Generalization Bounds for Neural Networks

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Sample Complexity: Infinite Hypothesis Spaces Agnostic Case

1) How many examples suffice to get UC whp (so success for ERM).

Theorem

$$m = O\left(\frac{1}{\varepsilon^2} \left[VCdim(H) + \log\left(\frac{1}{\delta}\right) \right] \right)$$

labeled examples are sufficient so that with probab. $1 - \delta$, all $h \in H$ with $|err_D(h) - err_S(h)| \le \epsilon$.

2) Statistical Learning Theory style:

With prob. at least $1 - \delta$, for all $h \in H$:

$$\operatorname{err}_{D}(h) \leq \operatorname{err}_{S}(h) + O\left(\sqrt{\frac{1}{2m}\left(\operatorname{VCdim}(H) + \ln\left(\frac{1}{\delta}\right)\right)}\right).$$

Tight bounds in the worst case.

VC-Dimension of Neural Networks

Theorem: H class of neural networks with L layers, W weights.

- Piecewise constant (linear threshold units): $VCdim(H) = \widetilde{O}(W)$. [Baum-Haussler, 1989]
- Piecewise linear (ReLUs): $VCdim(H) = \widetilde{O}(WL)$. [Bartlett-Harvey-Liaw-Mehrabian, 2017]
- Piecewise polynomial: $VCdim(H) = \widetilde{O}(WL^2).$ [Bartlett-Maiorov-Meir, 1998]

(Note: all final output values thresholded to $\{-1,1\}$) Nearly tight bounds.

Classic VCdim bounds have a strong explicit dependence on # of parameters in the network.

Trivial if # of parameters exceeds the number of examples.

How can we explain successful training of very deep networks?

- Stronger Data-Dependent Bounds
- Algorithm Does Implicit Regularization (finds local optima with special properties)
- Transfer Learning

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Data Dependent Generalization Bounds

Distribution/data dependent. Tighter for nice distributions.

Covering Numbers Generalization Bounds

See Anthony-Bartlett, "Neural Network Learning: Theoretical Foundations", 1999.

Rademacher Complexity Generalization Bounds

See Bousquet-Boucheron-Lugosi, "Introduction to Statistical Learning Theory", 2014.

Data-Dependent Bounds for Deep Networks

E.g., very recent papers:

 Via covering numbers: "Spectrally-normalized margin bounds for neural networks". [Bartlett-Foster-Telgarsky, NIPS 2017]

 Via Rademacher complexity: "Size-independent sample complexity of neural networks". [Golowich-Rakhlin-Shamir, COLT 2018]

Data-Dependent Bounds for Deep Networks

 Spectrally-normalized margin bounds for neural networks. [Bartlett-Foster-Telgarsky, NIPS 2017]

Theorem: With high probability, every f_W with $R_W \le R$ satisfies

$$\Pr(\mathsf{M}(\mathsf{f}_{\mathsf{W}}(\mathsf{X}),\mathsf{Y}) \leq 0) \leq \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}[\mathsf{M}(\mathsf{f}_{\mathsf{W}}(\mathsf{X}_{i}),\mathsf{Y}_{i}) \leq \gamma] + \widetilde{\mathsf{O}}\left(\frac{\mathsf{RL}}{\gamma \sqrt{n}}\right)$$

• Network with L layers, parameters $W_1, ..., W_L$:

$$f_W(\mathbf{x}) \coloneqq \sigma(W_L \sigma_{L-1}(W_{L-1} \dots \sigma_1(W_1 \mathbf{x}) \dots))$$

$$R_W \coloneqq \prod_{i=1}^L |W_i|_*^{2/3} \left(\sum_{i=1}^L \frac{||W_i||_{2,1}^{2/3}}{||W||_*^{2/3}}\right)^{3/2} \qquad [\sigma \text{ is 1-Lipschitz}]$$

$$\text{spectral norm}$$

[Golowich-Rakhlin-Shamir, COLT 2018] provide a related bound via a Rademacher complexity argument



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"Algorithmic Regularization in Over-parameterized Matrix Sensing and Neural Networks with Quadratic Activations". [Li-Ma-Zhang. COLT 2018]

Transfer Learning

"Risk Bounds for Transferring Representations With and Without Fine-Tuning". [McNamara-Balcan. ICML 2017]



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- Algorith

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Lots of open questions.