On Mixup Regularization

[Carratino et al., JMLR 2022]

-Summary-

Introduction – Current paper for mix-up theory

- There are some papers dealing with theoretical analysis of mix-up technique :

[Brief summary & idea]

1. How Does Mixup Help With Robustness And Generalization [Zhang et al., ICLR 2021]
   ① **Showed regularization effect of** mix-up using Taylor expansion on mix-up loss.
   ② Given adversarial attack size, **demonstrated mix up loss is the upper bound of adversarial loss.**
   ③ Under two-layer ReLU network setup with some assumption, they showed : Decreasing mix-up loss -> Decreasing ERM loss -> improve generalization performance as ERM minimization even using mix up training

Introduction – Current paper for mix-up theory

[Brief summary & idea]

2. Towards Understanding the Data Dependency of Mixup-style Training [Chidambaram et al., ICLR 2022]

   ① Showed why mix up technique still works even though model encounter very few true data points during training using theoretical analysis.

   ② Demonstrated that **if collinearity (= manifold intrusion) of mix up point is expected, then model cannot achieve zero training error even with very long training.**

   ③ On high dimensional dataset [MNIST, CIFAR-10/100], showed empirically that collinearity rarely occurs => reason why training loss -> 0 on CIFAR-10 mixup training (By computing minimum distance between each mixup points and points from classes other than the two mixed classes)

Introduction – Current paper for mix-up theory

[Brief summary & idea]

3. On Mixup Regularization [Carratino et al., JMLR 2022]
   ① Showed Mixup can be written as a perturbed ERM loss.
   ② **<u>Showed regularization effect</u>** of mix-up using Taylor expansion on various training case : Cross entropy loss / logistic regression loss / MSE loss
   (Slight different approach, but involves interesting terms to study)
   ③ Suggested '**Approximated Mixup'** by dropping out the regularization term, which is an intermediate compromise of Mixup and ERM training in the view or regularization. (Not our interest…)

<u>Our current goal</u> : Want to focus on part ① to study the detailed regularization effect of mix-up and find some reasonable intuition to modify original mix-up.
(to improve generalization performance)

Theorems on the paper [On Mixup Regularization]

- Learning problem & Notations:
  1. Training set : $S_n = \{(x_1, y_1), \dots (x_n, y_n)\}$,and $x_i \in \mathcal{X} \subset \mathbb{R}^d, \quad y_i \in \mathcal{Y} \subset \mathbb{R}^c$
  2. Sample mean : $\bar{x} = \frac{1}{\mathrm{n}} \sum_{i=1}^{n} x_i \, , \quad \bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$
  3. Sample covariance : $\Sigma_{xy} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})^T$
  4. ERM loss : $\mathcal{E}^{ERM}(f) = \frac{1}{n} \sum_{i=1}^{n} l\big(y_i, f(x_i)\big)$
  5. Mix-up loss : $\mathcal{E}^{Mixup}(f) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{i=1}^{n} \mathbb{E}_\lambda [l\big(\lambda y_i + (1-\lambda) y_j, f\big(\lambda x_i + (1-\lambda) x_j\big)\big)]$

Usually $\lambda \sim Beta(\alpha, \alpha)$

- Now, we reformulate mix-up loss as a perturbed ERM by following procedure.

Theorems on the paper [On Mixup Regularization]

1. Define $m_{ij}(\lambda) = l\left(\lambda y_i + (1-\lambda)y_j, f\left(\lambda x_i + (1-\lambda)x_j\right)\right)$ to simplify $\mathcal{E}^{Mixup}(f)$:

$$\mathcal{E}^{Mixup}(f) = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{i=1}^{n}\mathbb{E}_{\lambda}[m_{ij}(\lambda)]$$

Beta distribution constricted on given domain

2. Separate λ by symmetry of Beta distribution as follows :

$$\lambda = \pi\lambda_0 + (1-\pi)\lambda_1, \qquad \lambda_0 \sim Beta_{\left[0,\frac{1}{2}\right]}(\alpha,\alpha), \qquad \lambda_1 \sim Beta_{\left[\frac{1}{2},1\right]}(\alpha,\alpha), \qquad \pi \sim Bern\left(\frac{1}{2}\right)$$

Critical note : It is possible to use any pdf symmetric w.r.t 0.5 (restricted on [0,1]) for λ

3. Using the fact $\lambda_1' \coloneqq 1-\lambda_0 \sim Beta_{\left[\frac{1}{2},1\right]}(\alpha,\alpha)$, we further simplify as below :

$$\mathbb{E}_{\lambda}[m_{ij}(\lambda)] = \mathbb{E}_{\lambda_0,\lambda_1,\pi}[m_{ij}(\pi\lambda_0 + (1-\pi)\lambda_1)] = \frac{1}{2}[\mathbb{E}_{\lambda_1'}[m_{ji}(\lambda_1')] + \mathbb{E}_{\lambda_1}[m_{ij}(\lambda_1)]$$

Theorems on the paper [On Mixup Regularization]

4. Finally, we can simply $\mathcal{E}^{Mixup}(f)$ by following :

Recall : $m_{ij}(\lambda) = l\left(\lambda y_i + (1-\lambda)y_j, f\left(\lambda x_i + (1-\lambda)x_j\right)\right)$

$$\mathcal{E}^{Mixup}(f) = \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left[\mathbb{E}_{\lambda_1'}\left[m_{ji}(\lambda_1')\right] + \mathbb{E}_{\lambda_1}\left[m_{ij}(\lambda_1)\right]\right] = \frac{1}{n}\sum_{i=1}^{n} l_i$$

where $l_i = \mathbb{E}_{\theta,j}\left[l\left(\theta y_i + (1-\theta)y_j, f\left(\theta x_i + (1-\theta)x_j\right)\right)\right], \ \theta \sim Beta_{\left[\frac{1}{2},1\right]}(\alpha,\alpha), \ j \sim Unif([n])$

5. Define $\widetilde{x}_i \coloneqq \mathbb{E}_{\theta,j}\left[\theta x_i + (1-\theta)x_j\right]$ and $\widetilde{y}_i \coloneqq \mathbb{E}_{\theta,j}\left[\theta y_i + (1-\theta)y_j\right]$

6. Define $\delta_i \coloneqq \theta x_i + (1-\theta)x_j - \mathbb{E}_{\theta,j}\left[\theta x_i + (1-\theta)x_j\right]$

   $\epsilon_i \coloneqq \theta y_i + (1-\theta)y_j - \mathbb{E}_{\theta,j}\left[\theta y_i + (1-\theta)y_j\right]$

Note : $\mathbb{E}_{\theta,j}[\delta_i] = \mathbb{E}_{\theta,j}[\epsilon_i] = 0$

5. Then, $l_i = \mathbb{E}_{\theta,j}[l(\widetilde{y}_i + \epsilon_i, f(\widetilde{x}_i + \delta_i)]$

Theorems on the paper [On Mixup Regularization]

- Summarizing this result, we get following theorem :

Theorem 1 *Let $\theta \sim Beta_{[\frac{1}{2},1]}(\alpha, \alpha)$ and $j \sim Unif([n])$ be two random variables with $\alpha > 0$, $n > 0$ and let $\overline{\theta} = \mathbb{E}_\theta \theta$. For any training set $\mathcal{S}_n$, let $(\widetilde{x}_i, \widetilde{y}_i)$ for any $i \in [n]$ be the modified input/output pair given by*

$$\begin{cases} \widetilde{x}_i & = \overline{x} + \overline{\theta}(x_i - \overline{x}) \,, \\ \widetilde{y}_i & = \overline{y} + \overline{\theta}(y_i - \overline{y}) \,, \end{cases}$$

and $(\delta_i, \varepsilon_i)$ be the random perturbations given by:

$$\begin{cases} \delta_i & = (\theta - \overline{\theta})x_i + (1-\theta)x_j - (1-\overline{\theta})\overline{x} \,, \\ \varepsilon_i & = (\theta - \overline{\theta})y_i + (1-\theta)y_j - (1-\overline{\theta})\overline{y} \,. \end{cases}$$

Then for any $i \in [n]$, $\mathbb{E}_{\theta,j}\delta_i = \mathbb{E}_{\theta,j}\varepsilon_i = 0$, and for any function $f \in \mathcal{H}$,

$$\mathcal{E}^{Mixup}(f) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{\theta,j}\ell\left(\widetilde{y}_i + \varepsilon_i, f(\widetilde{x}_i + \delta_i)\right) .$$

Mixup loss as perturbed ERM

Theorems on the paper [On Mixup Regularization]

- Now, we want to approximate the mix-up loss via 2nd order Taylor expansion :

$$\mathcal{E}_Q^{Mixup}(f) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{\theta,j}[l_Q^{(i)}(\widetilde{y}_i + \epsilon_i, f(\widetilde{x}_i + \delta_i)]$$

where $l_Q^{(i)}$ is given as following :

$$\begin{aligned}\ell_Q^{(i)}\left(\widetilde{y}_i + \varepsilon, f(\widetilde{x}_i + \delta)\right) &= \ell\left(\widetilde{y}_i, f(\widetilde{x}_i)\right) + \nabla_y \ell\left(\widetilde{y}_i, f(\widetilde{x}_i)\right)\varepsilon + \nabla_u \ell\left(\widetilde{y}_i, f(\widetilde{x}_i)\right)\nabla_x f(\widetilde{x}_i)\delta \\ &+ \frac{1}{2}\left\langle \delta\delta^\top, \nabla f(\widetilde{x}_i)^\top \nabla_{uu}^2 \ell(\widetilde{y}_i, f(\widetilde{x}_i))\nabla f(\widetilde{x}_i) + \underline{\nabla_u \ell(\widetilde{y}_i, f(\widetilde{x}_i))\nabla^2 f(\widetilde{x}_i)}\right\rangle \\ &+ \frac{1}{2}\left\langle \varepsilon\varepsilon^\top, \nabla_{yy}^2 \ell(\widetilde{y}_i, f(\widetilde{x}_i))\right\rangle + \left\langle \varepsilon\delta^\top, \nabla_{yu}^2 \ell(\widetilde{y}_i, f(\widetilde{x}_i))\nabla f(\widetilde{x}_i)\right\rangle,\end{aligned}$$

Note : $< A, B > := Tr(A^T B)$ (Frobenius inner product)

This term : $1 \times c$ by c $\times |x| \times |x|$ calculation (tensor product)
In detail, it is the same as following :

$$\sum_{k=1}^{c} \nabla_u l\left(\widetilde{y}_i, f(\widetilde{x}_i)\right)^{(k)} \nabla^2 f(\widetilde{x}_i)^{(k)} \in \mathbb{R}^{|x|\times|x|}$$

Theorems on the paper [On Mixup Regularization]

- To proceed further, we define 3 covariance related term as belows :

Lemma 2 *Let $\overline{\theta}$ and σ^2 be respectively the mean and variance of a $Beta_{[\frac{1}{2},1]}(\alpha,\alpha)$ distributed random variable, and $\gamma^2 = \sigma^2 + (1-\overline{\theta})^2$. For any $i \in [n]$, let*

$$\Sigma^{(i)}_{\widetilde{x}\widetilde{x}} = \frac{\sigma^2(\widetilde{x}_i - \overline{x})(\widetilde{x}_i - \overline{x})^\top + \gamma^2 \Sigma_{\widetilde{x}\widetilde{x}}}{\overline{\theta}^2},$$

$$\Sigma^{(i)}_{\widetilde{y}\widetilde{y}} = \frac{\sigma^2(\widetilde{y}_i - \overline{y})(\widetilde{y}_i - \overline{y})^\top + \gamma^2 \Sigma_{\widetilde{y}\widetilde{y}}}{\overline{\theta}^2},$$

$$\Sigma^{(i)}_{\widetilde{x}\widetilde{y}} = \frac{\sigma^2(\widetilde{x}_i - \overline{x})(\widetilde{y}_i - \overline{y})^\top + \gamma^2 \Sigma_{\widetilde{x}\widetilde{y}}}{\overline{\theta}^2}.$$

Then, for any $i \in [n]$, the random perturbations defined in (6) satisfy

$$\mathbb{E}_{\theta,j}\delta_i\delta_i^\top = \Sigma^{(i)}_{\widetilde{x}\widetilde{x}}, \quad \mathbb{E}_{\theta,j}\varepsilon_i\varepsilon_i^\top = \Sigma^{(i)}_{\widetilde{y}\widetilde{y}}, \quad \text{and} \quad \mathbb{E}_{\theta,j}\delta_i\varepsilon_i^\top = \Sigma^{(i)}_{\widetilde{x}\widetilde{y}}.$$

Theorems on the paper [On Mixup Regularization]

- Further cleaning up the terms induces following approximation of Mixup loss :

Theorem 3 *For any twice continuously differentiable loss $\ell(y,u)$, the approximate Mixup risk at any twice differentiable $f \in \mathcal{H}$ satisfies*

$$\mathcal{E}_Q^{Mixup}(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(\widetilde{y}_i, f(\widetilde{x}_i)) + R_1(f) + R_2(f) + R_3(f) + R_4(f)\,,$$

where

$$R_1(f) = \frac{1}{2n}\sum_{i=1}^{n} \left\| \left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)^\top \left(\nabla^2_{uu}\ell(\widetilde{y}_i, f(\widetilde{x}_i))\right)^{\frac{1}{2}} \right\|^2_{\Sigma^{(i)}_{\widetilde{x}\widetilde{x}}}\,,$$

$$R_2(f) = \frac{1}{2n}\sum_{i=1}^{n} \left\langle \Sigma^{(i)}_{\widetilde{x}\widetilde{x}}, \nabla_u \ell(\widetilde{y}_i, f(\widetilde{x}_i))\nabla^2 f(\widetilde{x}_i) \right\rangle\,,$$

$$R_3(f) = -\frac{1}{2n}\sum_{i=1}^{n} \left\| \Sigma^{(i)}_{\widetilde{x}\widetilde{y}}\ \nabla^2_{yu}\ell(\widetilde{y}_i, f(\widetilde{x}_i))\ \left(\nabla^2_{uu}\ell(\widetilde{y}_i, f(\widetilde{x}_i))\right)^{-\frac{1}{2}} \right\|^2_{\left(\Sigma^{(i)}_{\widetilde{x}\widetilde{x}}\right)^{-1}}\,,$$

$$R_4(f) = \frac{1}{2n}\sum_{i=1}^{n} \left\langle \Sigma^{(i)}_{\widetilde{y}\widetilde{y}}, \nabla^2_{yy}\ell(\widetilde{y}_i, f(\widetilde{x}_i)) \right\rangle\,,$$

and

$$\forall i \in [n], \quad J^{(i)} = -\left(\nabla^2_{uu}\ell(\widetilde{y}_i, f(\widetilde{x}_i))\right)^{-1} \nabla^2_{uy}\ell(\widetilde{y}_i, f(\widetilde{x}_i))\Sigma^{(i)}_{\widetilde{y}\widetilde{x}}\left(\Sigma^{(i)}_{\widetilde{x}\widetilde{x}}\right)^{-1}.$$

Note : $\|A\|_Z^2 \coloneqq \langle A, ZA \rangle = Tr(A^T Z A)$
(Squared frobenius norm with metric Z)

<u>Hard to interpret</u>, but we can do something when loss is Cross-entropy loss

Theorems on the paper [On Mixup Regularization]

- If we use Cross-entropy loss $l^{CE}(y, u)$, we can get following facts :

$$
\boxed{
\begin{aligned}
\nabla_y \ell^{\mathrm{CE}}(y, u) &= -u^\top , \\
\nabla_u \ell^{\mathrm{CE}}(y, u) &= (\mathcal{S}(u) - y)^\top \\
\nabla^2_{yy} \ell^{\mathrm{CE}}(y, u) &= \mathbf{0}_c , \\
\nabla^2_{yu} \ell^{\mathrm{CE}}(y, u) &= -\mathbf{I}_c , \\
\nabla^2_{uu} \ell^{\mathrm{CE}}(y, u) &= H(u) .
\end{aligned}
}
$$

where $H(u) = diag\big(S(u)\big) - S(u)S(u)^T \in \mathbb{R}^{c \times c}$ [the Jacobian of softmax function (S)]

- By putting these terms into previous theorem, we achieve following approximate mix up loss on Cross entropy loss setup

Theorems on the paper [On Mixup Regularization]

Corollary 4 *Let $\mathcal{S} : \mathbb{R}^c \to \mathbb{R}^c$ be the softmax operator, i.e., for any $i \in [c]$ and $u \in \mathbb{R}^c$, $\mathcal{S}(u)_i = e^{u_i} / \sum_{j=1}^{c} e^{u_j}$, and let $H(u) = diag(\mathcal{S}(u)) - \mathcal{S}(u)\mathcal{S}(u)^\top \in \mathbb{R}^{c \times c}$. The approximate Mixup risk for the cross-entropy loss satisfies*

$$\mathcal{E}_Q^{Mixup}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell^{CE}(\tilde{y}_i, f(\tilde{x}_i)) + R_1^{CE}(f) + R_2^{CE}(f) + R_3^{CE}(f)\,,$$

where

$$R_1^{CE}(f) = \frac{1}{2n} \sum_{i=1}^{n} \left\| \left(\nabla f(\tilde{x}_i) - J^{(i)} \right)^\top H(f(\tilde{x}_i))^{\frac{1}{2}} \right\|^2_{\Sigma^{(i)}_{\tilde{x}\tilde{x}}}\,,$$

$$R_2^{CE}(f) = \frac{1}{2n} \sum_{i=1}^{n} \left\langle \Sigma^{(i)}_{\tilde{x}\tilde{x}}, \underline{(\mathcal{S}(f(\tilde{x}_i)) - \tilde{y}_i)}^\top \nabla^2 f(\tilde{x}_i) \right\rangle\,,$$

$$R_3^{CE}(f) = -\frac{1}{2n} \sum_{i=1}^{n} \left\| \Sigma^{(i)}_{\tilde{x}\tilde{y}}\, H(f(\tilde{x}_i))^{-\frac{1}{2}} \right\|^2_{\left(\Sigma^{(i)}_{\tilde{x}\tilde{x}}\right)^{-1}}\,,$$

This term is related with EL2N score.

=> Let's try upper bound analysis for each term

with

$$\forall i \in [n]\,, \quad J^{(i)} = H(f(\tilde{x}_i))^{-1} \Sigma^{(i)}_{\tilde{y}\tilde{x}} \left(\Sigma^{(i)}_{\tilde{x}\tilde{x}} \right)^{-1}.$$

Analysis beyond the paper

1. $R_1^{CE}(f)$ analysis : focus on $\left\| \left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)^T H\left(f(\widetilde{x}_i)\right)^{\frac{1}{2}} \right\|_{\Sigma_{\widetilde{x}\widetilde{x}}^{(i)}}^2$ term

2. Note the following :

$$
\begin{aligned}
\left\| \left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)^T H\left(f(\widetilde{x}_i)\right)^{\frac{1}{2}} \right\|_{\Sigma_{\widetilde{x}\widetilde{x}}^{(i)}}^2 &= Tr\left[H\left(f(\widetilde{x}_i)\right)^{\frac{1}{2}}\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)\Sigma_{\widetilde{x}\widetilde{x}}^{(i)}\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)^T H\left(f(\widetilde{x}_i)\right)^{\frac{1}{2}}\right] \\
&= Tr\left[\Sigma_{\widetilde{x}\widetilde{x}}^{(i)}\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)^T H\left(f(\widetilde{x}_i)\right)\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)\right] \\
&\le Tr\left(\Sigma_{\widetilde{x}\widetilde{x}}^{(i)}\right) \cdot Tr\left(H\left(f(\widetilde{x}_i)\right)\right) \cdot Tr\left[\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)^T\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)\right] \\
&\le Tr\left(\Sigma_{\widetilde{x}\widetilde{x}}^{(i)}\right) \cdot \mathcal{H}\left(S\left(f(\widetilde{x}_i)\right)\right) \cdot Tr\left[\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)^T\left(\nabla f(\widetilde{x}_i) - J^{(i)}\right)\right]
\end{aligned}
$$

As the entropy of prediction of $\widetilde{x}_i$ get higher (close to decision boundary ~ Hard example), It gets stronger regularization from mix-up

R_1^{CE} terms forces the Jacobian of $f(\widetilde{x}_i)$ to be close to $J^{(i)}$, which is interpreted as weighted Multivariate OLS estimator in this paper (MLOS ???)

Analysis beyond the paper

3. $R_2^{CE}(f)$ analysis : focus on $< \Sigma_{\tilde{x}\tilde{x}}^{(i)}, \ (S(f(\tilde{x}_i)) - \tilde{y}_i)^T \nabla^2 f(\tilde{x}_i) >$ term

4. Note the following :

$$
\begin{aligned}
< \Sigma_{\tilde{x}\tilde{x}}^{(i)}, \ (S(f(\tilde{x}_i)) - \tilde{y}_i)^T \nabla^2 f(\tilde{x}_i) > &= Tr\left[\Sigma_{\tilde{x}\tilde{x}}^{(i)} (S(f(\tilde{x}_i)) - \tilde{y}_i)^T \nabla^2 f(\tilde{x}_i)\right] \\
&\le Tr\left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right) \cdot Tr\left[(S(f(\tilde{x}_i)) - \tilde{y}_i)^T \nabla^2 f(\tilde{x}_i)\right] \\
&= Tr\left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right) \cdot (S(f(\tilde{x}_i)) - \tilde{y}_i)^T Tr^{tensor}\left(\nabla^2 f(\tilde{x}_i)\right) \\
&\le Tr\left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right) \underline{\left\|S(f(\tilde{x}_i)) - \tilde{y}_i\right\|_2} \cdot \underline{\left\|Tr^{tensor}\left(\nabla^2 f(\tilde{x}_i)\right)\right\|_2}
\end{aligned}
$$

where $Tr^{tensor}\left(\nabla^2 f(\tilde{x}_i)\right) = \begin{bmatrix} Tr\left(\nabla^2 f(\tilde{x}_i)^{(1)}\right) \\ \dots \\ Tr\left(\nabla^2 f(\tilde{x}_i)^{(c)}\right) \end{bmatrix} \in \mathbb{R}^c$

This term is EL2N score of expected mix-up point of x_i (=$\tilde{x}_i$). As the $\tilde{x}_i$ gets harder, the regularization effect of $\tilde{x}_i$ gets stronger.

R_2^{CE} terms forces the input Laplacian of $f(\tilde{x}_i)^{(k)}$ to be zero. ($k \in [c]$)
[Mustafal et al., ICLM 2020] claims that input hessian regularization improves robustness of model

Analysis beyond the paper

5. $R_3^{CE}(f)$ analysis : focus on $\left\| \Sigma_{\tilde{x}\tilde{y}}^{(i)} H(f(\tilde{x}_i))^{-\frac{1}{2}} \right\|^2_{\left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right)^{-1}}$ term

6. Note the following :

$$\left\| \Sigma_{\tilde{x}\tilde{y}}^{(i)} H(f(\tilde{x}_i))^{-\frac{1}{2}} \right\|^2_{\left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right)^{-1}} = Tr\left[H(f(\tilde{x}_i))^{-\frac{1}{2}} \Sigma_{\tilde{y}\tilde{x}}^{(i)} \left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right)^{-1} \Sigma_{\tilde{x}\tilde{y}}^{(i)} H(f(\tilde{x}_i))^{-\frac{1}{2}} \right]$$

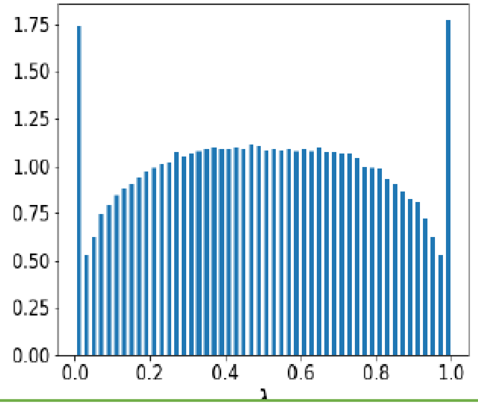
$$= Tr\left[\Sigma_{\tilde{y}\tilde{x}}^{(i)} \left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right)^{-1} \Sigma_{\tilde{x}\tilde{y}}^{(i)} H(f(\tilde{x}_i)) \right]$$

$$\leq Tr\left(\Sigma_{\tilde{y}\tilde{x}}^{(i)} \Sigma_{\tilde{x}\tilde{y}}^{(i)}\right) Tr\left(\left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right)^{-1}\right) \mathcal{H}\left(S(f(\tilde{x}_i))\right)$$

Since R_3^{CE} term regularize $\mathcal{H}\left(S(f(\tilde{x}_i))\right)$, the regularization effect of R_1^{CE} (~Jacobian regularization) becomes smaller as the training loss gets minimized

Regularize the entropy of prediction on $\tilde{x}_i$ and force the entropy to be lower as possible for expected mix-up point for x_i.

Towards stronger regularization



Learned λ distribution from MetaMixup

- Our natural question on Mix-up is 'Why we sample λ for $Beta(\alpha, \alpha)$?'
  (Obviously, this is the well-known distribution restricted on $[0,1]$)

- Some papers on mix-up shows test accuracy improvement via adopting new λ distribtuion:

  1. **RegMixup** [Pinto et al., NeurIPS 2022]
     : Propose to mix-up training with original training samples (with high $\alpha \sim 10$)

  2. **MetaMixup** [Mai et al., IEEE TNNLS]
     : Using Meta learning to learn good λ selection policy based on input x_i, demonstrated test accuracy improvement via W shaped λ distribution (learned from meta learning)

Towards stronger regularization

- Both paper showed the results by experiments, but we may be able to explain this phenomenon using our previous analysis on mix-up.

- Note the following terms appeared in $R_1^{CE}, R_2^{CE}, R_3^{CE}$: $Tr\left(\Sigma_{\tilde{y}\tilde{x}}^{(i)}\Sigma_{\tilde{x}\tilde{y}}^{(i)}\right)$ or $Tr\left(\Sigma_{\tilde{x}\tilde{x}}^{(i)}\right)$:

(Note : $\gamma^2 = \sigma^2 + \left(1-\bar{\theta}\right)^2$ and $\theta \sim Beta_{\left[\frac{1}{2},1\right]}(\alpha,\alpha)$)

- Recall :

$$\Sigma_{\widetilde{x}\widetilde{x}}^{(i)} = \frac{\sigma^2(\widetilde{x}_i - \overline{x})(\widetilde{x}_i - \overline{x})^\top + \gamma^2\Sigma_{\widetilde{x}\widetilde{x}}}{\overline{\theta}^2},$$

$$\Sigma_{\widetilde{y}\widetilde{y}}^{(i)} = \frac{\sigma^2(\widetilde{y}_i - \overline{y})(\widetilde{y}_i - \overline{y})^\top + \gamma^2\Sigma_{\widetilde{y}\widetilde{y}}}{\overline{\theta}^2},$$

$$\Sigma_{\widetilde{x}\widetilde{y}}^{(i)} = \frac{\sigma^2(\widetilde{x}_i - \overline{x})(\widetilde{y}_i - \overline{y})^\top + \gamma^2\Sigma_{\widetilde{x}\widetilde{y}}}{\overline{\theta}^2}.$$

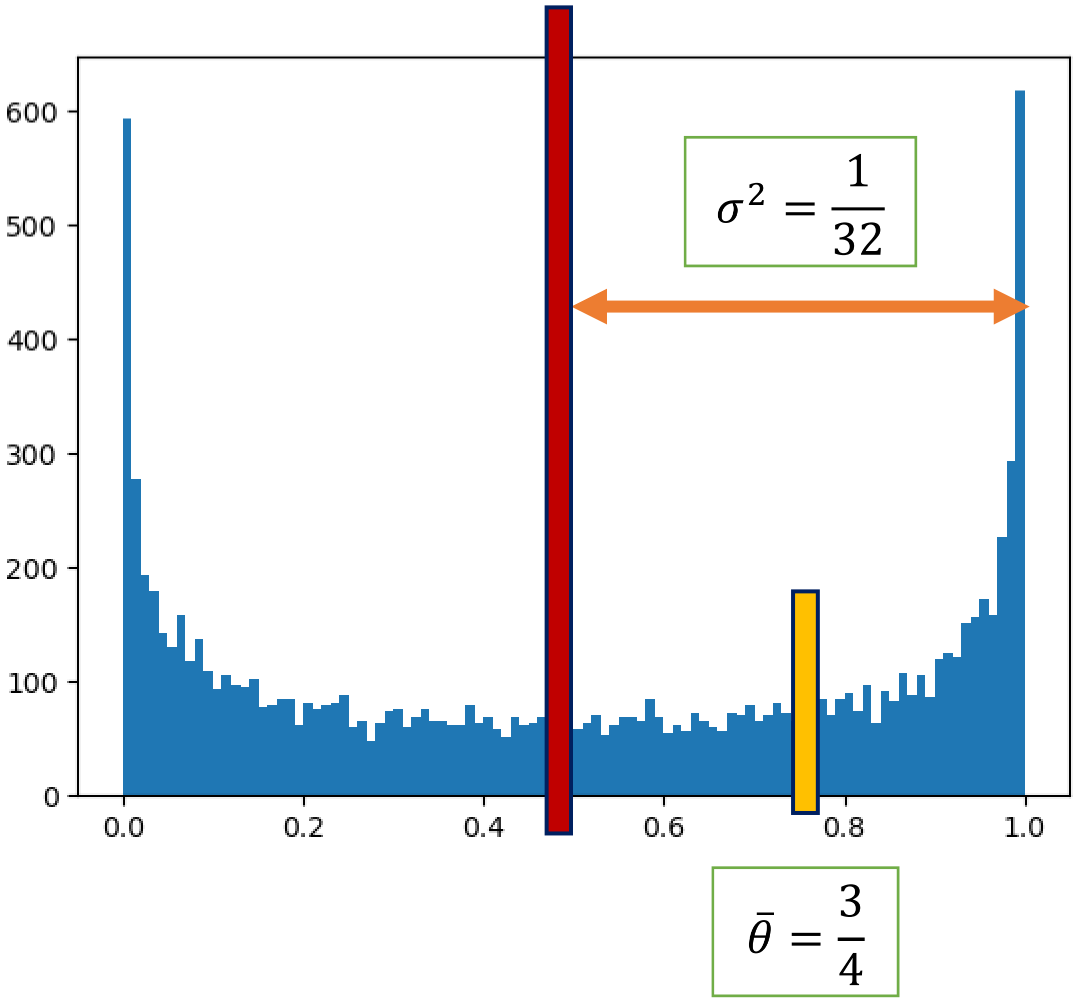
By maximizing, $\frac{\sigma^2}{\bar{\theta}^2}$ we can enhance the effect of regularization effect induced by all $R_1^{CE}, R_2^{CE}, R_3^{CE}$ term

Note : There is no problem to replace $Beta_{\left[\frac{1}{2},1\right]}$ distribution to any $[\frac{1}{2},1]$ restricted distribution symmetric to $\frac{1}{2}$. (This is our idea)

Towards stronger regularization

- (Experiment) Let $\lambda \sim Beta(0.5,0.5)$ as in naïve mixup.

$$dbeta(\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$



In other words, $p(\theta) = 2 \times dbeta(0.5,0.5)$.
Then,

$$\bar{\theta} = \mathbb{E}[\theta] = \frac{3}{4}$$

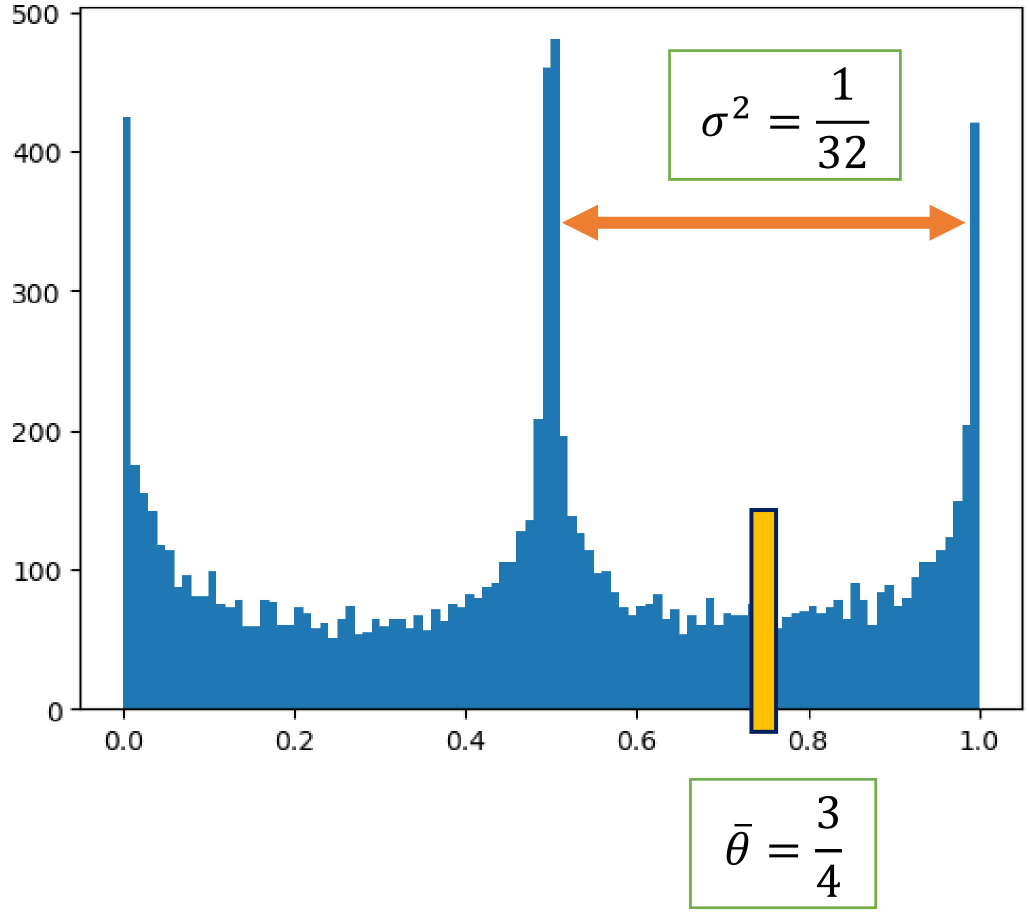
$$\sigma^2 = Var(\theta) = \frac{1}{4} Var(X) = \frac{1}{32}$$

Thus, $\frac{\sigma^2}{\bar{\theta}} = \frac{1}{24}$

Note : $X \sim Beta(\alpha,\alpha)$ => $Var(X) = \frac{1}{4(2\alpha+1)}$

Towards stronger regularization

- (Experiment) Let $\lambda|Z = \begin{cases} \frac{1}{2}X & Z = 0 \\ \frac{1}{2}(X+1) & Z = 1 \end{cases}$, where $X \sim Beta(0.5,0.5)$, $Z \sim Bern\left(\frac{1}{2}\right)$



In other words, $\theta = \frac{1}{2}(X+1)$.

Then,

$$\bar{\theta} = \mathbb{E}[\theta] = \frac{3}{4}$$

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Note : $X \sim Beta(\alpha, \alpha)$ => $Var(X) = \frac{1}{4(2\alpha+1)}$