Over-Training with Mixup May Hurt Generalization

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Three-Sentence Summary

- **Novel Observation**
  - Over-training with Mixup causes U-shaped test error curve.
- **Explanation**
  - Mixup induces label noise.
  - Overfitting to noise occcurs in over-training.

Background on Mixup

C-class classification setting

- Input space: $\mathcal{X} \subseteq \mathbb{R}^{d_0}$; Label space: $\mathcal{Y} = \{1, 2, \ldots, C\}$.
- Training set: $S = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$, where each $\mathbf{y}_i$ may be a one-hot vector.
- Predictor: $f_\theta : \mathcal{X} \to [0, 1]^C$; Loss: $\ell(\theta, \mathbf{x}, \mathbf{y})$;
  Empirical risk: $\hat{R}_S(\theta) := \frac{1}{n} \sum_{i=1}^n \ell(\theta, \mathbf{x}_i, \mathbf{y}_i)$.

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- Mixup synthetic dataset:

$$\widetilde{S}_\lambda := \{(\lambda\mathbf{x} + (1-\lambda)\mathbf{x}', \lambda\mathbf{y} + (1-\lambda)\mathbf{y}') : (\mathbf{x}, \mathbf{y}) \in S, (\mathbf{x}', \mathbf{y}') \in S\},$$

  where $\lambda \in [0, 1]$ is drawn from some prescribed distribution, independently across for all example pairs.
- "Mixup loss", is then

$$\mathbb{E}_\lambda \hat{R}_{\widetilde{S}_\lambda}(\theta) := \mathbb{E}_\lambda \frac{1}{|\widetilde{S}_\lambda|} \sum_{(\tilde{\mathbf{x}}, \tilde{\mathbf{y}}) \in \widetilde{S}_\lambda} \ell(\theta, \tilde{\mathbf{x}}, \tilde{\mathbf{y}})$$

Lower Bound on Mixup Loss

Lemma 1

Let $\ell(\cdot)$ be the cross-entropy loss, and $\{\lambda\}$ is drawn i.i.d. from $\mathrm{Beta}(1,1)$ (or the uniform distribution on $[0,1]$). Then for all $\theta \in \Theta$ and for any given training set S that is balanced,

$$\mathbb{E}_{\lambda} \hat{R}_{\widetilde{S}_{\lambda}}(\theta) \geq \frac{C-1}{2C},$$

where the equality holds iff $f_{\theta}(\tilde{\boldsymbol{x}}) = \tilde{\boldsymbol{y}}$ for each synthetic example $(\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}) \in \widetilde{S}_{\lambda}$.

For example, for 10-class classification tasks, the lower bound has value 0.45.

Observations: As the training loss continuously decays (left), the testing error first decreases then increases (right).

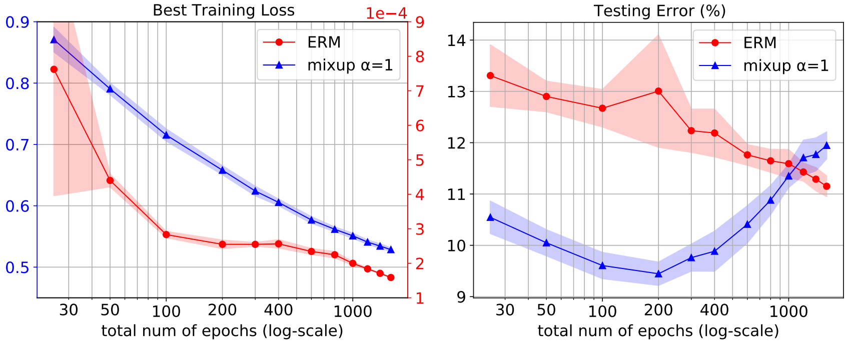

Figure 1: ResNet18 on CIFAR10

Observations

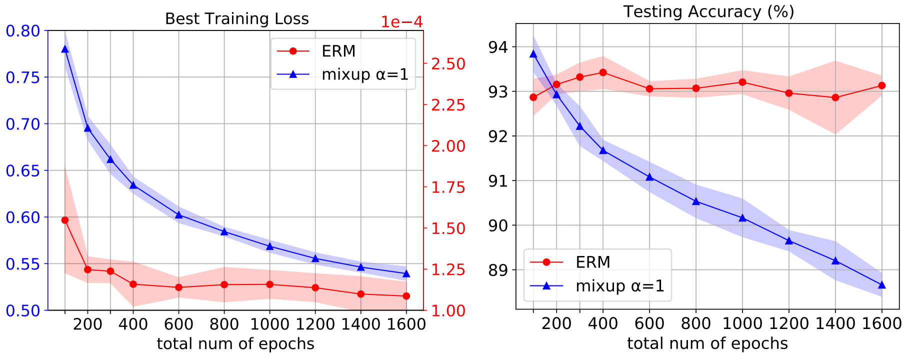

Figure 2: ResNet18 on SVHN (30%)

Observations

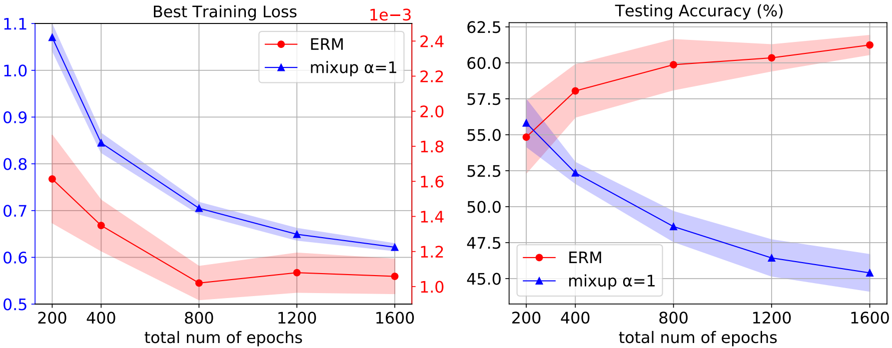

Figure 3: ResNet34 on CIFAR100

Also holds in

- ▷ different architecture, e.g., VGG16, ResNet34;
- ▷ different loss function, e.g., MSE;
- ▷ using other data augmentation (with reduced sample-size), e.g., “random crop” and “horizontal flip”;
- ▷ covariant shift, e.g., CIFAR10.1, CIFAR10.2.

Mixup Induces Label Noise

- Let $P(Y|X)$ be the ground-truth conditional distribution. Let $f : \mathcal{X} \to [0,1]^C$, where $f_j(\mathbf{x}) \triangleq P(Y = j|X = \mathbf{x})$.
  e.g., $\mathbf{y} = \arg\max_{j\in\mathcal{Y}} f_j(\mathbf{x})$.
- Let $\widetilde{X} \triangleq \lambda X + (1-\lambda)X'$. There are two ways to assign a label to $\widetilde{X}$
  - Ground-truth: $\widetilde{Y}_{\mathrm{h}}^* \triangleq \arg\max_{j\in\mathcal{Y}} f_j(\widetilde{X})$
  - Mixup: $\widetilde{Y}_{\mathrm{h}} \triangleq \arg\max_{j\in\mathcal{Y}} P(\widetilde{Y} = j|\widetilde{X})$
    where $P(\widetilde{Y} = j|\widetilde{X}) = \lambda f_j(X) + (1-\lambda) f_j(X')$ for each j.
- When the two assignments disagree, $\widetilde{Y}_{\mathrm{h}} \neq \widetilde{Y}_{\mathrm{h}}^*$, then Mixup-assigned label $\widetilde{Y}_{\mathrm{h}}$ is noisy.

Mixup Induces Label Noise

Theorem 1

For any fixed X, X' and $\widetilde{X}$ related by $\widetilde{X} = \lambda X + (1-\lambda)X'$ for a fixed $\lambda \in [0,1]$, the probability of assigning a noisy label is lower bounded by

$$\begin{aligned} P(\widetilde{Y}_{\mathrm{h}} \neq \widetilde{Y}^*_{\mathrm{h}} | \widetilde{X}) \geq & \mathrm{TV}(P(\widetilde{Y}|\widetilde{X}), P(Y|X)) \\ \geq & \frac{1}{2} \sup_{j \in \mathcal{Y}} \left| f_j(\widetilde{X}) - [(1-\lambda) f_j(X) + \lambda f_j(X')] \right|, \end{aligned}$$

where $\mathrm{TV}(\cdot,\cdot)$ is the total variation.

Training with Noisy Labels

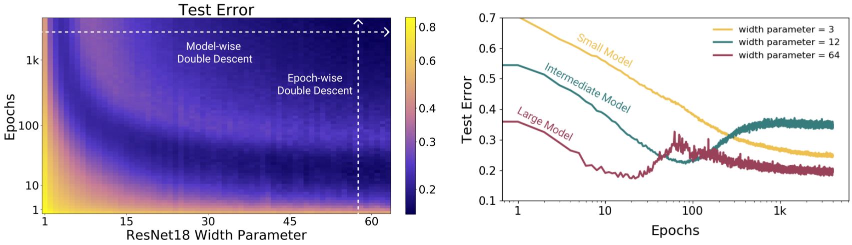

Figure 4: Double descent plots from *Nakkiran, Preetum, et al. "Deep Double Descent: Where Bigger Models and More Data Hurt." ICLR 2020.*

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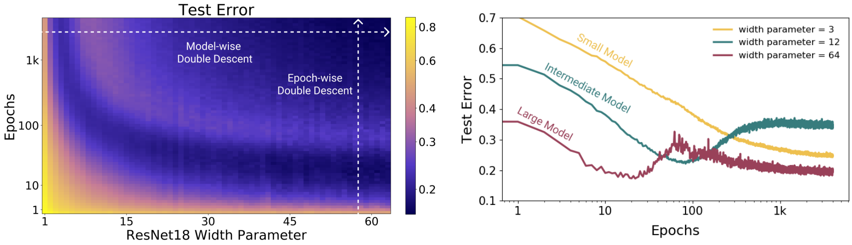

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Reasoning about U-shaped Curve

- DNN is no longer over-parameterized ($d < m$)
- Mixup creates noisy labels

Overfitting to noisy labels

Neural networks are trained with a fraction of random labels, they will

- first learn the clean data
- then will overfit to the data with noisy labels.

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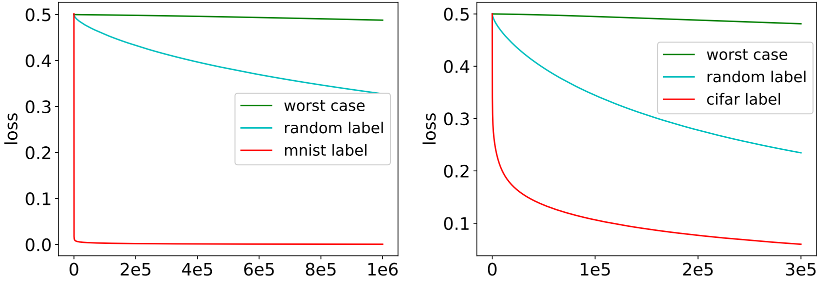

Figure 5: Convergence on clean data and noisy data from *Arora, Sanjeev, et al. "Fine-grained analysis of optimization and generalization for overparameterized two-layer neural networks." ICML 2019.*

A Case Study: Regression Setting With Random Feature Models

- Let $\mathcal{Y} = \mathbb{R}$ so $f : \mathcal{X} \to \mathbb{R}$.
- Let $\widetilde{Y}^* = f(\widetilde{X})$ and $Z \triangleq \widetilde{Y} - \widetilde{Y}^*$.
  Then Z is the data-dependent noise introduced by Mixup.
  e.g., if f is strongly convex with some parameter $\rho > 0$, then $Z \geq \frac{\rho}{2}\lambda(1-\lambda)||X - X'||_2^2$.

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- Given $\widetilde{S} = \{(\widetilde{X}_i, \widetilde{Y}_i)\}_{i=1}^m$ and $\theta^T\phi(X)$, where $\phi : \mathcal{X} \to \mathbb{R}^d$ is fixed and $\theta \in \mathbb{R}^d$. Using the MSE loss

$$\hat{R}_{\widetilde{S}}(\theta) \triangleq \frac{1}{2m}\left|\left|\theta^T\widetilde{\Phi} - \widetilde{\mathbf{Y}}^T\right|\right|_2^2,$$

where $\widetilde{\Phi} = [\phi(\widetilde{X}_1), \phi(\widetilde{X}_2), \ldots, \phi(\widetilde{X}_m)] \in \mathbb{R}^{d\times m}$ and $\widetilde{\mathbf{Y}} = [\widetilde{Y}_1, \widetilde{Y}_2, \ldots, \widetilde{Y}_m] \in \mathbb{R}^m$.

A Case Study: Regression Setting With Random Feature Models

Gradient flow:

$$\dot{\theta} = -\eta \nabla \hat{R}_{\widetilde{S}}(\theta) = \frac{\eta}{m} \widetilde{\Phi} \widetilde{\Phi}^T \left(\widetilde{\Phi}^\dagger \widetilde{\mathbf{Y}} - \theta \right), \tag{1}$$

where η is the learning rate and $\widetilde{\Phi}^\dagger = (\widetilde{\Phi}\widetilde{\Phi}^T)^{-1}\widetilde{\Phi}$ is the Moore–Penrose inverse of $\widetilde{\Phi}^T$ (only possible when $m > d$ i.e. under-parameterized regime).
e.g., ResNet-50: $d \leq 30$ million; CIFAR10: $m = n^2 \geq 200$ million.

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Lemma 2

Let $\theta^* = \widetilde{\Phi}^\dagger \widetilde{\mathbf{Y}}^*$ and $\theta^{\text{noise}} = \widetilde{\Phi}^\dagger \mathbf{Z}$ wherein $\mathbf{Z} = [Z_1, Z_2, \ldots, Z_m] \in \mathbb{R}^m$, the ODE of Eq. (1) has the following closed form solution

$$\theta_t - \theta^* = (\theta_0 - \theta^*) e^{-\frac{\eta}{m} \widetilde{\Phi}\widetilde{\Phi}^T t} + (\mathbf{I}_d - e^{-\frac{\eta}{m} \widetilde{\Phi}\widetilde{\Phi}^T t}) \theta^{\text{noise}}. \tag{2}$$

A Case Study: Regression Setting With Random Feature Models

Given $\widetilde{S}$, the expected population risk is

$$R_t \triangleq \mathbb{E}_{\theta_t, X, Y} \left|\left|\theta_t^T \phi(X) - Y\right|\right|_2^2 .$$

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Theorem 2 (Dynamic of Population Risk)

Given a synthesized dataset $\widetilde{S}$, assume $\theta_0\sim\mathcal{N}(0,\xi^2\mathrm{I}_d)$, $||\phi(X)||^2\leq C_1/2$ for some constant $C_1>0$ and $|Z|\leq\sqrt{C_2}$ for some constant $C_2>0$, then we have

$$R_t-R^*\leq C_1\sum_{k=1}^{d}\left[\left(\xi_k^2+\theta_k^{*2}\right)e^{-2\eta\mu_k t}+\frac{C_2}{\mu_k}\left(1-e^{-\eta\mu_k t}\right)^2\right]+2\sqrt{C_1R^*\zeta},$$

where $R^*=\mathbb{E}_{X,Y}\left|\left|Y-\theta^{*T}\phi(X)\right|\right|_2^2$, $\zeta=\sum_{k=1}^d\max\{\xi_k^2+\theta_k^{*2},\frac{C_2}{\mu_k}\}$ and μ_k is the k^{th} eigenvalue of the matrix $\frac{1}{m}\widetilde{\Phi}\widetilde{\Phi}^T$.

Random Matrix Theory?

If entries in Φ are i.i.d with zero mean, then the eigenvalues $\{\mu_k\}_{k=1}^{d}$ follow the Marchenko-Pasteur (MP) distribution in the limit $d, m \to \infty$ with $d/m = \gamma \in (0, +\infty)$, which is defined as

$$P^{MP}(\mu|\gamma) = \frac{1}{2\pi}\frac{\sqrt{(\gamma_+ - \mu)(\mu - \gamma_-)}}{\mu\gamma}\mathbf{1}_{\mu\in[\gamma_-,\gamma_+]},$$

where $\gamma_\pm = (1 \pm \gamma)^2$. Note that the P^{MP} are only non-zero when $\mu = 0$ or $\mu \in [\gamma_-, \gamma_+]$.

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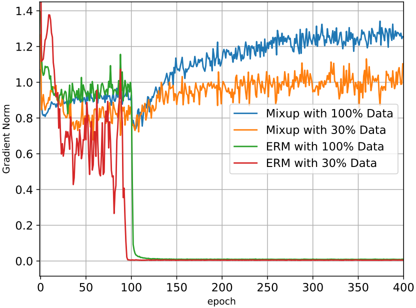
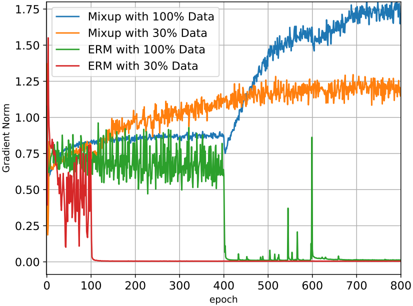
- When γ is close to one, the probability of extremely small eigenvalues is immensely increased.
- Let $d \ll m$ will alleviate the domination of the noise term in Theorem 2.
- Unfortunately columns in Φ are not independent.

Gradient Norm in Mixup Training Does Not Vanish





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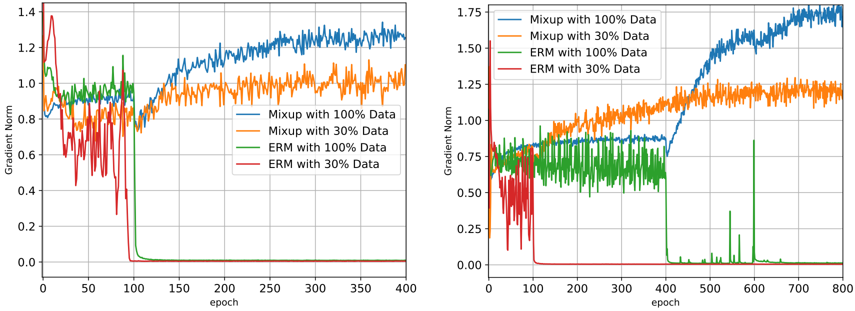

Take-home message:
A wrong objective/solution also helps, only the trajectory/dynamic matters.

Thank you!

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