

Generalization bounds

- Sample i.i.d dataset Z of size n from unknown distribution \mathcal{D} over \mathcal{Z} .
- Loss function $\ell: \Delta(\mathcal{F}) \times \mathcal{Z} \rightarrow [0,1]$ indicates quality of (randomized) $f \in \mathcal{F}$.

True: $L(A|Z; \mathcal{D}) = \mathbb{E}_{f \sim A|Z, Z' \sim \mathcal{D}}[\ell(f; Z')]$

Empirical: $L(A|Z; Z) = \mathbb{E}_{f \sim A|Z} \left[\frac{1}{n} \sum_{i=1}^n \ell(f; Z_i) \right]$

Standard PAC-Bayes/MI bounds

[McAllester 1998, 2003], [Audibert 2004], [Catoni 2007]

$$L(A|Z; \mathcal{D}) - L(A|Z; Z) \leq \text{whp \& } \mathbb{E} \sqrt{L(A|Z; Z) \cdot \frac{\text{KL}(A|Z \parallel \pi)}{n}}$$

independent of Z

[Russo and Zhou 2016], [Xu and Raginsky 2017]

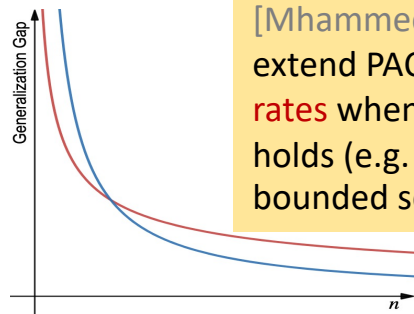
$$\mathbb{E}_Z [L(A|Z; \mathcal{D}) - L(A|Z; Z)] \leq \sqrt{\frac{2 \cdot I(A|Z; Z)}{n}}$$

Directions of improvement over standard

1. Do not capture **fast rates**: $\sim \sqrt{\frac{\text{COMPLEXITY}}{n}}$

Rewriting PAC-Bayes excess risk bounds:

$$R(A|Z; Z) + \left(\frac{\text{KL}(A|Z \parallel \pi)}{n} \right)^\gamma, \text{ where } \gamma \in \left[\frac{1}{2}, 1 \right].$$



[Mhammedi, Grünwald, Guedj 2019] extend PAC-Bayes to capture **fast rates** when a **Bernstein condition** holds (e.g. random label noise, bounded squared error loss).

2. Do not handle general **VC classes**: bound can be infinite for cases where Uniform Convergence implies generalization [Bassily, Moran, Nachum, Shafer, Yehudayoff 2018], [Livni and Moran 2020]

Conditional Mutual Information:

[Steinke and Zakyntinou 2020] extend MI to handle general **VC classes**, proposing $CMI_{\mathcal{D}}(A)$. Subsequently [Hellström and Durisi 2020] extend to PAC-Bayes.

Conditional, faster rate PAC-Bayes/MI bound

Theorem. If a γ -Bernstein condition holds, for arbitrary *almost exchangeable data-dependent priors* $\pi|\langle Z_0, Z_1 \rangle$

$$L(A(Z_0); \mathcal{D}) - L(A(Z_0); Z_0) \leq \left(2 - \frac{1}{\gamma} \right) \cdot R(A(Z_0); Z_0) + \left(\frac{\mathbb{E}_{Z_1} [\text{KL}(A(Z_0) \parallel \pi|\langle Z_0, Z_1 \rangle)]}{n} \right)^\gamma$$

$$\left. \begin{array}{l} \text{Real dataset } Z_0 \sim \mathcal{D}^n \\ \text{Ghost dataset } Z_1 \sim \mathcal{D}^n \end{array} \right\} \langle Z_0, Z_1 \rangle = \begin{array}{l} \{Z_{1,0}, Z_{1,1}\} \\ \{Z_{2,0}, Z_{2,1}\} \\ \vdots \\ \{Z_{n,0}, Z_{n,1}\} \end{array}$$

Claim (VC+New bound). For any class \mathcal{F} with $\text{VCdim}=d$, $\exists A$ (ERM with a consistency property) and prior π such that for any \mathcal{D} , $\text{KL}(A|Z_0 \parallel \pi|\langle Z_0, Z_1 \rangle) \leq d \log 2n$

Main Technical Lemma. Let $S \sim \text{Ber}(1/2)$, $\bar{S} = 1 - S$, and $|r_0|, |r_1| \leq 1$. Then for all $\eta < 1/4$, $r_{\bar{S}} - r_S \leq C \cdot \eta \cdot r_S^2$

Future directions

- Extend to unbounded (e.g. subgaussian) losses.
- Extend to *observable* bound (now might need to know γ, f^*, \mathcal{D})