Tight PAC-Bayesian generalization error bounds for deep learning

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Theory: High-probability PAC-Bayesian bound

From the data distribution we sample the training set, which the model transforms into a posterior, from which we sample the output hypothesis

$$\mathcal{D} \rightsquigarrow S \xrightarrow{\mathcal{M}} Q \rightsquigarrow h$$

We consider bounds on generalization error that hold with high probability over both sampling steps

The following **theorem** gives such a bound for the model producing the Bayesian posterior with 0/1 likelihood and any prior $P(h)$

> For any distribution P on any concept space $\mathcal{H}$ and any realizable distribution $\mathcal{D}$ on a space of instances we have, for $0 < \delta \leq 1$, and $0 < \gamma \leq 1$, that with probability at least $1-\delta$ over the choice of sample S of m instances, that with probability at least $1-\gamma$ over the choice of h:
>
> $$\ln\left(1-\epsilon(h)\right) < \frac{\ln \frac{1}{P(C(S))} + \ln m + \ln \frac{1}{\delta} + \ln \frac{1}{\gamma}}{m-1}$$
>
> where
>
> - $C(S)$ is the set of hypotheses in $\mathcal{H}$ consistent with the sample S and $P(C(S)) = \sum_{h \in C(S)} P(h)$
> - h is sampled from $Q(h) = \begin{cases} \frac{P(h)}{P(C(S))} & \text{if } h \in C(S) \\ 0 & \text{if } h \notin C(S) \end{cases}$

Proof: Essentially the same as that in (DA McAllister, 1999)

Following (G Valle-Perez et al., 2019), we make the following argument:

If SGD-trained neural networks:

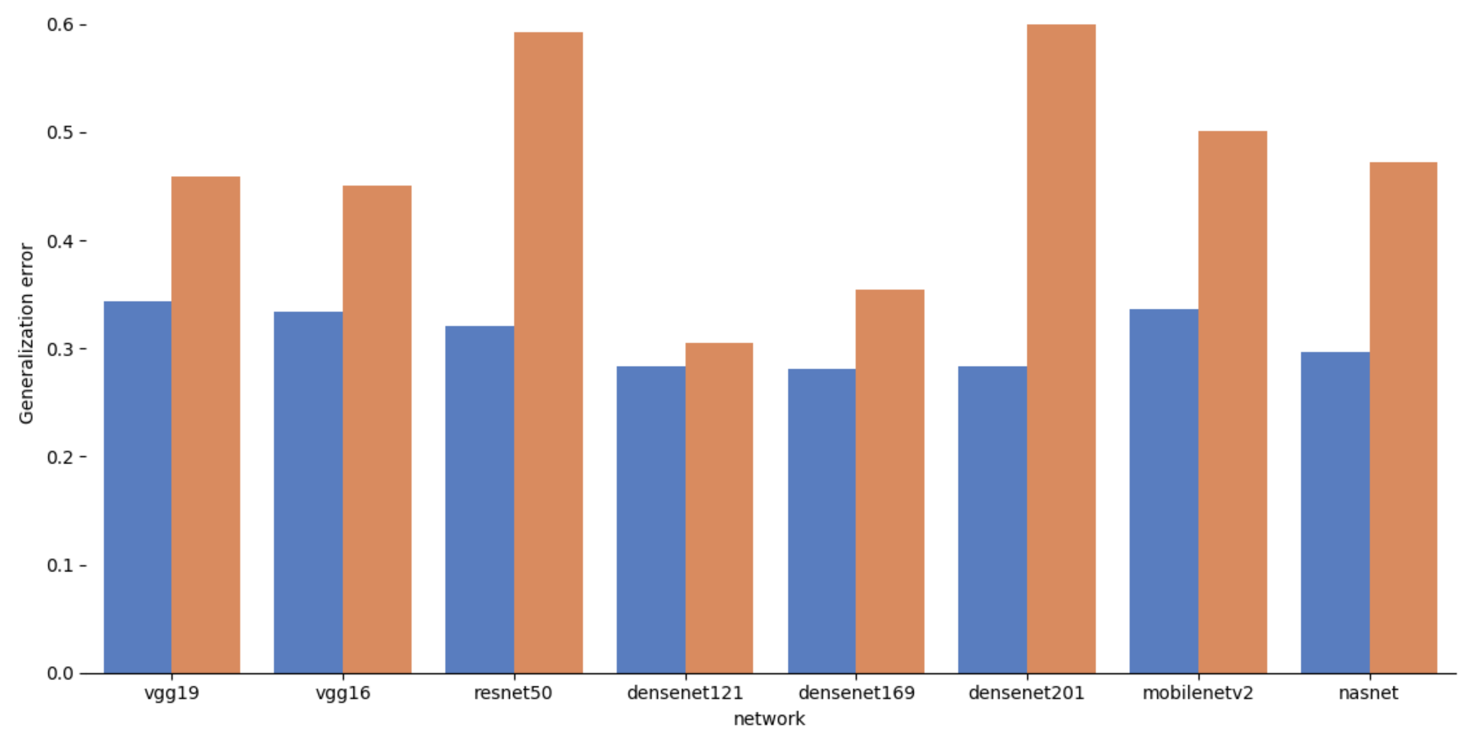
- Reach 0 training error (realizability + trainability)
- Sample the 0-training-error region of parameter space close to uniformly within a bounded domain (unbiasedness in parameter space)

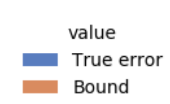
$\Longrightarrow$

SGD-trained neural networks approximate the above model, with prior $P(h)$ determined by the parameter-function map upon uniform sampling of inputs.

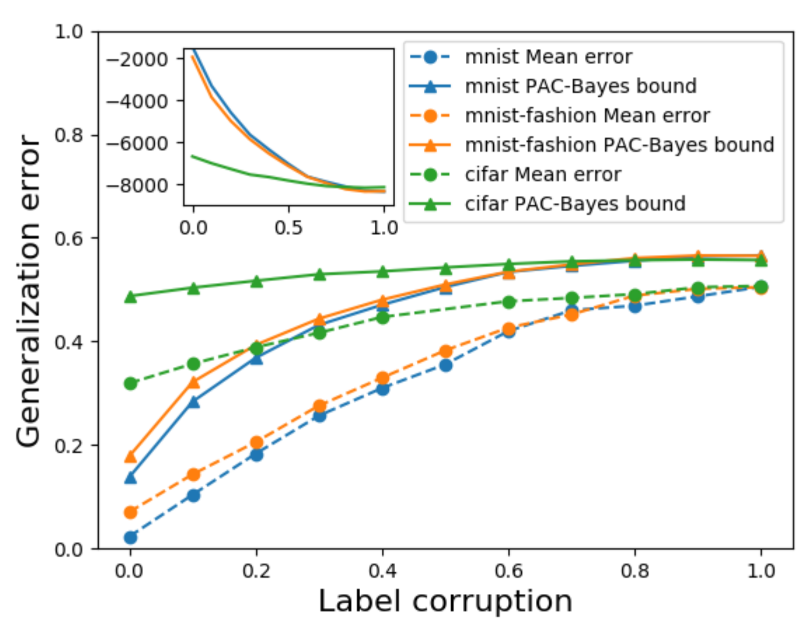
Experiments: Tighter bounds on deep learning architectures

We trained a range of neural network architectures on several standard datasets, and **compared the test error with the PAC-Bayes bound** calculated from the training data.

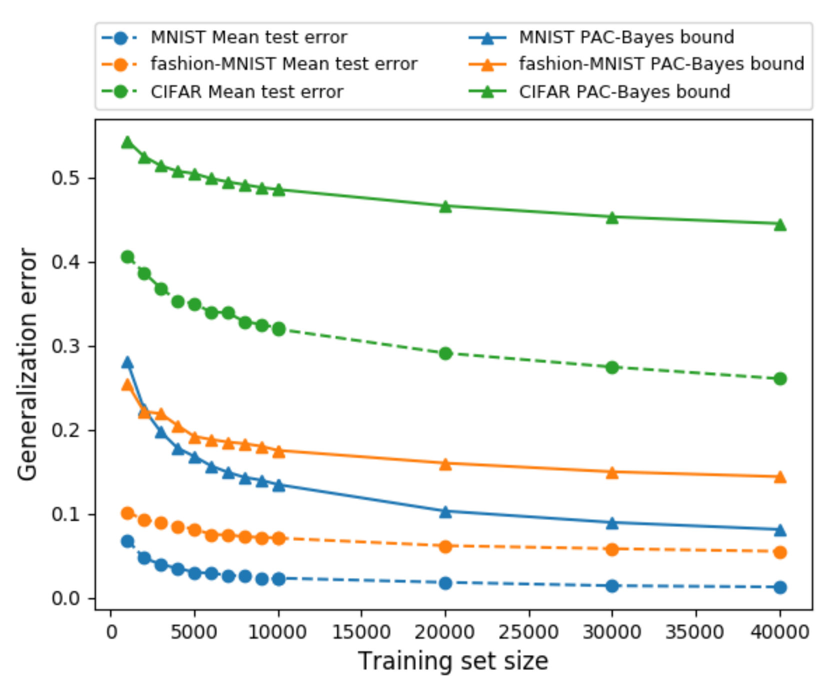




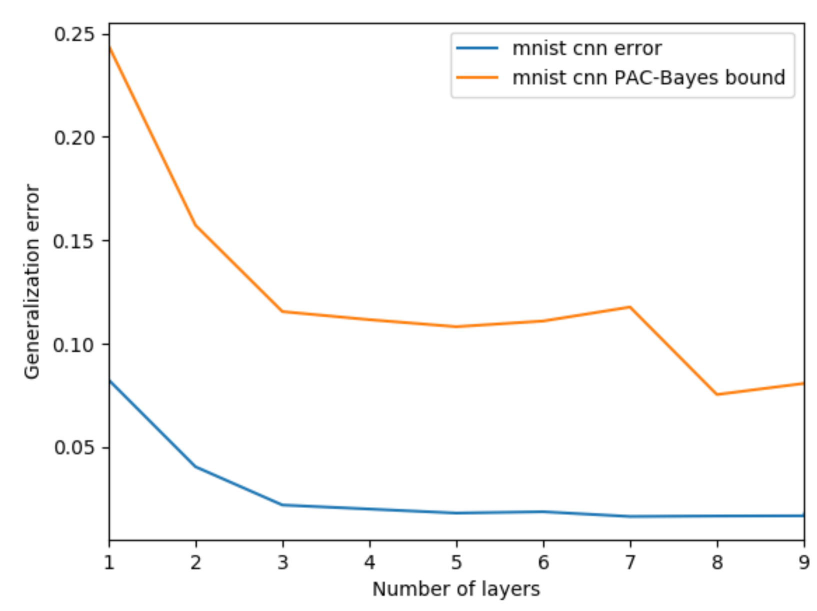
Error and bound, for different architectures trained on a sample of $10k$ images from CIFAR10 (with binarized labels)



Error and bound, versus label corruption (fraction of target labels which are randomized). Inset shows value of $P(C(S))$. Network is a 4-layer CNN without pooling.



Error and bound, versus training set size m, for a 4-layer CNN without pooling



Error and bound, versus number of layers for a CNN with max pooling, trained on a sample of $10k$ MNIST images

Implementation

Recent work (J Lee et al., 2017; A Garriga-Alonso et al., 2019; AGG Matthews et al., 2018, R Novak et al., 2019; G Yang, 2019) has shown that **the prior over functions** and marginal likelihood $P(C(S))$ upon i.i.d. Gaussian sampling of the weights, **can be approximated by a Gaussian process**, for sufficiently wide neural networks

The kernel in the Gaussian process for some architectures can be efficiently computed analytically. For other architectures, we use the **Monte Carlo approximation** proposed in (R Novak et al., 2019)

Refs:

Valle-Perez et al., 2019. Deep learning generalizes because the parameter-function map is biased towards simple functions. Published in ICLR 2019

J Lee et al., 2017. Deep neural networks as gaussian processes. arXiv preprint arXiv:1711.00165, 2017.

A Garriga-Alonso et al., 2019. Deep convolutional networks as shallow Gaussian processes. Published in ICLR 2019

R Novak et al., 2019. Bayesian Deep Convolutional Networks with Many Channels are Gaussian Processes. Published in ICLR 2019

AGG Mathews et al., 2018. Gaussian Process Behaviour in Wide Deep Neural Networks. Published in ICLR 2018

G Yang, 2019. Scaling Limits of Wide Neural Networks with Weight Sharing: Gaussian Process Behavior, Gradient Independence, and Neural Tangent Kernel Derivation. arXiv preprint arXiv:1902.04760, 2019

M Kääriäinen et al., 2005. A comparison of tight generalization error bounds. Published in ICML 2005

DA McAllister, 1999. Some pac-bayesian theorems. Machine Learning (1999) 37: 355

Conclusions

- **We obtain generalization error bounds for deep learning models which are tighter than previously published bounds**
- **For a given architecture, the bound closely follows the trends of the true error as the data is varied (different dataset, training set size, label corruption)**
- **The bound correlates with the true error as some architectural hyperparameters are varied (like layer depth)**
- **The bound doesn't appear to correlate so well with the true error when comparing more complicated architectures**

Full workshop paper:

https://guillefix.me/pacbayes

Limitations

- The bounds only formally apply in the asymptotic limit of infinite width. Making nonasymptotic bounds could prove difficult.
- The bounds depend on the choice of variance of the parameter distribution. This choice seems to have a significant effect only for sufficiently deep neural networks. Understanding how to best choose the variance for different hyperparameter choices is still an open question.
- How well can SGD be approximated by uniform sampling in the zero-error region is also an open question.
- The calculation of the marginal likelihood is approximate, using techniques which typically don't have rigorous guarantees (expectation propagation, MCMC). In this work we used expectation-propagation, but an MCMC approach is probably more accurate (at the expense of computation time).
- It isn't clear how tight PAC-Bayes itself is, as no matching lower bounds are available.
- As discussed by (Kääriäinen et al., 2005), the practical value of PAC-Bayesian versus test-set generalization error bounds may be limited. This is related to the above question of the tightness of the bounds.