{x}_i),y_i)$

Rademacher Complexity and Uniform Convergence

- Rademacher complexity reflects richness of function space
- $\epsilon_i \in \{-1, 1\}$ with probability $\frac{1}{2}$

$$\mathcal{R}(\mathcal{F}_\Theta) := \mathbb{E}_{\mathbf{x}_i, y_i, \epsilon_i}\left[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \epsilon_i f_\theta(\mathbf{x}_i)\right]$$

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Uniform Convergence Theorem
For b-uniformly bounded $\mathcal{L}$, with probability $> 1 - \delta$

$$\text{Uniform bound } \leq 2\mathcal{R}(\mathcal{L} \circ \mathcal{F}_\Theta) + \sqrt{\frac{2\log(1/\delta)}{n}}$$

- If $\mathcal{R}(\mathcal{L} \circ \mathcal{F}_\Theta) = o(1)$ then uniform bound $\xrightarrow{a.s.}$ 0 exponentially
- Rademacher complexity is tight

VC Dimension

- Largest n s.t. there is a $(\mathbf{x}_i)_{i=1}^n \in \mathcal{X}$ that we can assign any binary label $\{0,1\}^n$ to it using functions in $\mathcal{F}_\Theta$

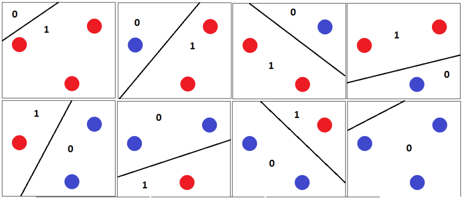

Figure 4: 2d linear classifier can shatter 3 points

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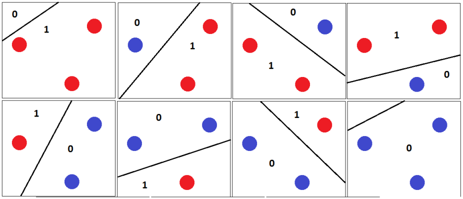

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> **Uniform VC Bound**
> For binary $\mathcal{L}$ (e.g. $yf(\mathbf{x}) < 0$) $\qquad \mathcal{R}(\mathcal{L} \circ \mathcal{F}_\Theta) \leq 2\sqrt{\frac{d_{\mathrm{VC}} \log(n+1)}{n}}$

- Very loose for rich function classes

Harvey's asymtotically tight VC Dimension Bound

Fully connected DNN

- Total number of parameters (weights and biases) M
- Depth L
- Number of neurons U
- $(p+1)$ piece polynomial activations with degree less than d

$$c.ML\log(M/L) \leq d_{\mathrm{VC}}(M,L) \leq C.ML\log M$$

- Tight for ReLU and leaky ReLU activations

$$d_{\mathrm{VC}}(M,L) = \mathcal{O}(MU\log(d+1)p)$$

Margin Bound

Classification margin

$$f(\mathbf{x}_i)_{y_i} - \max_{j \neq y_i} f(\mathbf{x}_i)_j$$

- Margin loss

$$\mathcal{L}_\gamma(f_{\hat{\theta}}, (\mathbf{x}_i, y_i)_{i=1}^n) := \frac{1}{n} \sum_{i=1}^n \mathbb{1}[f(\mathbf{x}_i)_{y_i} - \max_{j \neq y_i} f(\mathbf{x}_i)_j \leq \gamma]$$

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Margin Bound
With probability $> 1 - \delta$

$$\mathbb{P}[\arg\max_j f(\mathbf{x})_j \neq y] \leq \mathcal{L}_\gamma(f_{\hat{\theta}}, \ldots) + \frac{2}{\gamma} \mathcal{R}(\mathcal{F}_\Theta) + \mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{n}}\right)$$

Explaining SGD's Bias

After training DNNs on **real data**

- Aggregated updates have small singular values
- DNNs have bounded lipschitz constant
- Weights don't change much from initialization
    - Despite the long training time :)

$\implies$ Investigate complexity when wieghts have bounded norms

Feed Forward Network with Constraints (Neyshabur '18)

- $\|\mathbf{x}_i\|_2 \leq B$
- Depth L and width h
- Weight $\mathbf{W}_i$ for ith layer
- ReLU activations

Rademacher complexity of DNN with constrained lipschitz constant

$$\mathcal{O}\left(\frac{BL\sqrt{h}}{\sqrt{n}}\left(\prod_{i=1}^{L}\|\mathbf{W}_i\|_\sigma\right)\left(\sum_{i=1}^{L}\frac{\|\mathbf{W}_i-\mathbf{W}_{i,0}\|_F^2}{\|\mathbf{W}_i\|_\sigma^2}\right)^{1/2}\right)$$

Feed Forward Network with Constraints (Bartlett '17)

- $\|\mathbf{x}_i\|_2 \leq B$
- Depth L and width h
- Weight $\mathbf{W}_i$ for ith layer
- ρ_i-Lipschitz activations at ith layer

Rademacher complexity of DNN with constrained lipschitz constant

$$\mathcal{O}\left(\frac{B}{\sqrt{n}}\left(\prod_{i=1}^{L}\rho_i\|\mathbf{W}_i\|_\sigma\right)\left(\sum_{i=1}^{L}\frac{\|\mathbf{W}_i-\mathbf{W}_{i,0}\|_{2,1}^{2/3}}{\|\mathbf{W}_i\|_\sigma^{2/3}}\right)^{3/2}\right)$$

Feed Forward Network with Constraints (Neyshabur '19)

- $\|\mathbf{x}_i\|_2 \leq B$
- Two-layer ReLU NN
- First and second layer weights **U** and **V**
- k classes

Rademacher complexity of DNN with constrained distance norms

$$\mathcal{O}\left(\frac{B\sqrt{k}}{\sqrt{n}}\|\mathbf{V}\|_F\left(\|\mathbf{U}-\mathbf{U}_0\|_F+\|\mathbf{U}_0\|_\sigma\right)+\sqrt{\frac{h}{n}}\right)$$

Nagarajan's Arguments

- Consider high probability datasets $\mathcal{S}_\delta$
- Classifiers $h \in \mathcal{H}_\delta$ trained on $\mathcal{S}_\delta$ have low generalization error $\leq \epsilon$ w.h.p

If for every $h \in \mathcal{H}_\delta$ there is a dataset $S^{-}(h) \in \mathcal{S}_\delta$ that is misclassified w.h.p. $\implies$ $|\text{uniform bound}| \geq 1 - \epsilon$

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- Uniform convergence is all we have
  - Rademacher complexity
  - VC dim
  - PAC learning
  - Covering number

Connection to Adversarial Samples

- S^{-} is adversarial dataset for h
- In high dimensions almost all training samples can fool the classifier

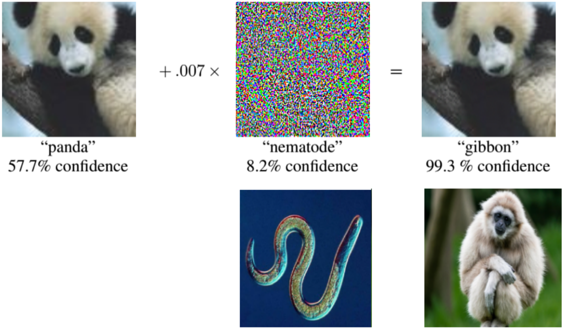

Figure 5: Just mutate with the right gene

- Is it high probability or does it fall off the data's manifold?

Nagarajan's Experiments

- Train a deep fc network with SGD batch size 1

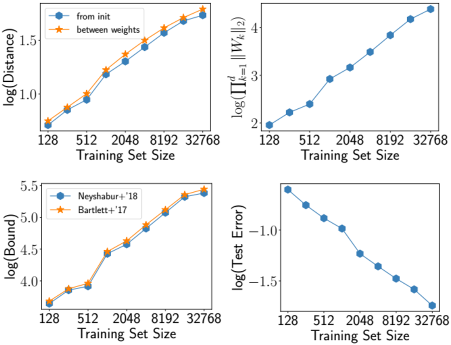

Figure 6: More noise stronger adversaries

DNNs have nothing better to do than memorize the noise in data

Compressability of SGD solution on real data

MNIST Classifier

- Removing unimportant singular values from weight updates

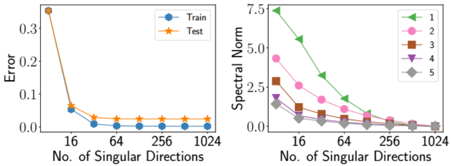

Figure 7: Too many useless singular directions

Compressed networks are more robust to adversarial examples

:)

Thank You

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