Using Region Tests to Evaluate PAC Bounds

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Neural Network Generalization

How well can a neural network make inferences from inputs not seen in the training data?

Notation and Definitions

- Feature space $\mathcal{X}$.
- Label space $\mathcal{Y}$.
- Input space $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$.
    - On which unknown distribution $\mathcal{D}$ is defined.
- Training data $S = \{(x_i, y_i)\}_{i=1}^m \overset{\text{i.i.d}}{\sim} \mathcal{D}^m$.
- Parameter space $\mathcal{W}$
- Hypothesis space $\mathcal{H} = \{h_\mathbf{w} : \mathbf{w} \in \mathcal{W}\}$.
    - The $h_\mathbf{w}$ are neural networks, with $\mathbf{w}$ being a vector of weights and biases.
- Loss function $l : \mathcal{Y} \times \mathcal{Y} \to [0, C]$.

Notations and Definitions

Definition

For a hypothesis $h_{\mathbf{w}}$ and set $S = \{(x_i, y_i)\}_{i=1}^{m}$ we define

- the error as $R(\mathbf{w}) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\left(l(h(x), y)\right)$, and
- the empirical error as $\hat{R}(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m} l(h_{\mathbf{w}}(x_i), y_i)$.

Note that $\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\mathbf{w})\right) = R(\mathbf{w})$.

Remarks

- We don't know $R(\mathbf{w})$.
- We train for low $\hat{R}(\mathbf{w})$.
- The generalization gap is $\left|R(\mathbf{w}) - \hat{R}(\mathbf{w})\right|$.

Goal

Bound the generalization gap with high probability.

Overview

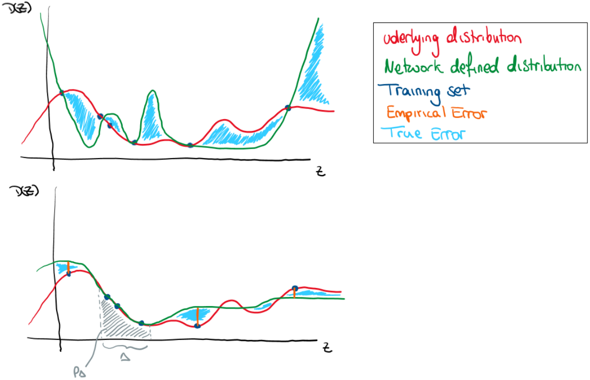


Figure: A sketch depicting the motivation of the investigation.

Assumption

Assumption

For a parameter $\mathbf{w}$ we can guarantee that $h_{\mathbf{w}}$ performs as expected on a region $\Delta \subset \mathcal{Z}$.

- For the 0-1 error this means $l_\Delta(\mathbf{w}) = 0$.

Questions

- How can we leverage this information to update our PAC bounds?
- How do these updates compare to increasing the size of the training data?

Leveraging the Assumption

We obtain information about the shape of $\mathcal{D}$ in the region Δ. Suppose we have a value for

$$p_\Delta = \mathbb{P}_{z\sim\mathcal{D}}(z \in \Delta) = \int_{z\in\Delta} \mathcal{D}(z)dz.$$

There are two potential improvements we can make to a PAC bound.

1. Tighten the bound, or
2. Improve the confidence with which the bound holds.

PAC Bound[1]

Theorem (PAC-Bound)

For a fixed $\mathbf{w} \in \mathcal{W}$*, let* $\delta \in (0,1)$ *then it follows that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}}\right) \geq 1-\delta.$$

[1] Alquier 2023.

Improving Bounds

Theorem

For $\mathbf{w} \in \mathcal{W}$ *and* $\delta \in (0,1)$ *we have that*

$$\mathbb{P}_{S \sim \mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + CB(m, p_\Delta, \delta) \middle| l_\Delta(\mathbf{w}) = 0\right) \geq 1 - \delta$$

for

$$B(m, p_\Delta, \delta) = \sqrt{\frac{\log\left(\frac{(1-p_\Delta)+\sqrt{(1-p_\Delta)^2+4\delta^{\frac{1}{m}}p_\Delta}}{2\delta^{\frac{1}{m}}}\right)}{2}}.$$

Remark

- With $p_\Delta = 0$ we recover Theorem PAC-Bound.
- With $p_\Delta = 1$ we note that $B(m, p_\Delta, \delta) > 0$.

Improving Confidence

Theorem

For $\mathbf{w} \in \mathcal{W}$ *and* $\delta \in (0, 1)$ *we have that*

$$\mathbb{P}_{S \sim \mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0 \right) \geq 1 - \left(\sum_{k=1}^{m} \binom{m}{k} \delta_k p_\Delta^{m-k} (1 - p_\Delta)^k \right)$$

where

$$\delta_k = \frac{1}{\left(\frac{1}{\delta}\right)^{\frac{m^2}{k^2}}}.$$

Remark

- With $p_\Delta = 0$ we recover Theorem PAC-Bound.
- With $p_\Delta = 1$ we get full confidence in our bound.

PAC-Bayes Framework

Bayesian Machine Learning

1. A prior distribution π is defined on the parameter space.
2. A learning algorithm forms the updated posterior distribution ρ from the training data.
3. Infer a parameter from the posterior distribution to define a learned network.

Added Assumption

A subset of the parameter space, $\Omega \subset \mathcal{W}$, such that for $\mathbf{w} \in \Omega$ we have that $l_\Delta(\mathbf{w}) = 0$.

Justifying the Assumption

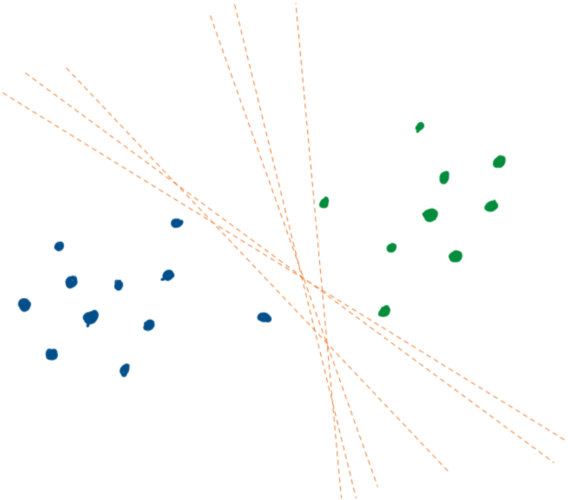


Figure: A sketch depicting the validity of our additional assumption.

Conditioned PAC-Bayes Bound

Theorem

For all $\lambda > 0$, $\rho \in \mathcal{M}(\mathcal{W})$ and $\delta \in (0,1)$, conditioned on the fact that $I_\Delta(\Omega)$ we have that

$$R(\rho) \leq \hat{R}(\rho) + \frac{\log\left(B(\lambda, m, p_\Delta, p_\Omega)\right) + \mathrm{KL}(\rho, \pi) + \log\left(\frac{1}{\delta}\right)}{\lambda},$$

holds with probability greater than $1-\delta$ over sampled training sets S where

$$B(\lambda, m, p_\Delta, p_\Omega) = p_\Omega \left(p_\Delta + (1 - p_\Delta) \exp\left(\frac{\lambda^2 C^2}{8m^2}\right)\right)^m + (1 - p_\Omega) \exp\left(\frac{\lambda^2 C^2}{8m}\right).$$

The original theorem was taken from Catoni 2009.

Experiment Details

- Define discrete underlying distribution.
- Sample m points randomly.
  - Approximating sample, S_A, with $m_A = \eta m$,
  - Training sample, S_T, with $m_T = (1-\zeta)(1-\eta)m$, and
  - Evaluation Sample, S_E, with $m_E = \zeta(1-\eta)m$ points.

1. Train on S_A with cross-entropy loss.
2. Determine correctly classified points of the underlying distribution, $\mathcal{C}$.
3. Sample $\mathcal{C}$ to determine Δ.
4. Approximate Δ using S_A.
5. Evaluate empirical 0-1 error using S_E.
6. Evaluate bound.

Approximating p_Δ

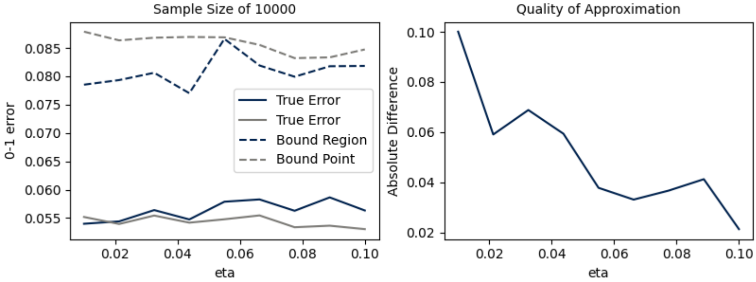
Let S_A be an $\mathrm{i.i.d}$ sample from $\mathcal{D}$.

1. Let $Z_i = \begin{cases} 1 & z_i \in \Delta \\ 0 & \text{otherwise,} \end{cases}$ so that $Z_i \sim \mathrm{Bern}(p_\Delta)$.
2. Let $\hat{p}_\Delta = \frac{1}{|S_A|} \sum_{z_i \in S_A} Z_i$.
3. Construct the $1 - \alpha$ one-sided Clopper-Pearson (exact) confidence interval
$$[q_B(\alpha, m_A\hat{p}_\Delta, m_A - m_A\hat{p}_\Delta + 1), 1],$$
where $q_B(\cdot, m_A\hat{p}_\Delta, m_A - m_A\hat{p}_\Delta + 1)$ is the quantile function for $\mathrm{Beta}(m_A\hat{p}_\Delta, m_A - m_A\hat{p}_\Delta + 1)$.

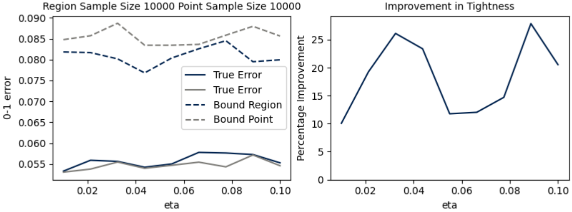
We can update our results accordingly

$$\mathbb{P}_{S\sim\mathcal{D}^m}\Big(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + B\big(q_B(\alpha, m_A\hat{p}_\Delta, m_A - m_A\hat{p}_\Delta + 1)\big)\Big) \geq 1 - (\delta + \alpha(1 - \delta)).$$

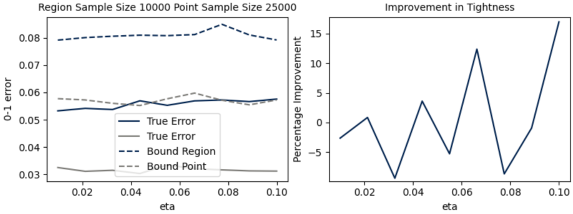
Bounds on MNIST



Comparison to Point Bounds



(a) 10000 samples to evaluate the point bound.



(b) 25000 samples to evaluate the point bound.

Uniform Bounds

Let

$$\mathcal{D}_\Delta(z) = \begin{cases} \frac{\mathcal{D}(z)}{p_\Delta} & z \in \Delta \\ 0 & \text{otherwise,} \end{cases} \quad \mathcal{D}_{\Delta'}(z) = \begin{cases} \frac{\mathcal{D}(z)}{1-p_\Delta} & z \in \Delta' \\ 0 & \text{otherwise.} \end{cases}$$

Then,

$$R(\mathbf{w}) = p_\Delta R_\Delta(\mathbf{w}) + (1 - p_\Delta) R_{\Delta'}(\mathbf{w}). \tag{1}$$

for

$$R_\Delta(\mathbf{w}) = \mathbb{E}_{z\sim\mathcal{D}_\Delta}(l_z(\mathbf{w})), \text{ and } R_{\Delta'}(\mathbf{w}) = \mathbb{E}_{z\sim\mathcal{D}_{\Delta'}}(l_z(\mathbf{w})).$$

Proposition

With notation as above we have that,

$$\mathbb{P}_{S\sim\mathcal{D}^m}\Big((1 - p_\Delta)R_{\Delta'}(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + B(\delta, m) - p_\Delta R_\Delta(\mathbf{w})\Big) \geq 1 - \delta,$$

for all $\mathbf{w} \in \mathcal{W}$ and $\delta \in (0, 1)$.

Experiment Details

1. Obtain a sample of size m from our data space according to a discrete underlying distribution.
2. Partition the data set according to some parameter ξ.
   2.1 Use ξm data points to determine the region Δ.
      - $\eta\xi m$ points to approximate p_Δ.
      - $(1-\eta)\xi m$ points to train a network to determine the region Δ.

   2.2 $(1-\xi)m$ points to evaluate our bound.
      - $(1-\zeta)(1-\xi)m$ points to train the model.
      - $\zeta(1-\xi)m$ points to evaluate the empirical errors for the bound.

Results

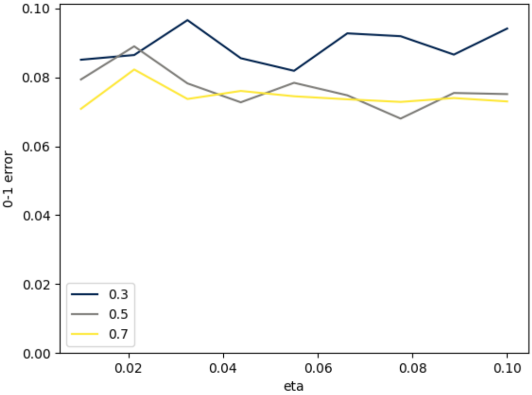


Figure: Plot of the value $\hat{R}(\mathbf{w}) + B(\delta, \zeta(1-\xi)m) - p_L R_\Delta(\mathbf{w})$ for $\zeta = 0.3$, and $\xi \in \{0.3, 0.5, 0.7\}$.

Summary

Conclusions

- Bounds can be updated using region-based performance certificates.
- Updating bounds with this information can break the uniformity of results.
- Improvements are comparable to significant increases in sample size.

Future Work

- Incorporate into other techniques for optimizing PAC bounds, such as data-informed priors, and compression bounds.
- Investigate informed sampling.
  - Updating the training process using the information from our assumptions.
- Perform more extensive experiments.
  - CIFAR10
  - Larger Networks

References

Catoni, Olivier (Jan. 2009). "A PAC-Bayesian approach to adaptive classification". In.

Alquier, Pierre (2023). *User-friendly introduction to PAC-Bayes bounds*.