Generalisation Bounds for Neural Networks

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Overview

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What is generalisation?

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- Assumption: the data (both for the training and testing) comes i.i.d. from a distribution D.
- Usually work in a *distribution-agnostic* setting.

What are generalisation bounds?

- *Classification setting*: input space $\mathcal{X}$ and output space $\mathcal{Y} := \{1, \ldots, k\}$ with a distribution D on $\mathcal{X} \times \mathcal{Y}$.

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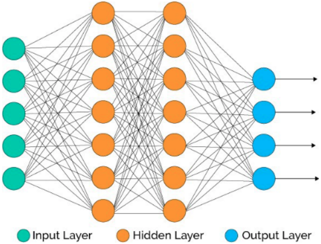
- Goal: to learn a function $f : \mathcal{X} \to \mathcal{Y}$ from a sample $S := \{(x_i, y_i)\}_{i=1}^m \subseteq \mathcal{X} \times \mathcal{Y}$.
- Generalisation bounds: bounding the difference between the expected and empirical losses of f with high probability over S.

What are generalisation bounds?



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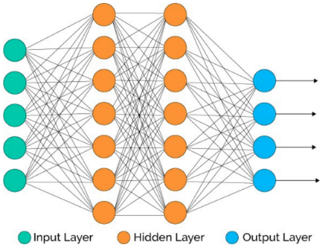

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$$L_0(f) := \mathbb{P}_{(x,y)\sim D}\left(f(x)_y \leq \max_{y' \neq y} f(x)_{y'}\right) \;,$$

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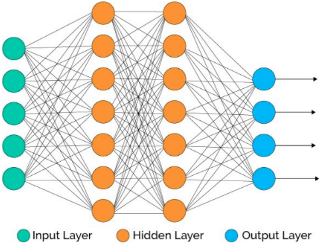

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and the empirical margin loss:

$$\widehat{L}_\gamma(f) := \frac{1}{m}\sum_{i=1}^{m} \mathbf{1}\left[f(x)_y \leq \gamma + \max_{y' \neq y} f(x)_{y'} \right] .$$

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    - Inspire new algorithms or regularisation techniques.

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Generalisation bounds (GB) for neural networks are usually obtained by

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2. Deriving a generalisation bound in terms of a complexity measure $M(H)$ (e.g. size of H, Rademacher complexity),
3. Upper bounding $M(H)$ in terms of model parameters (e.g., norm of weight matrices, number of layers, etc.).

General Strategies: Rademacher Complexity

Definition (Rademacher complexity)

Let G be a family of functions from a set $\mathcal{Z}$ to $\mathbb{R}$. Let $\sigma_1, \ldots, \sigma_m$ be Rademacher variables: $\mathbb{P}(\sigma_i = 1) = \mathbb{P}(\sigma_i = -1) = 1/2$. The *empirical Rademacher complexity* of G w.r.t. to a sample $S = \{z_i\}_{i=1}^m$ is

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Intuition: How much G correlates with random noise on S.

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Intuition: How much G correlates with random noise on S. Simple examples...

General Strategies: Rademacher Complexity

Theorem

Let G be a family of functions from Z to $[0,1]$, and let S be a sample of size m drawn from Z according to D. Let $L(g) = \mathbb{E}_{z \sim D}[g(z)]$ and $\widehat{L}_(g) = \frac{1}{m}\sum_{i=1}^{m} g(z_i)$. Then for any $\delta > 0$, with probability at least $1-\delta$ over S, for all functions $g \in G$,

$$L(g) \leq \widehat{L}(g) + 2\mathcal{R}_S(G) + O\left(\sqrt{\frac{\log(1/\delta)}{m}}\right) .$$

General Strategies: Rademacher Complexity

- Computing the empirical Rademacher complexity (RC) of a given H is usually hard or impractical.
- One usually derives Rademacher complexity upper bounds, for example by using the Dudley entropy integral.

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- Bounds that depend on the norm of the linear transformations [Bartlett, 1997].
- Spectrally-normalised margin-based bounds [Bartlett et al., 2017a].
- PAC-Bayesian approach to margin-based bounds [Neyshabur et al., 2017].

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Paper:

Stronger generalization bounds for deep nets via a compression approach.

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    - Can be adapted to convolutional neural networks.

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Definition

- $f : \mathbb{R}^d \to \mathbb{R}^k$.
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We say that f is (γ, S)-compressible via $G_{\mathcal{A}}$ if there exists $A \in \mathcal{A}$ such that for all x in the sample S,

$$\| f(x) - g_A(x) \|_\infty \leq \gamma \ .$$

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Theorem

Let $G_{\mathcal{A}} := \{g_A \mid A \in \mathcal{A}\}$, where A is a set of q parameters, each of which can have at most r discrete values. Let S be a training set of m samples. For any margin $\gamma > 0$, if f is (γ, S)-compressible via $G_{\mathcal{A}}$, then there exists $A \in \mathcal{A}$ such that w.h.p. over S,

$$L_0(g_A) \leq \widehat{L}_\gamma(f) + \mathcal{O}\left(\sqrt{\frac{q \log r}{m}}\right) \ .$$

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Theorem

Let $S \sim D^m$ and let $\gamma > 0$. A neural network of depth L with linear transformations $A_1, \ldots, A_L$. Then with high probability over S,

$$L_0(f) \leq \widehat{L}_\gamma(f) + \tilde{\mathcal{O}}\left(\sqrt{\frac{hL^2 \max_{x\in S}\|x\| \prod_{i=1}^L \|A_i\|_2^2 \sum_{i=1}^L \frac{\|A_i\|_F^2}{\|A_i\|_2^2}}{\gamma^2 m}}\right).$$

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Some remarks:

- γ is used both as the margin for the loss, and the approximation parameter for compressibility.
- Although the framework bounds the expected loss of the *compressed network* g_A by the empiricial loss of the *original network* f, one can show that g_A approximates f on the *whole input space* and not just S. This thus gives a generalisation bound for f.

Compressed networks: Method 2

Two main ideas:

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2. Randomly project the linear transformations onto lower-dimensional subspace (Johnson-Lindenstrauss transformation).
3. Use (1) and (2) to derive a tighter generalisation bound.

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- c (activation contraction): relates to the percentage of ReLU units that are activated (in practice $\approx 1/2$).
- *These properties relate to noise sensitivity and empirical observations.*

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- Use standard tools to get a generalisation bound:
  - Dudley entropy integral to bound the empirical Rademacher complexity of the margin loss function on the compressed network.

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Theorem

For any fully connected network f_A with $\rho_\delta \geq 3L$, and any margin $\gamma > 0$, the random projection algorithm generates weights $\tilde{A}$ s.t. with high probability over the training set,

$$L_0(f_{\tilde{A}}) \leq \widehat{L}_\gamma(f_A) + \tilde{O}\left(\sqrt{\frac{c^2 L^2 \max_{x \in S} \|f_A(x)\|_2^2 \sum_{i=1}^{L} \frac{1}{\mu_i^2 \mu_{i\rightarrow}^2}}{\gamma^2 m}}\right).$$

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  - Can we get better bounds? Currently: not useful in practice.
  - Can we develop notion and guarantees for adversarial generalisation? [Yin et al., 2018, Cullina et al., 2018]
  - Can *algorithmic stability* offer better bounds and explanations? [Bousquet and Elisseeff, 2002],[Hardt et al., 2016].

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