On the Generalization of Models Trained with SGD: Information-Theoretic Bounds and Implications

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Motivation

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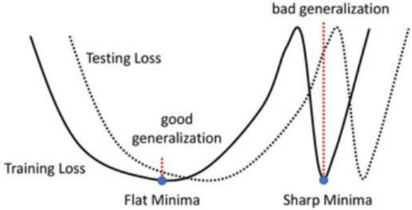
- Algorithm & Distribution-dependent $\Longrightarrow$ non-vacuous generalization bound

- Does the flatness have impact on the generalization?



Our work follows up on a recent work of

Gergely Neu, Gintare Karolina Dziugaite, Mahdi Haghifam, and Daniel M Roy. Information theoretic generalization bounds for stochastic gradient descent. In COLT, 2021

Problem Setup

- Training dataset: $S = \{Z_i\}_{i=1}^n \in \mathcal{Z}$, drawn i.i.d. from μ
- Hypothesis space: $\mathcal{W} \subseteq \mathbb{R}^d$
- Learning algorithm: $\mathcal{A} : \mathcal{Z}^n \to \mathcal{W}$ by $P_{W|S}$
- Loss: $\ell : \mathcal{W} \times \mathcal{Z} \to \mathbb{R}^+$
- We're interested in
  - Population risk: $L_\mu(w) \triangleq \mathbb{E}_{Z\sim\mu}[\ell(w,Z)]$
  - Empirical risk: $L_S(w) \triangleq \frac{1}{n}\sum_{i=1}^n \ell(w,Z_i)$
  - Expected generalization error: $\mathrm{gen}(\mu, P_{W|S}) \triangleq \mathbb{E}_{W,S}[L_\mu(W) - L_S(W)]$

Lemma 1 (Thm 1., Xu&Raginsky'2017)

Assume the loss $\ell(w, Z)$ is R-subgaussian[a] for any $w \in \mathcal{W}$. The generalization error of $\mathcal{A}$ is bounded by

$$|\mathrm{gen}(\mu, P_{W|S})| \le \sqrt{\frac{2R^2}{n} I(W;S)},$$

[a] A random variable X is R-subgaussian if for any ρ, $\log \mathbb{E} \exp\left(\rho\left(X - \mathbb{E}X\right)\right) \le \rho^2 R^2/2$.

Mutual information $I(W;S) \triangleq \mathrm{D_{KL}}(P_{W,S} || P_W \otimes P_S)$.

$\Longrightarrow$ Distribution-dependent and Algorithm-dependent

Stochastic Gradient Descent (SGD)

SGD updates:

$$W_t \triangleq W_{t-1} - \lambda_t g(W_{t-1}, B_t),$$

where

$$g(w, B_t) \triangleq \frac{1}{b} \sum_{z \in B_t} \nabla_w \ell(w, z),$$

- λ_t: learning rate
- b: batch size
- B_t denotes the batch used for the t^{th} update.

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Difficulty of using Xu's bound: $I(W_T; S) \to \infty$ in some cases

Auxiliary Weight Process (only exists in the analysis)

Let $\sigma_1, \sigma_2, \ldots, \sigma_T$ be a sequence of positive real numbers.

Define

$$\widetilde{W}_0 \triangleq W_0, \quad \text{and} \ \ \widetilde{W}_t \triangleq \widetilde{W}_{t-1} - \lambda_t g(W_{t-1}, B_t) + N_t, \ \text{for } t > 0,$$

where $N_t \sim \mathcal{N}(0, \sigma_t^2 \mathbf{I}_d)$ is a Gaussian noise.

$$\begin{array}{ccccccccccc} & & N_1 & & N_2 & & \cdots & & N_{T-1} & & N_T \\ & & \downarrow & & \downarrow & & & & \downarrow & & \downarrow \\ \widetilde{W}_0 & \to & \widetilde{W}_1 & \to & \widetilde{W}_2 & \to & \cdots & \to & \widetilde{W}_{T-1} & \to & \widetilde{W}_T \\ \| & \nearrow & & \nearrow & & \nearrow & & & & \nearrow & \\ W_0 & \to & W_1 & \to & W_2 & \to & \cdots & \to & W_{T-1} & \to & W_T \end{array}$$

Let $\Delta_t = \sum_{\tau=1}^{t} N_\tau$. Notice that $\widetilde{W}_t = W_t + \Delta_t$.

Xu's bound (Lemma 1) for noisy, iterative algorithm

- Learning algorithm $\widetilde{A}$ takes S as input and outputs $\widetilde{W}$
- Decomposition of the expected generalization gap:

$$
\begin{aligned}
&|\mathrm{gen}(\mu, P_{W_T|S})| \\
=& |\mathbb{E}_{W,S}[L_\mu(W_T) - L_S(W_T)]| \\
=& \left|\mathbb{E}_{W,S,\Delta}[L_\mu(W_T) - L_S(W_T) + L_\mu(\widetilde{W}_T) - L_S(\widetilde{W}_T) - L_\mu(\widetilde{W}_T) + L_S(\widetilde{W}_T)]\right| \\
=& \left|\mathrm{gen}(\mu, P_{\widetilde{W}_T|S}) + \mathop{\mathbb{E}}_{W_T,\Delta_T}\left[L_\mu(W_T) - L_\mu(\widetilde{W}_T)\right] + \mathop{\mathbb{E}}_{W_T,\Delta_T,S}\left[L_S(\widetilde{W}_T) - L_S(W_T)\right]\right|.
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\end{aligned}
$$

$$\Longrightarrow |\mathrm{gen}(\mu, P_{\widetilde{W}_T|S})| \leq \sqrt{\frac{2R^2}{n} I(\widetilde{W}_T; S)} < \infty$$

Information-theoretic bound for SGD

Lemma 2 (Thm.1, Neu et al'2021)

The generalization error of SGD is upper bounded by

$$|\mathrm{gen}(\mu, P_{W_T|S})| \leq \sqrt{\frac{4R^2}{n}\sum_{t=1}^{T}\frac{\lambda_t^2}{\sigma_t^2}\mathbb{E}\left[\Psi(W_{t-1}) + \widetilde{\mathbb{V}}_t(W_{t-1})\right]} + |\mathbb{E}\left[\gamma(W_T, S) - \gamma(W_T, S')\right]|$$

where

- Local gradient sensitivity:
  $\Psi(w_{t-1}) \triangleq \mathbb{E}\left[||\nabla_w \ell(w_{t-1}, Z) - \nabla_w \ell(w_{t-1} + \zeta, Z)||_2^2\right]$, $\zeta \sim \mathcal{N}(0, 2\sum_{i=1}^{t-1}\sigma_i^2 \mathrm{I}_d)$
- Gradient Dispersion/Variance: $\widetilde{\mathbb{V}}_t(w) \triangleq \mathbb{E}\left[||g(w, B_t) - \mathbb{E}\left[\nabla_w \ell(w, Z)\right]||_2^2\right]$
- Local value sensitivity: $\gamma(w, s) \triangleq \mathbb{E}\left[L_s(w + \Delta_T) - L_s(w)\right]$

Our main result

Let $\mathbb{V}_t(w) \triangleq \mathbb{E}\left[||g(w,B_t) - \mathbb{E}\left[\nabla_w \ell(W,Z)\right]||_2^2\right]$.

Theorem 1

The generalization error of SGD is upper bounded by

$$|\mathrm{gen}(\mu, P_{W_T|S})| \leq \sqrt{\frac{R^2}{n}\sum_{t=1}^{T}\frac{\lambda_t^2}{\sigma_t^2}\mathbb{E}\left[\mathbb{V}_t(W_{t-1})\right]} + \left|\mathbb{E}\left[\gamma(W_T,S) - \gamma(W_T,S')\right]\right|. \quad (1)$$

Assume $L_\mu(w_T) \leq \mathbb{E}_\Delta\left[L_\mu(w_T + \Delta_T)\right]$ *and* σ_t^2 *is independent of* t. *Denote by* H_{W_T} *the Hessian of the loss with respect to* W_T *and let* $\mathrm{Tr}(\cdot)$ *denote trace. Then*

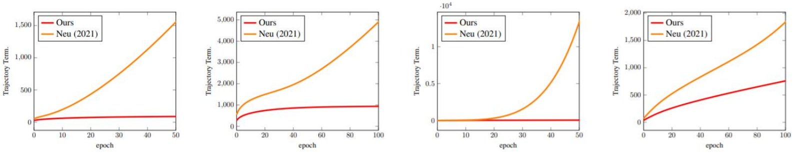
$$\mathrm{gen}(\mu, P_{W_T|S}) \leq \frac{3}{2}\left(\sum_{t=1}^{T}\frac{R^2\lambda_t^2 T}{n}\mathbb{E}\left[\mathbb{V}_t(W_{t-1})\right]\mathbb{E}\left[\mathrm{Tr}\left(\mathrm{H}_{W_T}(Z)\right)\right]\right)^{\frac{1}{3}} \quad (2)$$

$$|\mathrm{gen}(\mu, P_{W_T|S})| \leq \sqrt{\frac{R^2}{n}\sum_{t=1}^{T}\frac{\lambda_t^2}{\sigma_t^2}\mathbb{E}\left[\mathbb{V}_t(W_{t-1})\right]} + \left|\mathbb{E}\left[\gamma(W_T, S) - \gamma(W_T, S')\right]\right|.$$

- The first term: “trajectory term”; The second term: “flatness term”

$$|\text{gen}(\mu, P_{W_T|S})| \leq \sqrt{\frac{R^2}{n}\sum_{t=1}^{T}\frac{\lambda_t^2}{\sigma_t^2}\mathbb{E}\left[\mathbb{V}_t(W_{t-1})\right] + \left|\mathbb{E}\left[\gamma(W_T,S) - \gamma(W_T,S')\right]\right|}.$$

- The first term: “trajectory term”; The second term: “flatness term”
- Our bound improves the bound in Lemma 2:



(a) $\sigma = 10^{-5}$ (MNIST) (b) $\sigma = 10^{-6}$ (MNIST) (c) $\sigma = 10^{-5}$ (CIFAR10) (d) $\sigma = 10^{-6}$ (CIFAR10)

This improvement should come at no surprise, since $\Psi(W_{t-1})$ has the cumulative variance $2\sum_{i=1}^{t-1}\sigma_i^2 \mathrm{I}_d$

$$\text{gen}(\mu, P_{W_T|S}) \leq \frac{3}{2}\left(\sum_{t=1}^{T}\frac{R^2\lambda_t^2 T}{n}\mathbb{E}\left[\mathbb{V}_t(W_{t-1})\right]\mathbb{E}\left[\text{Tr}\left(\text{H}_{W_T}(Z)\right)\right]\right)^{\frac{1}{3}}$$

- Condition $L_\mu(w_T) \leq \mathbb{E}_{\Delta_T}\left[L_\mu(w_T + \Delta_T)\right] \Longrightarrow$ the perturbation does not decrease the population risk.
  Also assumed in [Foret, et al.'2021] in the derivation of a PAC-Bayesian bound.

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  Also assumed in [Foret, et al.'2021] in the derivation of a PAC-Bayesian bound.
- Eq.2 follows from Eq.1 by minimizing the bound over σ.
  Eq.2 can be computed easily and efficiently.

Application: Linear Networks

Regression setting:

- $Z = (X, Y)$
- $X \in \mathbb{R}^{d_0}$; Assume $||X|| = 1$
- Model $f(W, \cdot) : \mathbb{R}^{d_0} \to \mathbb{R}$
- $\ell(W, Z) = 1/2(Y - f(W, X))^2$

Theorem 2 (Linear Networks)

Let $f(W, X) = W^T X$. Then,

$$\mathrm{gen}(\mu, P_{W_T|S}) \leq 3 \left(\sum_{t=1}^{T} \frac{R^2 \lambda_t^2 T}{4n} \mathbb{E}\left[\ell(W_{t-1}, Z)\right] \right)^{\frac{1}{3}}.$$

Application: Two-Layer ReLU Networks

Theorem 3 (Two-Layer ReLU Networks)

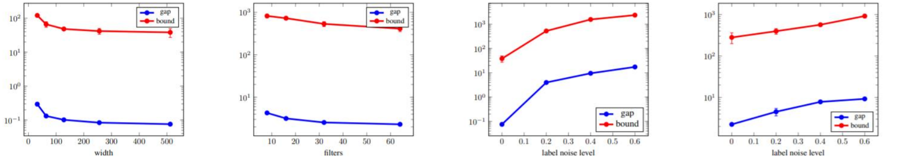
Following [Arora et al'2019], consider $f(W,X) = \frac{1}{\sqrt{m}}\sum_{r=1}^{m} A_r \mathrm{ReLU}(W_r^T X)$ *where* $A_r \sim \mathrm{unif}(\{+1,-1\})$. *We fix the second layer parameters during training. Then,*

$$\mathrm{gen}(\mu, P_{W_T|S}) \leq 3\left(\sum_{r=1}^{m}\mathbb{E}\left[\frac{\mathbb{I}_{r,i,T}}{m}\right]\sum_{t=1}^{T}\frac{R^2\lambda_t^2 T}{4n}\mathbb{E}\left[\sum_{r=1}^{m}\frac{\mathbb{I}_{r,i,t}}{m}\ell(W_{t-1},Z)\right]\right)^{\frac{1}{3}},$$

where $\mathbb{I}_{r,i,t} = \mathbb{I}\{W_{t-1,r}^T X_i \geq 0\}$ *and* $\mathbb{I}$ *is the indicator function.*

$\Longrightarrow$ Sparsely activated ReLU networks are expected to generalize better.

Experiment: Bound Verification of Thm 1



(a) MLP on MNIST (b) AlexNet on CIFAR10 (c) MLP on MNIST (d) AlexNet on CIFAR10

Figure 1: Estimated bound and empirical generalization gap ("gap") as functions of network width ((a) and (b)) and label noise level ((c) and (d)). Y-axis is in log scale.

Experiment: Epoch-wise Double Descent of Gradient Dispersion

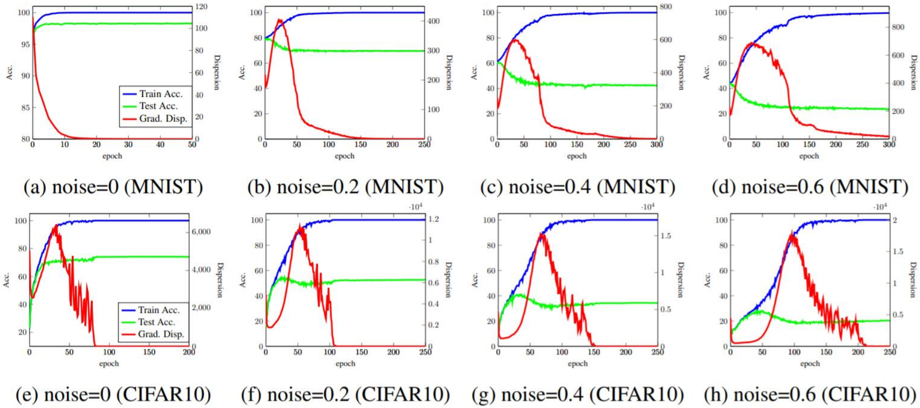
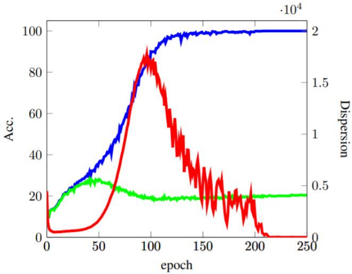


Figure 2: Dynamics of gradient dispersion, in relation to training/testing accuracy.

Three Learning Phases



- $\mathbb{V}$ rapidly descends; Both training acc. and test acc. increase; $\Longrightarrow$ "Generalization"
- $\mathbb{V}$ starts increasing until it reaches a peak value; Training acc. and testing acc. gradually diverge; $\Longrightarrow$ "Memorization"
- $\mathbb{V}$ descends again; Training and testing curves reach their respective maximum and minimum.

Implication: Dynamic Gradient Clipping

Algorithm 1 Dynamic Gradient Clipping

Require: Training set S, Batch size b, Loss function ℓ, Initial model parameter $\boldsymbol{w}_0$, Learning rate λ, Initial minimum gradient norm $\mathcal{G}$, Number of iterations T, Clipping parameter α, Clipping step T_c

for $t \leftarrow 1$ to T **do**
    Sample $\mathcal{B} = \{\boldsymbol{z}_i\}_{i=1}^{b}$ from training set S
    Compute gradient:
    $g_{\mathcal{B}} \leftarrow \sum_{i=1}^{b} \nabla_{\boldsymbol{w}} \ell(\boldsymbol{w}_{t-1}, \boldsymbol{z}_i)/b$
    if $t > T_c$ **then**
        if $||g_{\mathcal{B}}||_2 > \mathcal{G}$ **then**
            $g_{\mathcal{B}} \leftarrow \alpha \cdot \mathcal{G} \cdot g_{\mathcal{B}}/||g_{\mathcal{B}}||_2$
        else
            $\mathcal{G} \leftarrow ||g_{\mathcal{B}}||_2$
        end if
    end if
    Update parameter: $\boldsymbol{w}_t \leftarrow \boldsymbol{w}_{t-1} - \lambda \cdot g_{\mathcal{B}}$
end for

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    end if
  end if
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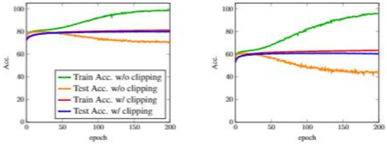
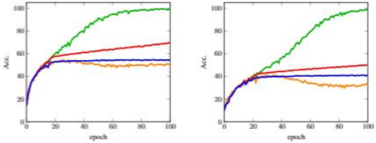


(a) noise=0.2 (MNIST) (b) noise=0.4 (MNIST)



(c) noise=0.2 (CIFAR10) (d) noise=0.4 (CIFAR10)

Implication: Gaussian Model Perturbation (GMP)

▷ We hope the empirical risk surface at w^* is flat, or insensitive to a small perturbation of w^*.

$$\min_w L_s(w) + \rho \mathop{\mathbb{E}}_{\Delta \sim \mathcal{N}(0,\sigma^2 \mathbf{I}_d)} [L_s(w+\Delta) - L_s(w)],$$

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  where ρ is a hyper-parameter.

- Replacing the expectation above with its stochastic approximation using k realizations of Δ gives rise to the following optimization problem.

$$\min_w \frac{1}{b} \sum_{z \in B} \left((1-\rho)\ell(w,z) + \rho \frac{1}{k} \sum_{i=1}^{k} (\ell(w+\delta_i, z)) \right).$$

Implication: GMP

Algorithm 2 Gaussian Model Perturbation Training

Require: Training set S, Batch size b, Loss function ℓ, Initial model parameter $\boldsymbol{w}_0$, Learning rate λ, Number of noise k, Standard deviation of Gaussian distribution σ, Lagrange multiplier ρ

while $\boldsymbol{w}_t$ not converged **do**

  Update iteration: $t \leftarrow t + 1$

  Sample $\mathcal{B} = \{\boldsymbol{z}_i\}_{i=1}^{b}$ from training set S

  Sample $\Delta_j \sim \mathcal{N}(0, \sigma^2)$ for $j \in [k]$

  Compute gradient:

  $g_{\mathcal{B}} \leftarrow \sum_{i=1}^{b} \left(\nabla_{\boldsymbol{w}} \ell(\boldsymbol{w}_t, z_i) + \rho \sum_{j=1}^{k} \left(\nabla_{\boldsymbol{w}} \ell(\boldsymbol{w}_t + \Delta_j, z_i) - \nabla_{\boldsymbol{w}} \ell(\boldsymbol{w}_t, z_i) \right) / k \right) / b$

  Update parameter: $\boldsymbol{w}_{t+1} \leftarrow \boldsymbol{w}_t - \lambda \cdot g_{\mathcal{B}}$

end while

- ▷ Empirical evidence shows that a small k (e.g., $k = 3$) already gives competitive performance.
- ▷ Implementing the $k + 1$ forward passes on parallel processors further reduces the computation load.

Implication: GMP on VGG16

Method	SVHN	CIFAR-10	CIFAR-100
ERM	96.86±0.060	93.68±0.193	72.16±0.297
Dropout	97.04±0.049	93.78±0.147	72.28±0.337
L. S.	96.93±0.070	93.71±0.158	72.51±0.179
Flooding	96.85±0.085	93.74±0.145	72.07±0.271
MixUp	96.91±0.057	**94.52±0.112**	73.19±0.254
Adv. Tr.	97.06±0.091	93.51±0.130	70.88±0.145
AMP[1]	**97.27±0.015**	94.35±0.147	74.40±0.168
GMP^{3}	<u>97.18±0.057</u>	94.33±0.094	<u>74.45±0.256</u>
GMP^{10}	97.09±0.068	<u>94.45±0.158</u>	**75.09±0.285**

Table 1: Top-1 classification accuracy acc.(%) of VGG16. We run experiments 10 times and report the mean and the standard deviation of the testing accuracy. Superscript denotes the number of sampled Gaussian noises during training.

[1] $\min_w L_s(w) + \rho \max_\delta L_s(w+\delta) - L_s(w)$

Implication: GMP on PreActResNet18

Method	SVHN	CIFAR-10	CIFAR-100
ERM	97.05±0.063	94.98±0.212	75.69±0.303
Dropout	97.20±0.065	95.14±0.148	75.52±0.351
L.S.	97.22±0.087	95.15±0.115	77.93±0.256
Flooding	97.16±0.047	95.03±0.082	75.50±0.234
MixUp	97.26±0.044	95.91±0.117	78.22±0.210
Adv. Tr.	97.23±0.080	95.01±0.085	74.77±0.229
AMP	**97.70±0.025**	**96.03±0.091**	**78.49±0.308**
GMP^3	97.43±0.037	95.64±0.053	78.05±0.208
GMP^{10}	97.34±0.058	95.71±0.073	78.07±0.170

Table 2: Top-1 classification accuracy acc.(%) of PreActResNet18.

Proof Sketch of Theorem 1 I

Recall that

$$|\mathrm{gen}(\mu, P_{W_T|S})| \leq \sqrt{\frac{2R^2}{n} I(\widetilde{W}_T; S)} + \left| \mathop{\mathbb{E}}_{W_T,S,S'} \left[\gamma(W_T, S) - \gamma(W_T, S')\right] \right|.$$

Notice that

$$\begin{aligned}
I(\widetilde{W}_T; S) =& I\left(\widetilde{W}_{T-1} - \lambda_T g(W_{T-1}, B_T) + N_T; S\right) \\
\leq& I\left(\widetilde{W}_{T-1}, -\lambda_T g(W_{T-1}, B_T) + N_T; S\right) && (3) \\
=& I(\widetilde{W}_{T-1}; S) + I\left(-\lambda_T g(W_{T-1}, B_T) + N_T; S|\widetilde{W}_{T-1}\right) && (4) \\
&\vdots \\
\leq& \sum_{t=1}^{T} I\left(-\lambda_t g(W_{t-1}, B_t) + N_t; S|\widetilde{W}_{t-1}\right), && (5)
\end{aligned}$$

Proof Sketch of Theorem 1 II

Lemma 3

Let X,Y and Δ be random variables which are all independent of $N \sim \mathcal{N}(0, \mathrm{I})$. Let $Z = Y + \Delta$, then for any σ and any function f, we have

$$I(f(Z,X) + \sigma N; X|Y) \leq \frac{1}{2\sigma^2}\mathbb{E}\left[||f(Z,X) - \mathbb{E}\left[f(Z,X)\right]||^2\right]$$

Thus,

$$\begin{aligned} I(-\lambda_t g(W_{t-1}, B_t) + \sigma_t N; S|\widetilde{W}_{t-1}) \leq & \frac{\lambda_t^2}{2\sigma_t^2}\mathbb{E}\left[||g(W_{t-1}, B_t) - \mathbb{E}\left[\nabla_w \ell(W_{t-1}, Z)\right]||^2\right] \\ = & \frac{\lambda_t^2}{2\sigma_t^2}\mathbb{E}\left[\mathbb{V}_t(W_{t-1})\right] \end{aligned}$$

Putting everything together we have the bound in Theorem 1.

Summary

- We derive tighter information-theoretic bounds for SGD
- Apply the bound to linear networks and two-layer ReLU networks
- Epoch-wise double descent of gradient dispersion is observed
- Design new regularization schemes, e.g., dynamic gradient clipping and GMP.

Thanks for listening!