Deep Neural Networks: From Flat Minima to Numerically Nonvacuous Generalization Bounds via PAC-Bayes

Daniel M. Roy
University of Toronto; Vector Institute

Joint work with

Gintarė K. Džiugaitė
University of Cambridge

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How does SGD work?

- Growing body of work arguing that SGD performs implicit regularization
- Problem: No matching generalization bounds that are nonvacuous when applied to real data and networks.
- We focus on “flat minima” – weights $w$ such that training error is “insensitive” to “large” perturbations
- We show the size/flatness/location of minima found by SGD on MNIST imply generalization using PAC-Bayes bounds
- Focusing on MNIST, we show how to compute generalization bounds that are *nonvacuous* for stochastic networks with millions of weights.
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- Focusing on MNIST, we show how to compute generalization bounds that are nonvacuous for stochastic networks with millions of weights.
- We obtain our (data-dependent, PAC-Bayesian) generalization bounds via a fair bit of computation with SGD. Our approach is a modern take on Langford and Caruana (2002).
Nonvacuous generalization bounds

risk: $L_D(h) := \mathbb{E}_{(x, y) \sim D}[\ell(h(x), y)]$, $\mathcal{D}$ unknown

empirical risk: $L_S(h) = \frac{1}{m} \sum_{i=1}^{m} \ell(h(x_i), y_i)$, $S = \{(x_1, y_1), \ldots, (x_m, y_m)\}$

generalization error: $L_D(h) - L_S(h)$

\[
\forall \mathcal{D} \quad \mathbb{P}_{S \sim D^m} \left( L_D(\hat{h}) - L_S(\hat{h}) < \epsilon(\mathcal{H}, m, \delta, S, \hat{h}) \right) > 1 - \delta
\]

generalization err. bound
SGD is $X$ and $X$ implies generalization

“SGD is Empirical Risk Minimization for large enough networks”
“SGD is (Implicit) Regularized Loss Minimization”
“SGD is Approximate Bayesian Inference”

No statement of the form “SGD is $X$” explains generalization in deep learning until we know that $X$ implies generalization under real-world conditions.
SGD is (not simply) empirical risk minimization

Training error of SGD at convergence.

Test error at convergence and for early stopping identical.

SGD $\approx$ Empirical Risk Minimization $\arg\min_{w \in \mathcal{H}} L_S(w)$

MNIST has 60,000 training data
Two-layer fully connected ReLU network has $>1$ m parameters
$\implies$ PAC bounds are vacuous
$\implies$ PAC bounds can’t explain this curve
Our focus: Statistical Learning Aspect

On MNIST, with realistic networks, …

▶ VC bounds don’t imply generalization
▶ Classic Margin + Norm-bounded Rademacher Complexity Bounds don't imply generalization
▶ Being “Bayesian” does not necessarily imply generalization (sorry!)

Using **PAC-Bayes bounds**, we show that size/flatness/location of minima, found by SGD on MNIST, imply generalization for MNIST.

Our bounds require a fair bit of computation/optimization to evaluate. Strictly speaking, they bound the error of a random perturbation of the SGD solution.
Flat minima...

training error in flat minima is “insensitive” to “large” perturbations

(Hochreiter and Schmidhuber, 1997)
Flat minima...

training error in flat minima is “insensitive” to “large” perturbations

(Hochreiter and Schmidhuber, 1997)

... meets the PAC-Bayes theorem (McAllister)

\[
\forall \mathcal{D} \forall P \exists \mathbb{P}_{S \sim \mathcal{D}^m} \left[ \forall Q \Delta(L_S(Q), L_D(Q)) \leq \frac{\text{KL}(Q||P) + \log \frac{\tau_{\Delta}(m)}{\delta}}{m} \right] \geq 1 - \delta
\]

For any data distribution, \( \mathcal{D} \),
For any “prior” randomized classifier \( P \),
with high probability over \( m \) i.i.d. samples \( S \sim \mathcal{D}^m \),
For any “posterior” randomized classifier \( Q \),

Generalization error of \( Q \) bounded approximately by \( \frac{1}{m} \text{KL}(Q||P) \)

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Controlling generalization error of randomized classifiers

Let $\mathcal{H}$ be a hypothesis class of binary classifiers $\mathbb{R}^k \rightarrow \{-1, 1\}$. A randomized classifier is a distribution $Q$ on $\mathcal{H}$. Its risk is

$$L_D(Q) = \mathbb{E}_{w \sim Q}[L_D(h_w)]$$

Among the sharpest generalization bounds for randomized classifiers are PAC-Bayes bounds (McAllester, 1999).

**Theorem (PAC-Bayes (Catoni, 2007)).**

Let $\delta > 0$ and $m \in \mathbb{N}$ and assume $L_D$ is bounded. Then

$$\forall P, \forall D, \mathbb{P}_{S \sim D^m}\left(\forall Q, L_D(Q) \leq 2L_S(Q) + 2\frac{KL(Q\|P) + \log \frac{1}{\delta}}{m}\right) \geq 1 - \delta$$
Our approach

given $m$ i.i.d. data $S \sim \mathcal{D}^m$
Our approach

given \( m \) i.i.d. data \( S \sim \mathcal{D}^m \)

empirical error surface
\[ w \mapsto L_S(h_w) \]
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- \( w_{\text{SGD}} \in \mathbb{R}^{472000} \)
weights learned by SGD on MNIST
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$\odot \hat{Q} = \mathcal{N}(w_{SGD} + w', \Sigma')$

stochastic neural net
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  weights learned by SGD on MNIST

$\hat{Q} = \mathcal{N}(w_{\text{SGD}} + w', \Sigma')$
  stochastic neural net

generalization/error bound: $\forall \mathcal{D} \quad \mathbb{P}_{S \sim \mathcal{D}^m} \left( L_{\mathcal{D}}(\hat{Q}) < 0.17 \right) > 0.95$
Optimizing PAC-Bayes bounds

Given data $S$, we can find a provably good classifier $Q$ by optimizing the PAC-Bayes bound w.r.t. $Q$.

For Catoni's PAC-Bayes bound, the optimization problem is of the form

$$\sup_Q -\tau L_S(Q) - KL(Q\|P).$$

**Lemma.** Optimal $Q$ satisfies

$$\frac{dQ}{dP}(w) = \frac{\exp(-\tau L_S(w))}{\int \exp(-\tau L_S(w))P(dw)}.$$  

**Observation.** Under log loss and $\tau = m$, the term $-\tau L_S(w)$ is the expected log likelihood under $Q$ and the objective is the ELBO.

**Lemma.** $\log \int \exp(-\tau L_S(w))P(dw) = \sup_Q -\tau L_S(Q) - KL(Q\|P)$.

**Observation.** Under log loss and $\tau = m$, l.h.s. is log marginal likelihood.

PAC-Bayes Bound optimization

\[
\inf_Q \left( \tilde{L}_S(Q) + \text{KL}(Q\|P) + \log \frac{1}{\delta} \right)
\]

Let \( \tilde{L}_S(Q) \geq L_S(Q) \) with \( \tilde{L}_S \) differentiable.

\[
\inf_Q m \tilde{L}_S(Q) + \text{KL}(Q\|P)
\]

Let \( Q_{w,s} = N(w, \text{diag}(s)) \).

\[
\min_w \in \mathbb{R}^d \min_s \in \mathbb{R}^d^+ m \tilde{L}_S(Q_{w,s}) + \text{KL}(Q_{w,s}\|P)
\]

Take \( P = N(w_0, \lambda I) \) with \( \lambda = c \exp\left\{ -\mu / b \right\} \).

\[
\min_w \in \mathbb{R}^d \min_s \in \mathbb{R}^d^+ m \tilde{L}_S(Q_{w,s}) + \text{KL}(Q_{w,s}\|N(w_0, \lambda I))
\]

\[
\leq 2 \log \left( \frac{b}{\lambda} \right) + \frac{1}{2} \left( \frac{1}{\lambda} \|s\|_1 + \frac{1}{\lambda} \|w-w_0\|_2^2 + d \log \frac{1}{\lambda} - \frac{1}{d} \cdot \log s - d \right).
\]
PAC-Bayes Bound optimization

\[
\inf_Q \quad L_S(Q) + \frac{KL(Q||P) + \log \frac{1}{\delta}}{m}
\]
PAC-Bayes Bound optimization

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Let \( \tilde{L}_S(Q) \geq L_S(Q) \) with \( \tilde{L}_S \) differentiable.
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\[ \inf_Q L_S(Q) + \frac{\text{KL}(Q\|P) + \log \frac{1}{\delta}}{m} \]

Let \( \tilde{L}_S(Q) \geq L_S(Q) \) with \( \tilde{L}_S \) differentiable.

\[ \inf_Q m\tilde{L}_S(Q) + \text{KL}(Q\|P) \]
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$$\inf_{Q} L_{S}(Q) + \frac{KL(Q||P) + \log \frac{1}{\delta}}{m}$$

Let $\tilde{L}_{S}(Q) \geq L_{S}(Q)$ with $\tilde{L}_{S}$ differentiable.

$$\inf_{Q} m \tilde{L}_{S}(Q) + KL(Q||P)$$

Let $Q_{w,s} = \mathcal{N}(w, \text{diag}(s))$. 
PAC-Bayes Bound optimization

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Let \( Q_{w,s} = \mathcal{N}(w, \text{diag}(s)) \).

\[
\min_{w \in \mathbb{R}^d, s \in \mathbb{R}_+^d} m \tilde{L}_S(Q_{w,s}) + \text{KL}(Q_{w,s}\|P)
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\[
\min_{w \in \mathbb{R}^d, s \in \mathbb{R}^d_+} m \tilde{L}_S(Q_{w,s}) + \text{KL}(Q_{w,s}\|P)
\]

Take \( P = \mathcal{N}(w_0, \lambda I_d) \) with \( \lambda = c \exp\{-j/b\} \).
PAC-Bayes Bound optimization

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\[
\min_{w \in \mathbb{R}^d, s \in \mathbb{R}^d_+, \lambda \in (0, c)} m \tilde{L}_S(Q_{w,s}) + \text{KL}(Q_{w,s}\|\mathcal{N}(w_0, \lambda I)) + 2 \log(b \log \frac{c}{\lambda})
\]
PAC-Bayes Bound optimization

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\]

\[
\frac{1}{2} \left( \frac{1}{\lambda} \|s\|_1 + \frac{1}{\lambda} \|w - w_0\|_2^2 + d \log \lambda - 1_d \cdot \log s - d \right).
\]
### Numerical generalization bounds on MNIST

<table>
<thead>
<tr>
<th># Hidden Layers</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>1 (R)</th>
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<tbody>
<tr>
<td>Train error</td>
<td>0.001</td>
<td>0.000</td>
<td>0.000</td>
<td>0.007</td>
</tr>
<tr>
<td>Test error</td>
<td>0.018</td>
<td>0.016</td>
<td>0.013</td>
<td>0.508</td>
</tr>
<tr>
<td>SNN train error</td>
<td>0.028</td>
<td>0.028</td>
<td>0.027</td>
<td>0.112</td>
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<tr>
<td>SNN test error</td>
<td>0.034</td>
<td>0.033</td>
<td>0.032</td>
<td>0.503</td>
</tr>
<tr>
<td>PAC-Bayes bound</td>
<td><strong>0.161</strong></td>
<td><strong>0.186</strong></td>
<td><strong>0.201</strong></td>
<td><strong>1.352</strong></td>
</tr>
<tr>
<td>KL divergence</td>
<td>5144</td>
<td>6534</td>
<td>7861</td>
<td>201131</td>
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<tr>
<td># parameters</td>
<td>472k</td>
<td>832k</td>
<td>1193k</td>
<td>472k</td>
</tr>
<tr>
<td>VC dimension</td>
<td>26m</td>
<td>66m</td>
<td>121m</td>
<td>26m</td>
</tr>
</tbody>
</table>

We have shown that type of flat minima found in practice can be turned into a generalization guarantee.

Bounds are loose, but only nonvacuous bounds in this setting.
Actually, SGD is pretty dangerous
Actually, SGD is pretty dangerous

- SGD achieves zero training error reliably
- Despite no explicit regularization, training and test error very close
- Explicit regularization has minor effect
- SGD can reliably obtain zero training error on randomized labels
  - Hence, Rademacher complexity of model class is near maximal w.h.p.

**Understanding Deep Learning Requires Re-Thinking Generalization**

Chiyuan Zhang*
Massachusetts Institute of Technology
chuyuan@mit.edu

Samy Bengio
Google Brain
bengio@google.com

Moritz Hardt
Google Brain
mrtz@google.com

Benjamin Recht†
University of California, Berkeley
brecht@berkeley.edu

Oriol Vinyals
Google DeepMind
vinyals@google.com
Entropy-SGD (Chaudhari et al., 2017)

Entropy-SGD replaces stochastic gradient descent on $L_S$ by stochastic gradient ascent applied to the optimization problem:

$$\arg\max_{w \in \mathbb{R}^d} F_{\gamma, \tau}(w; S),$$

where $F_{\gamma, \tau}(w; S) = \log \int_{\mathbb{R}^p} \exp \left\{ -\tau L_S(w') - \frac{\gamma}{2} ||w' - w||_2^2 \right\} \, dw'$. 

The local entropy $F_{\gamma, \tau}(\cdot; S)$ emphasizes flat minima of $L_S$. 

Dziugaite and Roy
Entroy-SGD optimizes PAC-Bayes bound w.r.t. prior

Entroy-SGD optimizes the local entropy

\[ F_{\gamma, \tau}(w; S) = \log \int_{\mathbb{R}^p} \exp \left\{ -\tau L_S(w') - \tau \frac{\gamma}{2} \|w' - w\|^2 \right\} \, dw'. \]
Entropy-SGD optimizes PAC-Bayes bound w.r.t. prior

Entropy-SGD optimizes the local entropy

\[ F_{\gamma, \tau}(w; S) = \log \int_{\mathbb{R}^p} \exp \left\{ -\tau L_S(w') - \tau \frac{\gamma}{2} \| w' - w \|_2^2 \right\} \, dw'. \]

**Theorem.** Maximizing \( F_{\gamma, \tau}(w; S) \) w.r.t. \( w \) corresponds to minimizing PAC-Bayes risk bound w.r.t. prior’s mean \( w \).
Entropy-SGD optimizes PAC-Bayes bound w.r.t. prior

Entropy-SGD optimizes the local entropy

$$F_{\gamma, \tau}(w; S) = \log \int_{\mathbb{R}^p} \exp \left\{ -\tau L_S(w') - \frac{\gamma}{2} \|w' - w\|^2_2 \right\} \, dw'.$$

**Theorem.** Maximizing $F_{\gamma, \tau}(w; S)$ w.r.t. $w$ corresponds to minimizing PAC-Bayes risk bound w.r.t. prior’s mean $w$.

**Theorem.** Let $\mathbb{P}(S)$ be an $\epsilon$-differentially private distribution. Then

$$\forall D, \mathbb{P}_{S \sim D^m} \left( (\forall Q) \, \text{KL}(L_S(Q) || L_D(Q)) \leq \frac{\text{KL}(Q || \mathbb{P}(S)) + \ln 2m + 2 \max\{\ln \frac{3}{\delta}, m \epsilon^2\}}{m - 1} \right) \geq 1 - \delta.$$

We optimize $F_{\gamma, \tau}(w; S)$ using SGLD, obtaining $(\epsilon, \delta)$-differential privacy.

SGLD is known to converge weakly to the $\epsilon$-differentially private exponential mechanism. Our analysis makes a coarse approximation: privacy of SGLD is that of exponential mechanism.
Conclusion

- We show that the size/flatness/location of minima (that were found by SGD on MNIST) imply generalization using PAC-Bayes bounds;
- We show Entropy-SGD optimizes the prior in a PAC-Bayes bound, which is not valid;
- We give a differentially private version of PAC-Bayes theorem and modify Entropy-SGD so that prior is privately optimized.


