Studying generalization in deep learning via PAC-Bayes

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Joint work with

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- I'll focus on the role of the prior P.

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- Introduce three principles for studying generalization using PAC-Bayes framework.
- Describe their application to computing risk bounds on Q concentrated near w_{SGD}.
- Show how same ideas can be applied to self-bounded learning.

PAC-Bayes yields risk bounds for Gibbs classifiers

Let $\mathcal{H}$ be weight space (which determine classifiers).
Let $\ell : \mathcal{H} \times Z \to [0, 1]$ be our loss function.

Risk and empirical risk

For $h \in \mathcal{H}$,

$$L_{\mathcal{D}}(h) = \mathbb{E}_{z \sim \mathcal{D}}[\ell(h, z)] \qquad \textit{risk}$$

$$L_S(h) = \frac{1}{n} \sum_{i=1}^{n} \ell(h, z_i) \qquad \textit{empirical risk}$$

Gibbs classifier

A *Gibbs classifier* is a probability distribution on $\mathcal{H}$.

The *risk* of a Gibbs classifier Q is defined to be the average risk under $w \sim Q$, i.e.,

$$L_{\mathcal{D}}(Q) = \mathbb{E}_{h \sim Q}[L_{\mathcal{D}}(h)] = \mathbb{E}_{z \sim \mathcal{D}} \mathbb{E}_{h \sim Q}[\ell(h, z)].$$

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Theorem (PAC-Bayes; Catoni 2007)

McAllester 1999, Shawe-Taylor and Williamson 1997

Assume $L_S(\cdot) \in [0, 1]$.

$\mathbb{R}^d$

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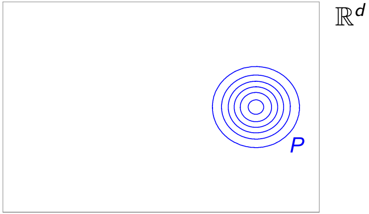

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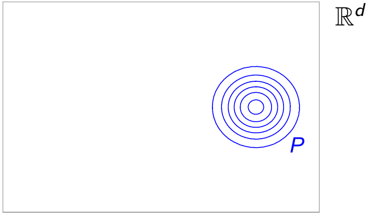
   Now we know the empirical risk surface $L_S(\cdot)$.



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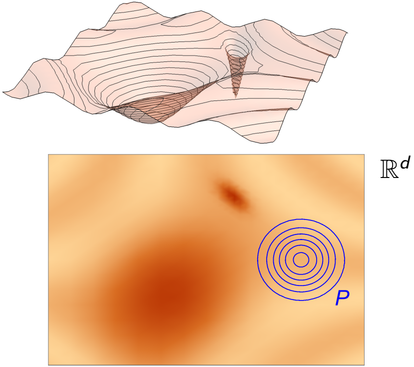

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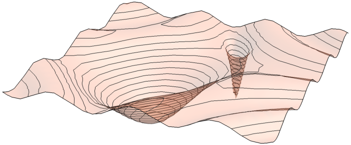
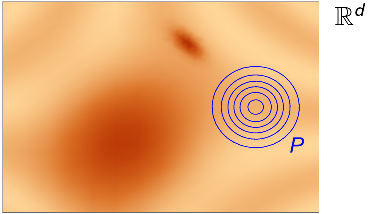
4. Then, with probability at least $(1-\delta)$,

$$\forall Q,\ L_{\mathcal{D}}(Q) \leq L_S(Q) + \sqrt{\frac{\mathrm{KL}(Q||P) + \ln m/\delta}{2m}}.$$





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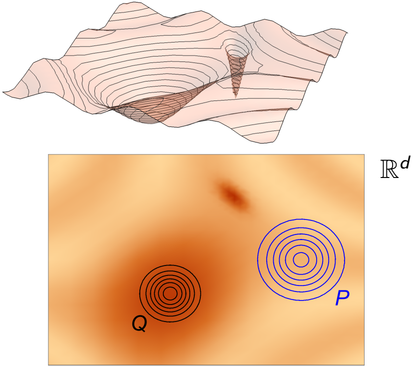

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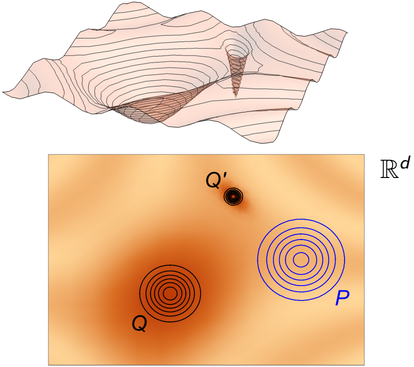

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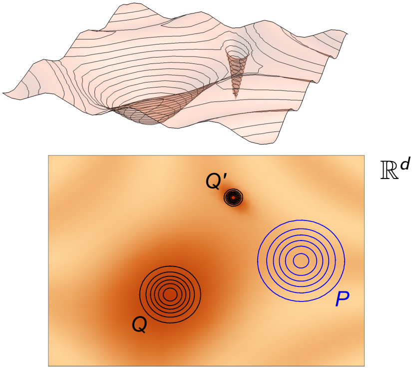
$$\forall Q,\ 2(L_{\mathcal{D}}(Q) - L_S(Q))^2 \le \frac{\mathrm{KL}(Q||P) + \ln m/\delta}{m}.$$



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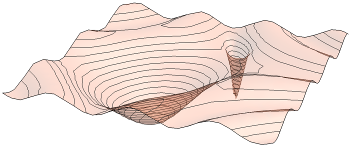

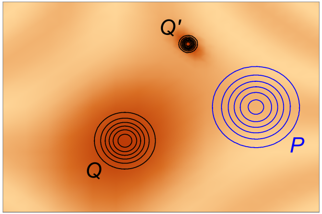

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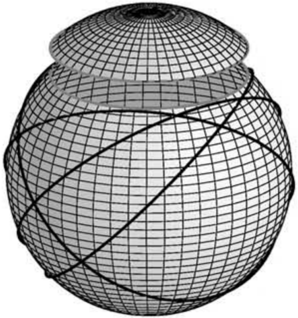

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Theorem (Neyshabur et al. 2019). *Fix margin $\gamma > 0$ and confidence $\delta > 0$. For each $h \in \mathcal{H}$, let $Q(h)$ be a distribution on $\mathcal{H}$ satisfying, with probability $\geq \frac{1}{2}$ over $h' \sim Q(H)$,*

$$\sup_z \|f_h(z) - f_{h'}(z)\|_\infty \leq \frac{\gamma}{4}.$$

Then, with probability at least $(1-\delta)$,

$$\forall h \in \mathcal{H},\ L_{\mathcal{D}}(h) \leq L_\gamma(h) + 4\sqrt{\frac{\mathrm{KL}(Q(h)||P) + \ln \frac{6m}{\delta}}{m+1}}$$

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- **Disintegrated versions of PAC-Bayes**
  Catoni (2007)
- ...
- **PAC-Bayes + Generic Chaining**
  Miyaguchi (2019)

Recap: Towards a nonvacuous bound on SGD

$$\forall Q,\ \Delta\Big(L_S(Q), L_{\mathcal{D}}(Q)\Big) \leq \frac{\mathrm{KL}(Q||P) + \ln \mathcal{I}^{\Delta}(m)/\delta}{m}.$$

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  - **Use all the data + differential privacy**
    (D. and Roy 2018a)

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which yields the following PAC-Bayes bound: with probability $\geq 1-\delta$,

$$\Delta\big(L_S(Q'), L_{\mathcal{D}}(Q')\big) \leq \frac{1}{m}\left(\frac{\gamma}{\sqrt{m}}\sqrt{\ln\frac{4\sqrt{m}}{\delta}} + \frac{\gamma^2}{4m} + \ln\frac{4\sqrt{m}}{\delta}\right)$$

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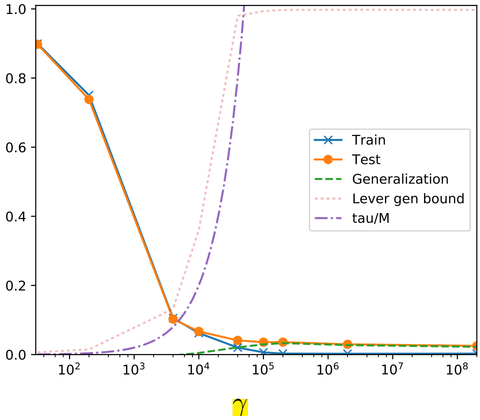

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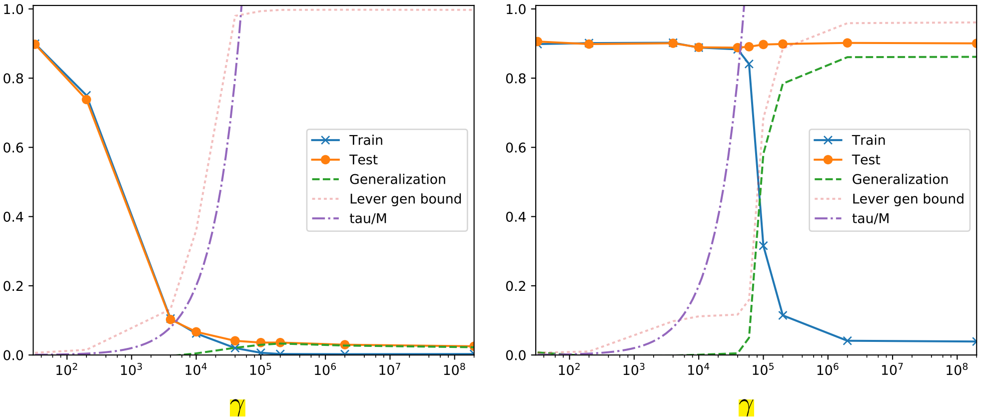

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Theorem (D. and Roy, 2018a). *Let $\mathscr{P}(S)$ be an ϵ-differentially private prior. Then, with probability $\geq 1-\delta$ over an i.i.d. sample S from an unknown distribution,*

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- Challenge: ϵ-differential privacy for $\epsilon \ll 1$ is hard to achieve.

Distribution-dependent approximations of optimal priors via privacy

- Summary: Lever et al. bound vacuous once γ large enough to fit random labels.
- Recall: PAC-Bayes prior P can depend on data distribution $\mathcal{D}$ but not data. But data is our only handle on $\mathcal{D}$.
- Idea: If we use the data S to choose a prior $\mathscr{P}(S)$, but in a way that is *stable* to changes to S, then $\mathscr{P}(S)$ is "almost" independent from S.

Theorem (D. and Roy, 2018a). *Let $\mathscr{P}(S)$ be an ϵ-differentially private prior. Then, with probability $\geq 1-\delta$ over an i.i.d. sample S from an unknown distribution,*

$$(\forall Q)\ \Delta(L_S(Q), L_{\mathcal{D}}(Q)) \leq \frac{\mathrm{KL}(Q||\mathscr{P}(S)) + \ln \frac{4\sqrt{m}}{\delta}}{m} + \epsilon^2/2 + \epsilon\sqrt{\frac{\ln 4/\delta}{2m}}$$

- Challenge: ϵ-differential privacy for $\epsilon \ll 1$ is hard to achieve.
- Solution: We show that being close in Wasserstein to a private mechanism suffices to yield a generalization bound.
- See different approach based on stability by Rivasplata et al. (2018).

A question of interpretation

$$\Delta\Big(L_S(Q(S)), L_{\mathcal{D}}(Q(S))\Big) \leq \frac{\mathrm{KL}(Q(S)||P^*) + \ln \mathcal{I}^{\Delta}(m)/\delta}{m}.$$

- Numerous approaches exist to approximate $P^* = \mathbb{E}[Q(S)]$ analytically, with data, and with privacy/stability.

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Theorem (D., Roy, Hsu, Gharbieh 2019+). *Informally, there's a distribution, loss, and learning algorithm such that a PAC-Bayes bound with oracle prior $P^*(S') = \mathbb{E}[Q(S)]$ is vacuous, but same bound on a subset $S \setminus S'$ with data-dependent oracle prior $P^*(S') = \mathbb{E}[Q(S)|S']$ is nonvacuous.*

Recap: Towards a nonvacuous bound on SGD

$$\Delta\Big(L_{S\setminus S'}(Q(S)), L_{\mathcal{D}}(Q(S))\Big) \leq \frac{\mathrm{KL}(Q(S)||P^*(S')) + \ln \mathcal{I}^{\Delta}(|S \setminus S'|)/\delta}{|S \setminus S'|}.$$

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How might we approximate $P^*(S') = \mathbb{E}[Q(S)|S']$?

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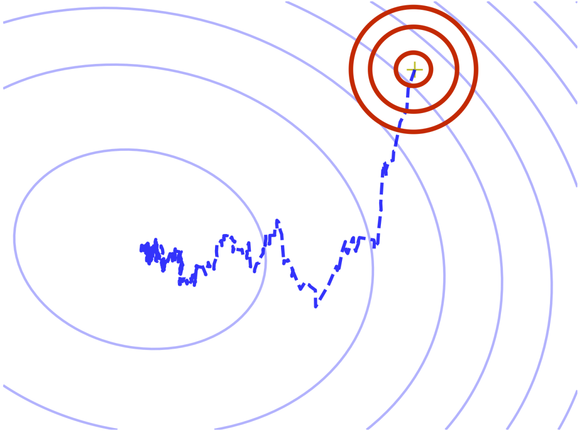
- We will approximate $\bar{w}(S', U)$ by running SGD *on the subset* S' to convergence. By design, SGD on S' will match the initial behavior of SGD on S.

Example: SGD on S' predicting SGD on S



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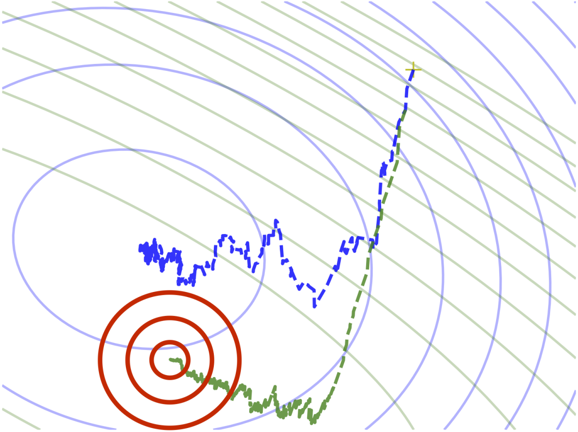

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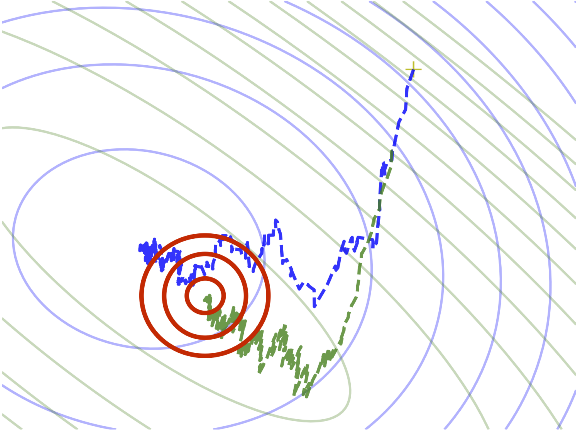

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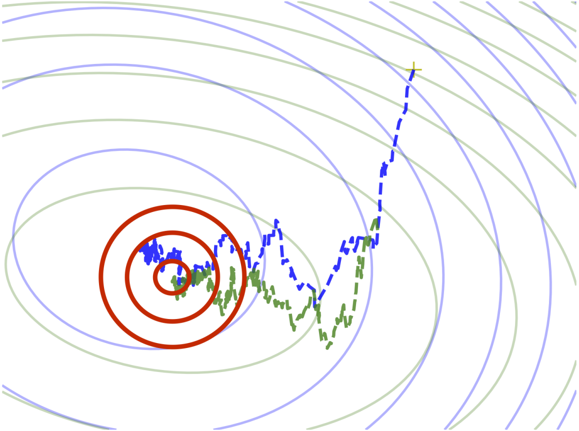
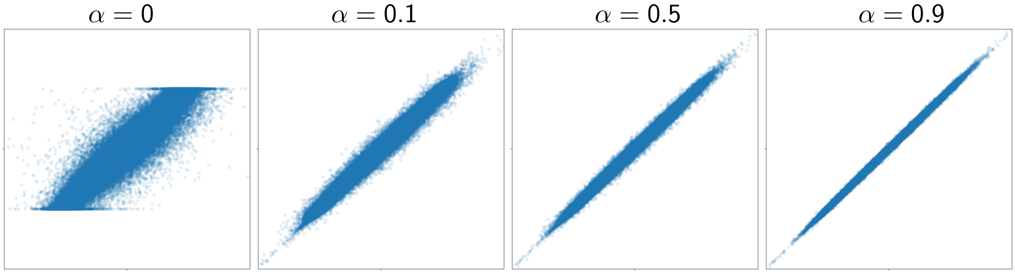
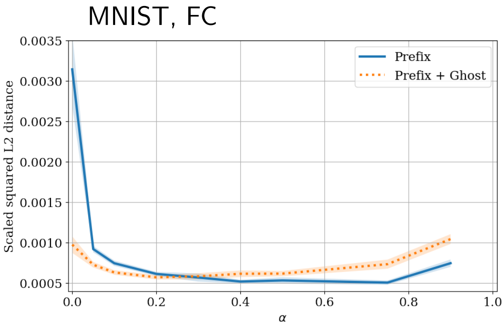


How well are we predicting the weights learned by SGD?

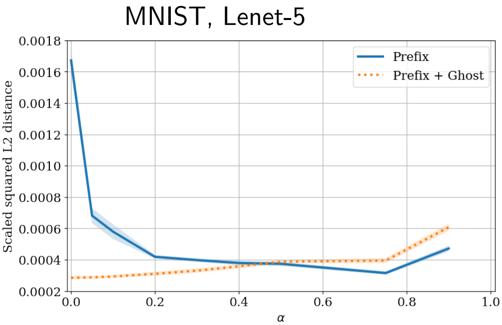


MNIST, FC (2 hidden layers).

Data-dependent oracle priors for neural networks



$\alpha = |S'|/|S|$



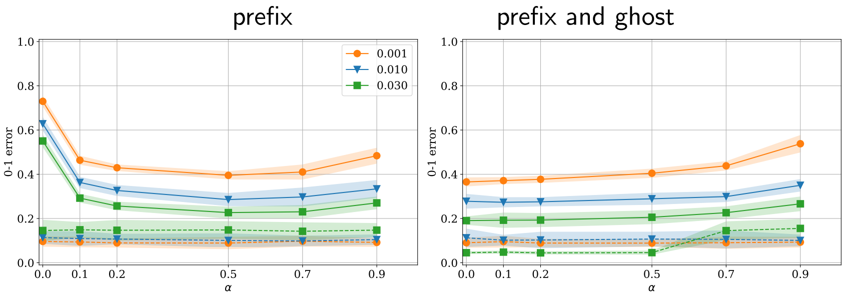
$\alpha = |S'|/|S|$

Scaled squared L2 $= \frac{\|w_{\mathrm{SGD}} - \bar{w}\|_2^2}{(1-\alpha)|S|}$.

Similar results found for networks trained on Fashion-MNIST and CIFAR10 datasets.

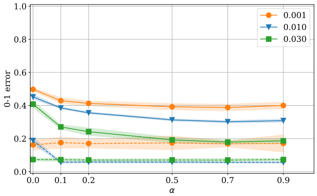
Coupled data-dependent approximate oracle priors and posteriors

Gaussian Lenet5 networks with **means equal to SGD trained on 30k examples from MNIST**.

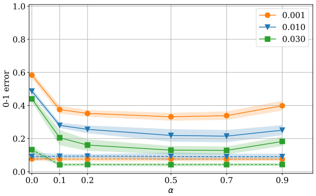


Gaussian network bounds for Coupled data-dependent priors

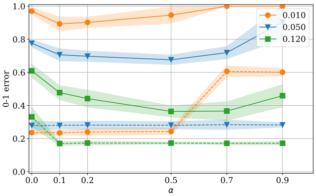
MNIST, FC;



MNIST, LeNet-5;



Fashion-MNIST, LeNet-5;



Test error and PAC-Bayes generalization bounds with isotropic prior covariance. The best test error bound on MNIST, Lenet5 (approximately 11%) is significantly better than the 46% bound by Zhou et al., 2018.

Oracle access to optimal prior covariance

For a Gaussian prior P_Λ with diagonal covariance $\Lambda = \mathrm{diag}(\lambda_i)$, the KL term is

$$\mathrm{KL}(Q(S)||P_\Lambda(S')) = \frac{1}{2}(w_{\mathsf{SGD}} - \bar{w})'\Lambda(w_{\mathsf{SGD}} - \bar{w}) + \frac{1}{2}\sum_i \Psi(\lambda_i, s_i)$$

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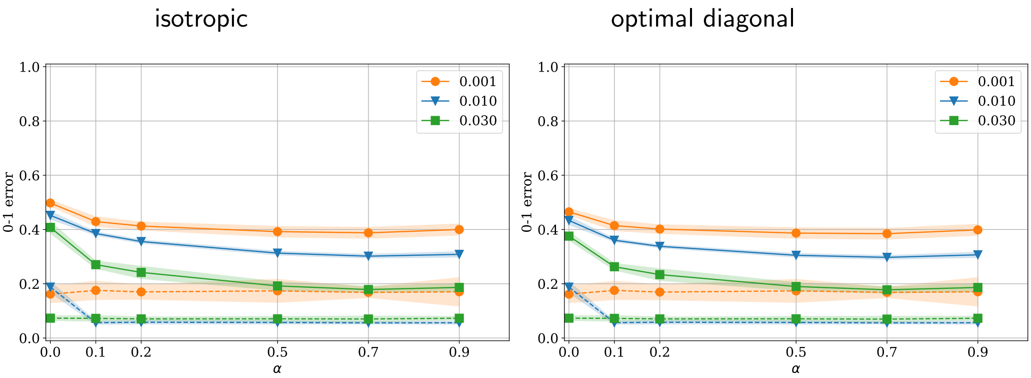
- This bound represents the best we could hope to achieve and allows us to test limits of proposed mean prediction $\bar{w}(S', U)$.

Gaussian network bounds with oracle data-dependent prior covariance

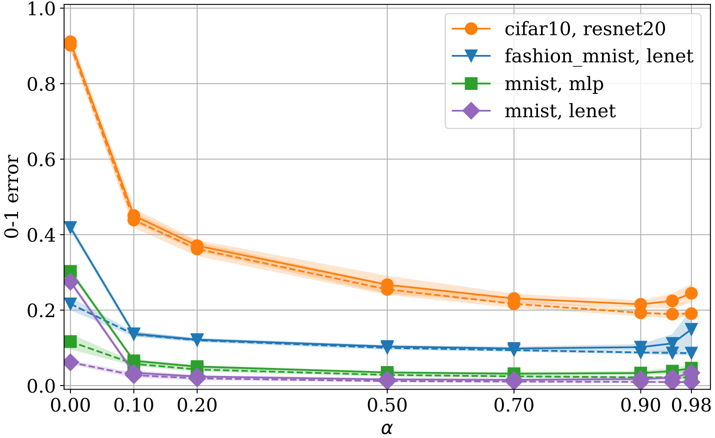
MNIST, Lenet-5.



The bounds are hypothetical.

Directly optimizing Variational data-dependent PAC-Bayes generalization bound.

Apply these same ideas (data-dependency and coupling) to self-bounded learning.



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- We're still far from studying SGD itself: Stochastic neural networks in our studies were severely underfit due to looseness of the KL term during PAC-Bayes optimization. Need to understand the pareto-optimal frontier.
- Study of Gibbs classifiers "concentrated" near SGD weights may be a fruitful (suggestive) test bed for generalization ideas.