MixupE: Understanding and Improving Mixup from Directional Derivative Perspective

Abstract

Mixup is a popular data augmentation technique for training deep neural networks where additional samples are generated by linearly interpolating pairs of inputs and their labels. This technique is known to improve the generalization performance in many learning paradigms and applications. In this work, we first analyze Mixup and show that it implicitly regularizes infinitely many directional derivatives of all orders. Based on this new insight, we propose an improved version of Mixup, theoretically justified to deliver better generalization performance than the vanilla Mixup. To demonstrate the effectiveness of the proposed method, we conduct experiments across various domains such as images, tabular data, speech, and graphs. Our results show that the proposed method improves Mixup across various datasets using a variety of architectures, for instance, exhibiting an improvement over Mixup by 0.8% in ImageNet top-1 accuracy.

1 INTRODUCTION

Deep Neural Networks (DNNs) represent a class of very powerful function approximators, and large-scale DNNs have achieved state-of-the-art performance in many application areas such as computer vision [Krizhevsky et al., 2012], natural language understanding [Devlin et al., 2018], speech recognition [Hinton et al., 2012], reinforcement learning [Silver et al., 2016], and natural sciences [Jumper et al., 2021]. In a supervised learning setting, typically, DNNs are trained to minimize their average error on the training samples. This training principle is known as Empirical Risk Minimization (ERM) [Vapnick, 1998].

Although being a simple training principle, training neural networks with ERM have a major problem: in the absence of regularization techniques, instead of learning meaningful concepts, neural networks trained with ERM are prone to *memorize* training data [Arpit et al., 2017]. This results in poor generalization to test samples, which come from a distribution slightly different from the training samples. To address this limitation of ERM, recently Mixup [Zhang et al., 2018] has been proposed as an alternative training principle. In a nutshell, instead of training a neural network on individual samples and their corresponding outputs, Mixup trains a neural network on the linear interpolation of the samples and the corresponding linear interpolation of the outputs.

Mathematically, let us suppose that $\mathbf{x}_i$ and $\mathbf{x}_j$ are input vectors corresponding to two randomly drawn samples i and j from the training distribution, and $\mathbf{y}_i$ and $\mathbf{y}_j$ are their one-hot encoded labels. Then, Mixup constructs a training sample as $\tilde{\mathbf{x}} = \lambda \mathbf{x}_i + (1-\lambda)\mathbf{x}_j$ and $\tilde{\mathbf{y}} = \lambda \mathbf{y}_i + (1-\lambda)\mathbf{y}_j$, where $\lambda \in [0, 1]$. Training with this kind of synthetic samples encourages the model to learn a function where linear interpolation in the input vectors leads to the linear interpolation of the corresponding targets. This kind of constraint limits the model complexity, and thus limits their ability to memorize training samples. Mixup can be interpreted as a data-agnostic *data augmentation* technique that does not require expert knowledge for creating additional training samples. Mixup can also be interpreted from the viewpoint of *Vicinal Risk Minimization* (VRM) principle [Chapelle et al., 2000]. In this view, Mixup proposes a generic vicinal distribution based on the interpolation of training samples and their associated targets, and the additional training samples are drawn from such vicinal distribution around each training sample [Zhang et al., 2018].

Despite its simplicity and minimal computation overhead, Mixup and its variants have been shown to achieve state-of-the-art in many tasks such as but not limited to, image classification [Yun et al., 2019, Kim et al., 2020, Faramarzi et al., 2020], object detection [Jeong et al., 2021], speech recognition [Lam et al., 2020, Tomashenko et al., 2018], text classification [Guo et al., 2019, Zhang et al., 2020], and medical image segmentation [Panfilov et al., 2019]. Re-

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cently, Mixup was theoretically analyzed and shown to be approximately equivalent to adding a second-order regularization term to the standard loss function [Zhang et al., 2021]. However, if the benefit of Mixup can be explained by a second-order regularization, the following natural question arises: why we cannot replace Mixup with this second-order regularization directly? Unfortunately, the answer is no because the second-order terms are input-specific thus yielding a complicated form.

In this paper, we show that Mixup is equivalent to implicitly adding infinitely many regularization terms on the directional derivatives of all orders instead of a complex second-order form as [Zhang et al., 2021] for ERM. Our analysis provides a feasible insight to design the regularization in practice. Based on this novel insight, this paper proposes to explicitly enhance the implicit regularization effect of Mixup on the directional derivatives. Instead of computing all infinite regularization terms, we approximate the dominant term from accessible results in each forward propagation. We name this method as *MixupE* (**Mixup E**nhanced). Figure 1 shows the training and test loss of ERM, Mixup, and *MixupE* on CIFAR-100 dataset trained with Wide-Resnet-28-10 [Zagoruyko and Komodakis, 2016] architecture. We can see that *MixupE* has higher training loss, implying that it works as a stronger regularizer than Mixup and ERM. This subsequently results in better generalization (lower test loss) than Mixup and ERM.

To understand the benefits of *MixupE* empirically, we conduct experiments on a variety of datasets, such as images, tabular data and speech data, using various architectures such as LeNet [LeCun et al., 1998], VGG [Simonyan and Zisserman, 2014], ResNet [He et al., 2016], Vision Transformer [ViT, Dosovitskiy et al., 2020], and CoAtNet [Dai et al., 2021]. In our experiments, we consistently see the *MixupE* has better generalization error than Mixup and ERM.

2 METHODS

In this section, we derive our method with a new mathematical understanding of Mixup. We begin in Section 2.1 with the notation used to present our theory and method. Mixup is then shown to implicitly regularize infinitely many directional derivatives of all orders in Section 2.2. This theoretical insight allows us to enhance the regularization effect on the directional derivatives. In Section 2.3, we present an algorithm to strengthen the regularization effect of Mixup based on a theoretical derivation and justify the theoretical improvement over Mixup.

2.1 NOTATION

We denote by $\mathbf{z} = (\mathbf{x}, \mathbf{y})$ the input and output pair where $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d$ and $\mathbf{y} \in \mathcal{Y} \subseteq \mathbb{R}^C$. Let $f_\theta(\mathbf{x}) \in \mathbb{R}^C$ be the output of the logits (i.e., the last layer before the softmax or sigmoid) of the model parameterized by θ. We use $\ell(\theta, \mathbf{z}) = h(f_\theta(\mathbf{x})) - \mathbf{y}^\top f_\theta(\mathbf{x})$ to denote the loss function where

$$h(f_\theta(\mathbf{x})) = \begin{cases} \log\left(\sum_j \exp(f_\theta(\mathbf{x})_{(j)})\right) & \text{Softmax} \\ \log\left(1 + \exp\left(f_\theta(\mathbf{x})\right)\right) & \text{Sigmoid} \end{cases} \tag{1}$$

Let $g(\cdot)$ be the activation function. We use $\mathbf{x}_{(i)}$ to index i-th element of the vector $\mathbf{x}$ and $\mathbf{x}_j$ to represent j-th variable in a set.

Mixup Given a training dataset $S = ((\mathbf{x}_i, \mathbf{y}_i))_{i=1}^n$ of size n with $\mathbf{x}_i \in \mathcal{X}$ and $\mathbf{y}_i \in \mathcal{Y}$, we define the Mixup version of the input and output pair by $\tilde{\mathbf{z}}_{i,j}(\lambda) = (\tilde{\mathbf{x}}_{i,j}(\lambda), \tilde{\mathbf{y}}_{i,j}(\lambda))$ where $\tilde{\mathbf{x}}_{i,j}(\lambda) = \lambda \mathbf{x}_i + (1-\lambda)\mathbf{x}_j$ and $\tilde{\mathbf{y}}_{i,j}(\lambda) = \lambda \mathbf{y}_i + (1-\lambda)\mathbf{y}_j$ with the Mixup coefficient $\lambda \in [0, 1]$. Then, we denote the standard empirical loss by $L_n^{std}(\theta, S) = \frac{1}{n}\sum_{i=1}^n l(\theta, \mathbf{z}_i)$ and the Mixup loss by $L_n^{\text{mix}}(\theta, S) = \frac{1}{n^2}\sum_{i,j=1}^n \mathbb{E}_{\lambda \sim \text{Beta}(\alpha,\beta)} l(\theta, \tilde{\mathbf{z}}_{ij}(\lambda))$ where $\text{Beta}(\alpha, \beta)$ represents the beta distribution with its parameters $\alpha, \beta > 0$. We define a mixture of beta distributions as $\mathcal{D}_\lambda = \frac{\alpha}{\alpha+\beta}\text{Beta}(\alpha+1, \beta) + \frac{\beta}{\alpha+\beta}\text{Beta}(\beta+1, \alpha)$ where the coefficients are the drawing probabilities. Let $a_\lambda = 1 - \lambda$ and $[n] = \{1, \ldots, n\}$.

2.2 MOTIVATION FROM IMPLICIT REGULARIZATION OF MIXUP

Here we show a theorem that optimizing the vanilla Mixup loss induces an implicit regularization on directional derivatives of the model f_θ.

Theorem 1. *Let $\ell(\theta, \mathbf{z}) \triangleq h(f_\theta(\mathbf{x})) - \mathbf{y}^\top f_\theta(\mathbf{x})$ be the loss function and $\forall \theta \in \Theta$ functions $f_\theta(\cdot)$ in a C^k manifold. Then the implicit regularization of Mixup is:*

$$\begin{aligned} L_n^{mix}(\theta, S) &= L_n^{std}(\theta, S) \\ &+ \frac{1}{n}\sum_{i=1}^n \mathbb{E}_{\substack{\lambda \sim \mathcal{D}_\lambda \\ \mathbf{x}' \sim \mathcal{D}_X}} \Bigg(\sum_{k=1}^K \frac{a_\lambda^k}{k!} \mathbf{J}_{h \circ f_\theta}^k(\mathbf{x}_i) \Delta_i^{\otimes k} \\ &- a_\lambda \mathbf{y}_i^\top \Delta_i + a_\lambda^K \hat{\psi}_{i,\mathbf{x}'}(a_\lambda) \Bigg) \end{aligned} \tag{2}$$

where $\mathbf{J}_{h \circ f_\theta}(\mathbf{x}_i) = g(f_\theta(\mathbf{x}_i))^\top \mathbf{J}_{f_\theta}(\mathbf{x}_i)$ and

$$\Delta_i = \sum_{k=1}^K \frac{a_\lambda^{k-1}}{k!} \mathbf{J}_{f_\theta}^k(\mathbf{x}_i)(\mathbf{x}' - \mathbf{x}_i)^{\otimes k} + a_\lambda^{K-1} \psi_{i,\mathbf{x}'}(a_\lambda). \tag{3}$$

Remark 1. $\hat{\psi}_{i,\mathbf{x}'}$ and $\psi_{i,\mathbf{x}'}$ are the remainder terms in Taylor expansion of order $\mathcal{O}(K)$ and with probability 1, $\lim_{a_\lambda \to 0} \hat{\psi}_{i,\mathbf{x}'}(a_\lambda) = 0$, $\lim_{a_\lambda \to 0} \psi_{i,\mathbf{x}'}(a_\lambda) = 0$. For cross-entropy loss $h(z) = \log\left(\sum_k \exp(z_k)\right)$, the derivative of each element is $\frac{\partial h(\mathbf{z})}{\partial \mathbf{z}_{(t)}} = [\sum_j \exp(\mathbf{z}_{(j)})]^{-1} \exp(\mathbf{z}_{(t)}) = g(\mathbf{z})_{(t)}$, Similarly, the logistic loss has same derivative form

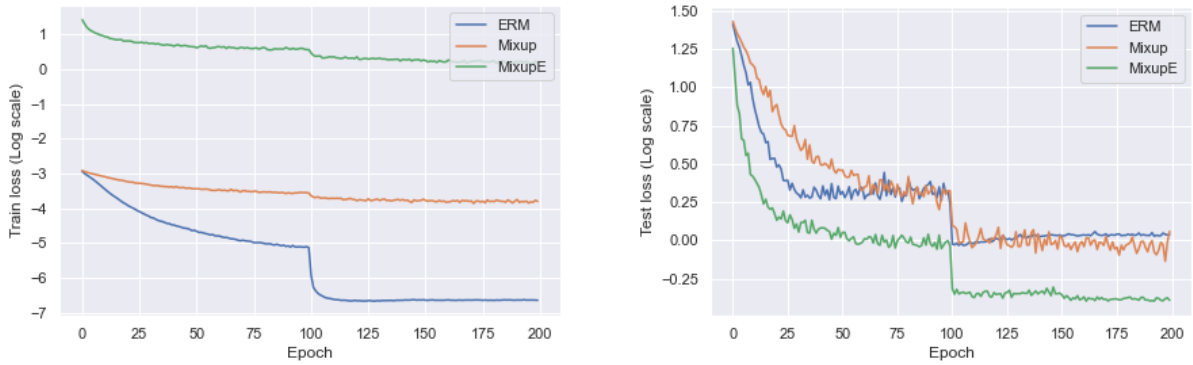

Figure 1: Comparison of train and test loss of ERM, Mixup, and *MixupE*. We see that *MixupE* has higher training loss but better test loss than Mixup and ERM.

$\frac{\partial h(z)}{\partial z} = (1 + \exp(z))^{-1}\exp(z) = g(z)$. Therefore, for both cases, we have the Jacobian w.r.t $\mathbf{x}_i$ $\mathbf{J}_{h \circ f_\theta}(\mathbf{x}_i) = g(f_\theta(\mathbf{x}_i))^\top \mathbf{J}_{f_\theta}(\mathbf{x}_i) \in \mathbb{R}^{1\times d}$.

The proof of Theorem 1 is given in Appendix A. Theorem 1 provides the following novel insight: while we can understand the implicit regularization of Mixup, we cannot replace it by explicitly computing the regularizer, because it involves infinite terms. Instead, it is expected to follow the Mixup to propose an efficient closed-form regularization.

In this view, Theorem 1 provides a theoretical motivation to further improve Mixup by enhancing its regularization effect in terms of directional derivatives. For computational efficiency, we propose to strengthen the first-order term while letting Mixup implicitly take care of the higher-order terms. In Theorem 1, the regularization effect of Mixup on the first-order directional derivatives ($k = 1$) is captured by $\frac{1}{n}\mathbb{E}_{\lambda\sim\mathcal{D}_\lambda}[a_\lambda]\sum_{i=1}^n q(\mathbf{x}_i)$, where

$$q(\mathbf{x}_i) = (g(f_\theta(\mathbf{x}_i)) - \mathbf{y}_i)^\top \mathbf{J}_{f_\theta}(\mathbf{x}_i)(\mathbb{E}[\mathbf{x}'] - \mathbf{x}_i) \quad (4)$$

and $\partial f_\theta(\mathbf{x}_i) \in \mathbb{R}^{C\times d}$. Since $0 < a_\lambda < 1$ and very small, the first-order derivative dominates the rest terms. Therefore, it turns out to be a stitch in time saves nine. Furthermore, $q(\mathbf{x}_i)$ can be approximated by

$$\hat{q}(\mathbf{x}_i) = (\mathbf{y}_i - g(f_\theta(\mathbf{x}_i)))^\top f_\theta(\mathbf{x}_i), \quad (5)$$

which lessens the computational burden by removing the derivatives of f_θ. This approximation $q(\mathbf{x}_i) = \hat{q}(\mathbf{x}_i)$ holds true when $\mathbb{E}_{\mathbf{x}'\sim\mathcal{D}_X}[\mathbf{x}'] = 0$ and $\mathbf{J}_{f_\theta}(\mathbf{x}_i)\mathbf{x}_i = f_\theta(\mathbf{x}_i)$. To this end, we can normalize the training dataset with zero means to realize the first condition. The second condition can be guaranteed from the linear model, i.e deep neural networks with ReLU activation. Thus we have the approximation that $q(\mathbf{x}_i) \approx \hat{q}(x_i)$ and $\mathbf{J}_{f_\theta}(\mathbf{x}_i)\mathbf{x}_i \approx f_\theta(\mathbf{x}_i)$.

However, there is an issue of negativity in the implicit (first-order) regularization of Mixup. Let $\alpha_{k,i} = (g(f(\mathbf{x}_i)_{(k)}) - \mathbf{y}_i)\zeta_{k,i}$, (4) can be rewritten as

$$q(\mathbf{x}_i) = \sum_{j=1}^{C} \alpha_{j,i}\|\mathbf{J}_{f_\theta}(\mathbf{x}_i)_{(j)}\|_2 \|\mathbb{E}_{\mathbf{x}'\sim\mathcal{D}_X}[\mathbf{x}'] - \mathbf{x}_i\|_2 \quad (6)$$

where $f(\mathbf{x}_i)_{(j)}$ is the j-th coordinate of $f(\mathbf{x}_i)$ and coefficient $\zeta_{j,i}$ is the cosine similarity between $\partial f(\mathbf{x}_i)_{(j)} \in \mathbb{R}^d$ and $\mathbb{E}_{\mathbf{x}'\sim\mathcal{D}_X}[\mathbf{x}'] - \mathbf{x}_i$. If $\alpha_{j,i}$ is positive, then Mixup tends to minimize all first-order directional derivatives $\|\mathbf{J}_{f_\theta}(\mathbf{x}_i)_{(j)}\|_2, j \in [C]$. However, if $\alpha_{j,i}$ is negative, Mixup has an unintended effect of maximizing $\|\mathbf{J}_{f_\theta}(\mathbf{x}_i)_{(j)}\|_2$. Figure 2 shows that the minimum values of α are negative for some sample x_i and coordinate k in the initial phase of Mixup training. We show these values for both Preactresnet18 and Preactresnet50 architectures on CIFAR10 dataset.

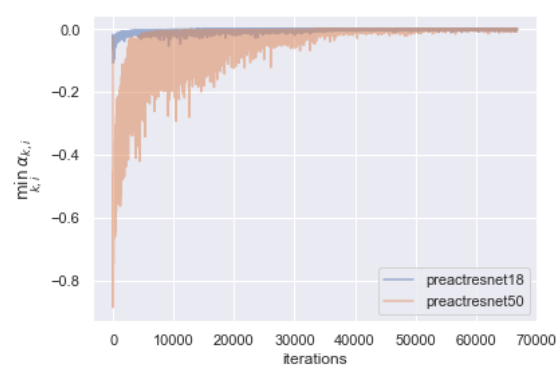

Figure 2: Minimum value of α over the coordinate k and sample i for different iterations during the training.

2.3 PROPOSED MIXUPE

To avoid the unintended effect of maximizing $\|\mathbf{J}_{f_\theta}(\mathbf{x}_i)_{(j)}\|_2$ in the initial phase of Mixup training, the proposed method adds the following term to the original loss to strengthen the

Algorithm 1 Algorithm of *MixupE*

Require: Model $f_\theta : \mathbb{R}^d \to \mathbb{R}^C$. Hyperparameters α, β for beta distribution (mean $\overline{\lambda}$). Loss function ℓ.

while Training epochs $< N$ **do**
  for Batch of data $X \in \mathbb{R}^{m\times d}, Y \in \mathbb{R}^{m\times C}$ in training set of size m **do**
    Sample $\lambda \sim \text{Beta}(\alpha, \beta)$
    Mixup data with $\tilde{X}, \tilde{Y} \leftarrow \lambda(X, Y) + a_\lambda \text{Permute}(X, Y)$
    Mixup Loss $L_n^{mix}(\theta, X) = \ell(f_\theta(\tilde{X}), \tilde{Y})$
    Compute first-order directional derivatives that $\hat{q}(X) = f_\theta(X) \otimes (Y - \text{Softmax}(f_\theta(X)))$
    Get additional loss $R(\theta, X)$ via (5)
    $\mathcal{L} \leftarrow \hat{\eta}\left(L_n^{mix}(\theta, S) + \eta R(\theta, S)\right)$ via (7)
    Optimize parameters θ with loss $\mathcal{L}$
  end for
end while

vanilla Mixup:

$$R(\theta, S) = \frac{\mathbb{E}_{\lambda\sim\mathcal{D}_\lambda}[a_\lambda]}{n} \sum_{i=1}^{n} |\tilde{q}(\mathbf{x}_i)|, \tag{7}$$

where $\tilde{q} = q$ for the accurate version and $\tilde{q} = \hat{q}$ for the approximate version. The functions q and $\hat{q}$ are defined in equations (4) and (5). The approximate version does not require computation of the directional derivatives and the additional computational cost is negligible because $f_\theta(\mathbf{x}_i)$ is known for the original loss and the value of $\mathbb{E}_{\lambda\sim\mathcal{D}_\lambda}[a_\lambda]$ is a fixed number over epochs: e.g., $\mathbb{E}_{\lambda\sim\mathcal{D}_\lambda}[a_\lambda] = 1 - \frac{\alpha+1}{2\alpha+1}$ when $\text{Beta}(\alpha, \alpha)$ is used for Mixup. To justify the rationality of our proposed regularization, we consider a degenerate case. Given a mixup distribution $\text{Beta}(\alpha, \beta)$, if $\alpha, \beta \to 0$, we have that $R(\theta, S) \to 0$ as $\mathbb{E}_{\lambda\sim\mathcal{D}_\lambda}[a_\lambda] \to 0$. In this case, Mixup behaves closely to ERM (i.e., mixup coefficient λ goes to 0). Then additional term $R(\theta, S)$ vanishes and is consistent with the behavior of vanilla Mixup. However, introducing $R(\theta, S)$ brings the artifacts when computing the training loss. In line with the original mixup training, we rescale the loss magnitude as before. Overall, we propose an explicit regularization $R(\theta, S)$ for vanilla Mixup to strengthen the implicit effect, namely *MixupE*, where the total loss is defined as below:

$$\mathcal{L}(\theta, S) := \hat{\eta}\left(L_n^{mix}(\theta, S) + \eta R(\theta, S)\right) \tag{8}$$

$$\hat{\eta} = \frac{|L_n^{mix}(\theta, S)|}{|L_n^{mix}(\theta, S) + \eta R(\theta, S)|} \tag{9}$$

where $\hat{\eta}$ is a scaling factor that depends on the magnitudes of $L_n^{mix}(\theta, S)$ and $R(\theta, S)$. Note that $\eta > 0$ is the only hyperparameter of the proposed method.

The whole algorithm of *MixupE* is shown in Algorithm 1. Extending Mixup to *MixupE* requires one additional forward pass on the *original* (non-mixed) sample for computing the additional loss term and requires one additional hyperparameter η in comparison to Mixup. We note that the Algorithm 1 shows how to apply *MixupE* when the training sample is in the form of a fixed shape tensor (for example, images, tabular data). If applying *MixupE* to training samples that have irregular (not fixed) topology, such as graphs, sequences, and trees, we need first to project the input samples to a fixed shape hidden states using an encoder network. After this projection, *MixupE* can be applied in the usual form.

Theoretical justification: To validate the rationality of the *MixupE*, we focus on justifying the generalization improvement over Mixup. Considering the vanilla Mixup as the original unconstrained problem, then the constraint Θ in the dual problem of *MixupE* will be

$$\Theta = \{\mathbf{x} \to f_\theta(\mathbf{x}) | \sup_{\mathbf{x}} \hat{q}(\mathbf{x}) \leq \gamma\} \tag{10}$$

Following Zhang et al. [2021], we consider Generalized Linear Model $h(f_\theta(\mathbf{x})) = A(\theta^\top \mathbf{x})$ for *MixupE*. For simplicity, we assume $\mathbf{y}$ can be represented by $(\theta^*)^\top \mathbf{x}$. Thus, there exists a diagonal matrix Σ of size d such that $\theta^* = \Sigma\theta$. We proved the following generalization gap:

Theorem 2. *Suppose $A(\cdot)$ is L_A-Lipchitz continuous, $\mathcal{X}, \mathcal{Y}$ and Θ are all bounded, the label of GLM is $\mathbf{y} = (\Sigma\theta)^\top \mathbf{x}$, then there exist constants $L, B > 0$, such that for all θ satisfying $\sup_{\mathbf{x}} \hat{q}(\mathbf{x}) \leqslant \gamma$, we have*

$$\begin{aligned}\mathcal{L}(\theta, S) \leq \hat{\eta}\eta L_n^{mix}(\theta, S) + \frac{2\hat{\eta}\eta L L_A(L_A + \sqrt{\gamma\overline{\sigma}})}{\overline{\sigma}\sqrt{n}} \\ + B\sqrt{\frac{\log(1/\delta)}{2n}}\end{aligned} \tag{11}$$

and $\overline{\sigma} = \sup_\Sigma \frac{\text{tr}(\Sigma)}{d}$ with probability at least $1 - \delta$.

See proof in Appendix B. Note that for vanilla Mixup, the general parameter constraint i.e $\|\theta\|^2 \leq \gamma$ will be up to $\sqrt{\gamma \cdot \text{MaxNorm}(\mathbf{x})/n}$ which depends on the maximum norm of data which can be much larger than the second term in the above inequality. In addition, $\overline{\sigma}$ is the average value of the maximum correction matrix to the ground truth which can be large as well. (we discuss the detail in Appendix B). It tells us that the regularized version of Mixup leads to better generalization due to the constraint on parameter space and validates the rationality of *MixupE*.

3 RELATED WORK

Mixup [Zhang et al., 2018, Tokozume et al., 2017] and its numerous variants have seen remarkable success in supervised learning problems, as well as other problems such as semi-supervised learning [Verma et al., 2021a, Berthelot et al., 2019], unsupervised learning using autoencoders [Beckham et al., 2019, Berthelot* et al., 2019], adversarial

learning [Lamb et al., 2019, Lee et al., 2020, Pang* et al., 2020], graph-based learning [Verma et al., 2019b], computer vision [Yun et al., 2019, Jeong et al., 2021, Panfilov et al., 2019, Faramarzi et al., 2020], natural language [Guo et al., 2019, Zhang et al., 2020] and speech [Lam et al., 2020, Tomashenko et al., 2018].

Mixup [Zhang et al., 2018] creates synthetic training samples by linear interpolation in the input vectors and their corresponding labels. The follow-up work of Mixup can be categorized into two main categories: (a) methods that propose a *non-linear* interpolation in the input vector (or hidden vectors), examples of this category include Yun et al. [2019], Faramarzi et al. [2020], Kim et al. [2020], Zhang et al. [2020], Verma et al. [2021b]. (b) methods that extend linear interpolation based Mixup training to various learning paradigms or applications, examples of this class include Mixup based training for supervised learning [Verma et al., 2019a], semi-supervised learning [Verma et al., 2021a, Berthelot et al., 2019], for adversarial training [Lamb et al., 2019], for node classification [Verma et al., 2019b], and for natural language processing [Guo et al., 2019]. The method proposed in this work can be applied to any of the methods in the latter category, and we leave experimental evaluation of *MixupE* applied to these methods for future work.

Theoretically, Mixup has been analyzed in Zhang et al. [2021] in which the authors show that it is approximately equivalent to adding a second-order regularizer to improve robustness and generalization. They did not propose a method based on the theory. In contrast, this paper shows that it is equivalent to adding infinite regularizations on the directional derivatives of all orders, and used this theory to propose a new method.

4 EXPERIMENTS

We present a range of experiments to back up the methodological claims, demonstrate versatility across benchmark problems, and show practical applicability on images, tabular data, and speech problems.

4.1 IMAGE DATASETS

For small-scale image datasets, we consider CIFAR-10, CIFAR-100, SVHN, and Tiny-ImageNet. We run our experiments using a variety of architectures including PreActResNet18, PreActResNet34, PreActResNet50, PreActResNet101 [He et al., 2016], and Wide-Resnet-28-10 [Zagoruyko and Komodakis, 2016].

Throughout our experiments, we use SGD+Momentum optimizer with batch-size 100, learning rate 0.1, momentum 0.9 and weight-decay 10^{-4}, with step-wise learning rate decay. We train all the networks for all the datasets for 200 epochs and the learning rate is annealed by a factor of 10 at epochs 100 and 150.

Hyperparameters α and η: For Mixup on CIFAR-10 and CIFAR-100 datasets, we used the value $\alpha = 1.0$ as recommended in Zhang et al. [2018]. For Mixup on SVHN and Tiny-ImageNet datasets, we experimented with the α values 1.0 and 0.2 respectively as recommended in Verma et al. [2019a]. We experimented with the $\eta \in \{0.0001, 0.001, 0.01, 0.1\}$, and obtained the best results using $\eta = 0.001$ for most of the experiments, and using $\eta = 0.0001$ for the remaining experiments.

Results: We show results for the CIFAR-10 (Table 1a), CIFAR-100 (Table 1b), SVHN (Table 2a), and Tiny-ImageNet (Table 2b) datasets. We see that *MixupE* consistently outperforms baseline methods ERM and Mixup across all the datasets and architectures.

Sensitivity to hyperparameter η: To validate that the method is not overly sensitive to the newly introduced hyperparameter η, we conducted experiments for *MixupE* with the value of $\eta \in \{0.0001, 0.001, 0.01, 0.1\}$ with Preactresnet50 architecture and CIFAR100 dataset. This experiment was repeated five times with different initializations. We got the mean test error (in %) of $20.23, 20.84, 21.01, 20.87$ for the η values of $0.0001, 0.001, 0.01, 0.1$, respectively, vs the mean test-error 23.03 for Mixup. This suggests that the proposed method *MixupE* is not overly sensitive to the hyperparameter η and works better than Mixup for a large range of η values.

For a large-scale image classification dataset, we consider ImageNet [Deng et al., 2009], using three architectures: ResNet [He et al., 2016], Vision Transformer [ViT, Dosovitskiy et al., 2020], and CoAtNet [Dai et al., 2021]. In particular, we use ResNet-50, ViT-B/16, and CoAtNet-0. We choose these architectures for experiments because they are fast to train, and they respectively represent the three families of image classification models: convolution-based models, attention-based models, and hybrid models.

Except for the Mixup-related hyperparameters α and η, all training hyperparameters for these models follow their original paper. Specifically, all models are trained and evaluated at the resolution of 224x224. Our ResNet-50 is trained with a SGD+Momentum with the momentum coefficient of 0.9, while our ViT-B/16 and CoAtNet-0 are both trained with AdamW [Loshchilov and Hutter, 2018], $\beta_1 = 0.9$ and $\beta_2 = 0.99$. An L_2 weight decay of 10^{-4} is applied to our ResNet-50, while the larger weight decays of 0.05 and 0.3 are applied to our CoAtNet-0 and ViT-B/16, respectively.

All models were trained for 100K steps, with a global batch size of 4096. Throughout these 100K training steps, the learning rate starts from 0 and warms up linearly to its peak value – which is 1.6 for ResNet-50 and 0.001 for ViT and CoAtNet – and then decreases to 1/1000 times the peak

Table 1: Classification errors on (a) CIFAR-10 and (b) CIFAR-100. Standard deviations over five repetitions. Best performing methods in **bold**.

(a) CIFAR-10

PreActResNet50	Test Error (%)
ERM	$4.71_{\pm 0.062}$
Mixup	$4.53_{\pm 0.041}$
MixupE	$\mathbf{3.53}_{\pm 0.047}$
PreActResNet101	
ERM	$4.21_{\pm 0.069}$
Mixup	$4.43_{\pm 0.049}$
MixupE	$\mathbf{3.35}_{\pm 0.049}$
Wide-Resnet-28-10	
ERM	$4.24_{\pm 0.101}$
Mixup	$3.03_{\pm 0.091}$
MixupE	$\mathbf{2.94}_{\pm 0.048}$

(b) CIFAR-100

PreActResNet50	Test Error (%)
ERM	$24.68_{\pm 0.349}$
Mixup	$23.03_{\pm 0.471}$
MixupE	$\mathbf{20.23}_{\pm 0.507}$
PreActResNet101	
ERM	$23.20_{\pm 0.362}$
Mixup	$23.05_{\pm 0.383}$
MixupE	$\mathbf{18.86}_{\pm 0.376}$
Wide-Resnet-28-10	
ERM	$22.20_{\pm 0.108}$
Mixup	$19.38_{\pm 0.113}$
MixupE	$\mathbf{17.12}_{\pm 0.111}$

Table 2: Classification error on SVHN and classification accuracy on Tiny-Imagenet. Standard deviations over five repetitions. Best performing methods in **bold**.

(a) Classification Error on SVHN

PreActResNet50	Test Error (%)
ERM	$4.71_{\pm 0.062}$
Mixup	$4.53_{\pm 0.041}$
MixupE	$\mathbf{3.53}_{\pm 0.047}$
PreActResNet101	
ERM	$4.21_{\pm 0.069}$
Mixup	$4.43_{\pm 0.049}$
MixupE	$\mathbf{3.35}_{\pm 0.049}$
Wide-Resnet-28-10	
ERM	$4.24_{\pm 0.101}$
Mixup	$3.03_{\pm 0.091}$
MixupE	$\mathbf{2.94}_{\pm 0.048}$

(b) Classification Accuracy on Tiny-ImageNet

PreActResNet18	top-1	top-5
ERM	$54.97_{\pm 0.52}$	$72.71_{\pm 0.48}$
Mixup	$54.64_{\pm 0.43}$	$72.53_{\pm 0.51}$
MixupE	$\mathbf{62.21}_{\pm 0.39}$	$\mathbf{82.09}_{\pm 0.41}$
PreActResNet34		
ERM	$57.25_{\pm 0.48}$	$72.58_{\pm 0.53}$
Mixup	$57.79_{\pm 0.39}$	$76.15_{\pm 0.42}$
MixupE	$\mathbf{65.37}_{\pm 0.31}$	$\mathbf{83.77}_{\pm 0.35}$
PreActResNet50		
ERM	$55.91_{\pm 0.61}$	$73.50_{\pm 0.57}$
Mixup	$54.86_{\pm 0.46}$	$73.11_{\pm 0.43}$
MixupE	$\mathbf{67.22}_{\pm 0.38}$	$\mathbf{85.14}_{\pm 0.36}$

value following the cosine schedule. For models with batch normalization, i.e., ResNet-50 and CoAtNet-0, the batch statistics during training are computed globally. We also apply a Polyak moving average with the rate of 0.999 on all parameters, *including* the batch normalization cumulative statistics in the case of ResNet-50 and CoAtNet-0.

Hyperparameters α and η: we use the Mixup rate $\alpha = 0.2$ for ResNet-50, following the suggestions from Zhang et al. [2018]. Since ViT-B/16 and CoAtNet-0 were invented after Mixup, we first tune the value of α and found that $\alpha = 0.4$ offers a sweet spot for these models. Fixing $\alpha = 0.2$ for ResNet-50 and $\alpha = 0.4$ for ViT-B/16 and CoAtNet-0, we then tune the values for η with ResNet-50. We find that $\eta = 10^{-3}$ is best for ResNet-50 while the smaller value of $\eta = 5 \times 10^{-4}$ is best for ViT-B/16 and CoAtNet-0.

ImageNet results: Table 3 presents our results. We observe that *MixupE* consistently outperforms Mixup across the three architectures in our experiments. Notably, the gains of *MixupE* – in terms of top-1 accuracy – are larger for ViT-B/16 and CoAtNet-0 than for ResNet-50, *i.e.* +0.7 and +0.8 compared to +0.5, even though the top-1 accuracy of the Mixup baselines for ViT-B/16 and CoAtNet-0 are higher. We note that other extensions of Mixup, such as CutMix [Yun et al., 2019], PuzzleMix [Kim et al., 2020], and PatchUp [Faramarzi et al., 2020] use *non-linear* mixing of samples, thus they are not directly comparable with *MixupE*. We leave an experimental comparison of *MixupE* with these methods using a common implementation scheme (architecture and training/validation protocol) as a future work.

A note on implementation and runtime. Despite these im-

Table 3: ImageNet accuracy of various models. Each experiment was run for 3 times.

Models	MixUp Type	Top-1	Top-5
ResNet-50	None	$76.2_{\pm 0.5}$	$93.6_{\pm 0.3}$
	MixUp	$77.2_{\pm 0.2}$	$94.0_{\pm 0.1}$
	MixupE	$\mathbf{77.7}_{\pm 0.2}$	$\mathbf{94.4}_{\pm 0.1}$
ViT-B/16	None	$79.1_{\pm 0.2}$	$95.1_{\pm 0.1}$
	MixUp	$79.7_{\pm 0.2}$	$95.4_{\pm 0.1}$
	MixupE	$\mathbf{80.4}_{\pm 0.1}$	$\mathbf{95.8}_{\pm 0.1}$
CoAtNet-0	None	$79.8_{\pm 0.2}$	$95.1_{\pm 0.1}$
	MixUp	$80.8_{\pm 0.3}$	$95.5_{\pm 0.1}$
	MixupE	$\mathbf{81.6}_{\pm 0.2}$	$\mathbf{95.7}_{\pm 0.2}$

provements, *MixupE* requires twice as many forward passes as compared to normal Mixup. As shown in Algorithm 1, the extra computation stems from the forward pass through the original (non-mixed) samples X, *i.e.* $f_\theta(X)$. For larger models running on ImageNet, this cost can lead to significantly slower experiment time. To alleviate the computational burden, we "batch" this extra pass through the non-mixup data into the pass through the mixup data. Thanks to this trick, our implementation of *MixupE* is only 1.3 times slower than Mixup.

4.2 TABULAR DATASETS

We consider a number of tabular environments drawn from the UCI dataset [Lichman et al., 2013], namely *Arrhythmia, Letter, Balance-scale, Mfeat-factors, Mfeat-fourier, Mfeat-karhunen, Mfeat-morphological, Mfeat-zernike, CMC, Optdigits, Pendigits, Iris, Mnist_784, Abalone* and *Volkert*.

We consider the same setting as Zhang et al. [2018] where the network is a fully-connected multi-layer perceptron (MLP) with two hidden layers, each with 128 dimensions, with ReLU activations for non-linearity. We train this network with the Adam optimizer using the cross-entropy loss with the default learning rate of 0.001 and a batch size of 100, for 25 epochs. We feed in the categorical part of the data as one-hot inputs, and for any samples with missing features in the dataset, we fill it with the mean (for continuous) or mode (for discrete) of those features.

Hyperparameters α and η: We consider the hyperparameters from the set $\alpha \in \{0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1.0, 2.0, 5.0\}$ and $\eta \in \{0.0001, 0.001, 0.01, 0.1, 1.0\}$ and run five seeds for each of the combinations and algorithms. Then, the value of (α, η) is chosen based on the best validation accuracy, corresponding to which we report the test accuracy for that particular dataset.

Results: Table 4 presents our results for a subset of the tabular datasets (see appendix) for results on all datasets).

Table 4: Classification Test Error (%) on tabular datasets from UCI repository. Results are averaged over five trials.

Dataset	Method		
	ERM	Mixup	*MixupE*
Arrhythmia	$\mathbf{34.60}_{\pm 3.10}$	$35.49_{\pm 3.88}$	$34.85_{\pm 3.99}$
Letter	$4.56_{\pm 0.27}$	$\mathbf{3.71}_{\pm 0.18}$	$4.04_{\pm 0.20}$
Balance-scale	$3.87_{\pm 1.03}$	$3.70_{\pm 1.00}$	$\mathbf{3.68}_{\pm 0.97}$
Mfeat-factors	$2.74_{\pm 0.81}$	$\mathbf{2.44}_{\pm 0.42}$	$2.56_{\pm 0.64}$
Mfeat-fourier	$17.69_{\pm 1.76}$	$17.80_{\pm 1.56}$	$\mathbf{17.57}_{\pm 1.60}$
Mfeat-karhunen	$3.74_{\pm 0.58}$	$3.06_{\pm 0.29}$	$\mathbf{2.47}_{\pm 0.32}$
Mfeat-morph	$25.00_{\pm 2.10}$	$\mathbf{24.62}_{\pm 1.83}$	$24.66_{\pm 1.30}$
Mfeat-zernike	$17.58_{\pm 1.72}$	$\mathbf{15.19}_{\pm 1.73}$	$15.55_{\pm 0.62}$
CMC	$45.77_{\pm 1.49}$	$46.67_{\pm 1.83}$	$\mathbf{45.42}_{\pm 2.05}$
Optdigits	$1.48_{\pm 0.19}$	$\mathbf{1.15}_{\pm 0.21}$	$1.33_{\pm 0.14}$
Pendigits	$1.03_{\pm 0.25}$	$0.76_{\pm 0.19}$	$\mathbf{0.72}_{\pm 0.16}$
Iris	$9.06_{\pm 7.01}$	$8.14_{\pm 6.48}$	$\mathbf{7.29}_{\pm 6.95}$
Mnist_784	$2.83_{\pm 0.11}$	$2.57_{\pm 0.05}$	$\mathbf{2.56}_{\pm 0.14}$
Abalone	$35.05_{\pm 0.61}$	$35.07_{\pm 0.69}$	$\mathbf{34.91}_{\pm 0.70}$
Volkert	$33.26_{\pm 0.62}$	$32.74_{\pm 0.76}$	$\mathbf{32.54}_{\pm 0.61}$

We observe that *MixupE* outperforms the standard Mixup as well as ERM across multiple datasets.

4.3 SPEECH DATASET

To have a rigorous comparison with Zhang et al. [2018], similar to their work, for speech dataset we use Google commands dataset [Warden, 2018]. This dataset consists of 65000 one-second long utterances of 30 short words such as *yes, no, up, down, left, right, stop, go, on, off*, by thousands of different people. 30 short words correspond to 30 classes. We preprocess the utterances by first extracting the normalized spectrograms from the original waveform at a sampling rate of 16 kHz, followed by zero-padding the spectrograms to equalize their size at 160×101. This preprocessing step is exactly same as Zhang et al. [2018]. Furthermore, similar to Zhang et al. [2018], we use LeNet [LeCun et al., 1998] and VGG-11 and VGG-13 [Simonyan and Zisserman, 2014] architectures. We train all the models for 20 epochs using Adam optimizer with a learning rate of 0.001 and batch-size of 100.

Hyperparameters α and η: For all the architectures, we first find the best value of hyperparameter α for Mixup from the set $\alpha \in \{0.1, 0.2, 0.5, 1.0, 2.0\}$. We observed that $\alpha = 0.2$ works best consistently for all architectures. For *MixupE*, we used the best α values from Mixup, and only fine-tuned the η hyperparameter using $\eta \in \{0.001, 0.01, 0.1, 1.0\}$. In our experiments $\eta = 0.01$ works best for all the experi-

Table 5: Classification Test Error (%) on Google Speech Command Dataset [Warden, 2018]. We run each experiment five times

Architecture	**Method**		
	ERM	Mixup	*MixupE*
LeNet	$10.43_{\pm 0.052}$	$10.12_{\pm 0.041}$	$\mathbf{10.02}_{\pm 0.042}$
VGG-11	$6.04_{\pm 0.059}$	$4.63_{\pm 0.047}$	$\mathbf{3.93}_{\pm 0.050}$
VGG-13	$5.77_{\pm 0.053}$	$4.68_{\pm 0.039}$	$\mathbf{3.84}_{\pm 0.040}$

ments.

Results: In Table 5, we observe that *MixupE* improves the test error of Mixup for different architectures. Moreover, the improvement is more significant for larger architectures such as VGG-11 and VGG-13 than LeNet.

4.4 GRAPH DATASETS

For graph classification, we consider the *MUTAG, NCI1, PTC, PROTEINS, IMDB-BINARY* and *IMDB-MULTI* datasets. We use the experimental settings defined in Xu et al. [2018] as the baseline system, where Mixup and *MixupE* is performed after encoding the graph to a fixed dimensional vector, that is, at the graph-level readout stage. Each system here relies on 5 graph neural network layers that give rise to the readout, which is then operated on by a non-linear MLP. The models are trained for 350 epochs using Adam optimizer with a learning rate of 0.01, which is halved every 50 epochs. For the hyperparameters, we consider $\alpha \in \{0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1.0, 2.0, 5.0\}$ and $\eta \in \{0.0001, 0.001, 0.01, 0.1, 1.0\}$. Corresponding to each model setting, we perform 10-fold validation and identify which epoch and hyperparameters give the best test accuracy, and report the final mean and standard deviation of the algorithm on it over the ten folds. We refer the readers to Table 6, which shows the benefits of using *MixupE* on the graph datasets.

4.5 ABLATION EXPERIMENTS

In *MixupE*, we have proposed to add an additional loss term derived from the first-order derivative (7) to the Mixup Loss 8. A natural question arises: what would be the performance of adding this term to the ERM loss? We conduct an ablation study to investigate this question. Specifically, we compare the following four methods : 1) ERM, 2) Mixup, 3) ERM+additional loss, 4) Mixup+additional loss (*MixupE*). The test error on CIFAR100 dataset using the Preactresnet50 architecture for the above mentioned method is shown in Table 7.

Results in Table 7 show that adding the additional loss term of Equation 7 improves the test accuracy in Mixup. This is consistent with our argument in Section 2.2 that Mixup can have an unintended effect of maximizing $\|\mathbf{J}_{f_\theta}(\mathbf{x}_i)_{(j)}\|_2$. Furthermore, we observe that Mixup+additional loss (*MixupE*) performs better than ERM+additional loss; this indicates that the implicit regulraization of higher order directional derivative through Mixup training is important for better test errors, thus justifying our proposed method.

Table 6: Classification Test Error (%) on graph datasets from the TUDatasets benchmark when following the setup of Xu et al. [2018]. Results are obtained from 10-fold validation.

Dataset	**Method**		
	ERM	Mixup	*MixupE*
MUTAG	$10.15_{\pm 0.06}$	$10.67_{\pm 0.05}$	$\mathbf{10.06}_{\pm 0.06}$
NCI1	$17.79_{\pm 0.02}$	$18.59_{\pm 0.02}$	$\mathbf{17.74}_{\pm 0.01}$
PTC	$38.37_{\pm 0.09}$	$\mathbf{34.87}_{\pm 0.08}$	$35.50_{\pm 0.08}$
PROTEINS	$25.43_{\pm 0.04}$	$24.44_{\pm 0.04}$	$\mathbf{23.72}_{\pm 0.04}$
IMDBBINARY	$25.60_{\pm 0.03}$	$25.30_{\pm 0.03}$	$\mathbf{25.20}_{\pm 0.03}$
IMDBMULTI	$50.33_{\pm 0.03}$	$49.27_{\pm 0.04}$	$\mathbf{48.53}_{\pm 0.03}$

Table 7: Ablation experiments to understand the effect of the additional loss term in Equation 7. Each experiment was run for 5 times.

Method	**Test Error**
ERM	24.68
Mixup	23.03
ERM+additional loss	22.42
Mixup+additional loss (*MixupE*)	20.23

5 CONCLUSION AND LIMITATIONS

In this work, we have theoretically derived a new method to improve Mixup. Our theory shows that Mixup is a computationally efficient way to regularize directional derivatives of all orders. Our method is mathematically designed to strengthen the regularization effect of Mixup with a generalization improvement guarantee Theorem 2. The proposed method *MixupE* outperforms Mixup on several datasets such as image, tabular, and speech datasets, trained with various networks. The improvement in test error is more significant for networks with larger capacities. As a limitation, our method requires one additional forward pass in the network during training than Mixup, but only suffers an extra 30% time cost than Mixup. While we only approximate the first-order term for the computational efficiency, our results suggest a promising future research direction to enhance Mixup by studying higher-order terms in Theorem 1

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