# On the Benefits of Defining Vicinal Distributions in Latent Space

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## Abstract

*The vicinal risk minimization (VRM) principle is an empirical risk minimization (ERM) variant that replaces Dirac masses with vicinal functions. Mixup Training (MT), a popular choice of vicinal distribution, improves generalization performance of models by introducing globally linear behavior in between training examples. Apart from generalization, recent works have shown that mixup trained models are relatively robust to input perturbations/corruptions and at same time are calibrated better than their non-mixup counterparts. In this work, we investigate the benefits of defining these vicinal distributions like mixup in latent space of generative models rather than in input space itself. We propose a new approach - VarMixup (Variational Mixup) - to better sample mixup images by using the latent manifold underlying the data. Our empirical studies on CIFAR-10, CIFAR-100 and Tiny-ImageNet demonstrates that models trained by performing mixup in the latent manifold learned by VAEs are inherently more robust to various input corruptions and are significantly better calibrated than vanilla mixup.*

## 1. Introduction

In most successful applications, Deep Neural Networks are trained to minimize the average error over the training dataset known as the Empirical Risk Minimization (ERM) principle [28]. However, various empirical and theoretical studies have shown that minimizing Empirical Risk over training datasets in over-parameterized settings leads to their memorization and thus poor generalization on examples just outside the training distribution. To mitigate this problem of memorization in over-parameterized neural networks, Vicinal Risk Minimization (VRM) was proposed which essentially chooses to train networks on similar but different examples to the training data. This technique more popularly known as data augmentation [22], requires one to define a vicinity or neighbourhood around each training example (eg. in terms of brightness, contrast, imperceptible noise, etc.). Once defined, more examples can be sampled from their vicinity to enlarge the support of training distribution.

One of the popular choices to create the vicinal distribution is Mixup. Mixup Training (MT) [34] has emerged as a popular technique to train models for better generalisation in the last couple of years. Recent works have also shown that the idea of Mixup and Mixup training can be leveraged during inference [20] and in many existing techniques like data augmentation [12], adversarial training [16], etc. to improve the robustness of models to various input perturbations [25, 31] and corruptions [12]. Other efforts on Mixup [26] have shown that Mixup-trained networks are significantly better calibrated and less prone to over-confident predictions on out-of-distribution than ones trained in the regular fashion. We mention other recent efforts in area of mixup and distinguish ourselves from them in the Appendix A.1.

Although still in its early phase, the above efforts [34, 29, 20, 26] also indicate a trend to viewing Mixup from perspectives of robustness and calibration. In this work, we take another step in this direction and propose a new vicinal distribution/sampling technique called *VarMixup (Variational Mixup)* to sample better Mixup images during training to induce robustness as well as improve predictive uncertainty of models. In particular, we hypothesize that the latent unfolded manifold underlying the data (through a generative model, a Variational Autoencoder in our case) is linear by construction (manifolds unfold the locally linear structure of a high-dimensional data space), and hence more suitable for the defining vicinal distributions involving linear interpolations, such as Mixup. Importantly, we show that this choice of the distribution for Mixup plays an important role towards robustness and predictive uncertainty (Section 3).

## 2. Background on Vicinal Risk Minimization

We denote a neural network as $F_w : \mathbb{R}^{c\times h\times w} \rightarrow \mathbb{R}^k$, with weight parameters $w$. $F_w$ takes an image $x \in \mathbb{R}^{c\times h\times w}$ and outputs logits, $F_w^i(x)$ for each class $i \in \{1...k\}$. Without loss of generality, we assume the classification task with $\mathcal{L}$ as the standard cross-entropy loss function. $p_{actual}$ de-

notes the training data distribution, and the optimal weight parameter $w^*$ is obtained by training the network using standard empirical risk minimization [28], i.e. $w^* = _w \mathbb{E}_{(\mathbf{x},y)\sim p_{actual}} [\mathcal{L}(F_w(\mathbf{x}), y)]$, where $y$ is the true label associated with input $x$.

Given the data distribution $p_{actual}$, a neural network $F_w$ and loss function $\mathcal{L}$, the *expected risk* (average of loss function over $p_{actual}$) is given by

$$R(F_w) = \int \mathcal{L}(F_w(x), y) \cdot dp_{actual}(x, y)$$

In practice, the true distribution $p_{actual}$ is unknown, and is approximated by the training dataset $D = \{(x_i, y_i)\}_{i=1}^N$, which represents the *empirical distribution*:

$$p_\delta(x, y) = \frac{1}{N} \cdot \sum_{i=1}^{N} \delta(x = x_i, y = y_i)$$

Here, $\delta(x = x_i, y = y_i)$ is the Dirac delta function centered at $(x_i, y_i)$. Using $p_\delta$ as an estimate to $p_{actual}$, we define *expected empirical risk* as

$$R_\delta(F_w) = \frac{1}{N} \cdot \sum_{i=1}^{N} \mathcal{L}(F_w(x_i), y_i)$$

Minimizing $R_\delta(F_w)$ to find optimal $F_{w^*}$ is typically termed *Empirical Risk Minimization (ERM)* [28]. However overparametrized neural networks can suffer from memorizing, leading to undesirable behavior of network outside the training distribution, $p_\delta$ [32, 25]. Addressing this concern, [27] and [5] proposed *Vicinal Risk Minimization (VRM)*, where $p_{actual}$ is approximated by a vicinal distribution $p_v$, given by

$$p_v(x, y) = \frac{1}{N} \cdot \sum_{i=1}^{N} v(x, y|x_i, y_i)$$

where $v$ is the *vicinal distribution* that calculates the probability of a data point $(x, y)$ in the vicinity of other samples $(x_i, y_i)$.
Thus, using $p_v$ to approximate $p_{actual}$, *expected vicinal risk* is given by

$$R_v(F_w) = \frac{1}{N} \cdot \sum_{i=1}^{N} g(F_w, \mathcal{L}, x_i, y_i)$$

where $g(F_w, \mathcal{L}, x_i, y_i) = \int \mathcal{L}(F_w(x), y) \cdot dv(x, y|x_i, y_i)$. The superiority of VRM over ERM has been theoretically as well as empirically verified by many recent works [19, 4, 9, 33].

Popular examples of vicinal distributions include: (i) *Gaussian Vicinal distribution*: Here, $v_{gaussian}(x, y|x_i, y_i) = \mathcal{N}(x - x_i, \sigma^2) \cdot \delta(y = y_i)$, which is equivalent to augmenting the training samples with Gaussian noise; and (ii) *Mixup Vicinal distribution* : Here $v_{mixup}(x, y|x_i, y_i) = \frac{1}{n} \cdot \sum_{j=1}^{N} \mathbb{E}_\lambda[\delta(x = \lambda \cdot x_i + (1 - \lambda) \cdot x_j, y = \lambda \cdot y_i + (1 - \lambda) \cdot y_j)]$, where $\lambda \sim \beta(\eta, \eta)$ and $\eta > 0$.

## 3. Our Approach: VarMixup (Variational Mixup)

In this work, we build on the recent success of using Mixup as a vicinal distribution by proposing the use of the latent spaces learned by a generative deep neural network model. The use of generative models such as Variational Autoencoders (VAEs) [15] to capture the latent space from which a distribution is generated provides us an unfolded manifold (the low-dimensional latent space), where the linearity in between training examples is more readily observed. Defining vicinal distributions by using neighbors on this latent manifold, which is more linear in the low-dimensional space, learned by generative models provides us more effective linear interpolations than the ones in input space. We hence leverage such an approach to capture the induced global linearity in between examples, and define Mixup vicinal distributions on this latent surface.

To capture the latent manifold of the training data through a generative model, we opt for a Variational Autoencoder (VAE). VAE [15] is an autoencoder which is trained using Variational Inference, which serves as an implicit regularizer to ensure that the obtained latent space allows us to generate new data from the same distribution as training data.

We denote the encoding and decoding distribution of VAE as $q_\phi(z|x)$ and $p_\theta(x|z)$ respectively, parametrized by $\phi$ and $\theta$ respectively. Given $p(z)$ as the desired prior distribution for encoding, the general VAE objective is given by the loss function:

$$\begin{aligned}\mathcal{L}_{VAE} = &-\gamma \cdot D(q_\phi(z)\|p(z)) \\ &+ \mathbb{E}_{x\sim p_{actual}} \mathbb{E}_{z\sim q_\phi(z|x)}[\log(p_\theta(x|z))]\end{aligned} \tag{1}$$

Here, $D$ is any strict divergence, meaning that $D(q\|p) \geq 0$ and $D(q\|p) = 0$ if and only if $q = p$, and $\gamma > 0$ is a scaling coefficient. The second term in the objective acts as a image reconstruction loss and $q_\phi(z) = \mathbb{E}_{x\sim p_{actual}}[q_\phi(z|x)]$. The original VAE [15] uses KL-divergence in Eqn 1. However, using KL-divergence in Eqn 1 has some shortcomings, as pointed out in [6, 23, 36, 24]. KL-divergence encourages the encoding $q_\phi(z|x)$ to be a random sample from $p(z)$ for each $x$, making them uninformative about the input. Also, it is not strong enough a regularizer compared to the reconstruction loss and tends to overfit data, consequently, learning a $q_\phi(z|x)$ that has high variance. Both the aforementioned shortcomings can affect the encoding distribution by making them uninformative of inputs with high variance. Since we use VAEs to better capture a linear latent manifold and subsequently define interpolations there, a bad latent distribution can affect our method significantly. We hence use a variant *Maximum Mean Discrepancy VAE* (MMD-VAE)[36] which uses a MMD Loss [7] instead of KL-divergence, and hence optimizes the following objec-

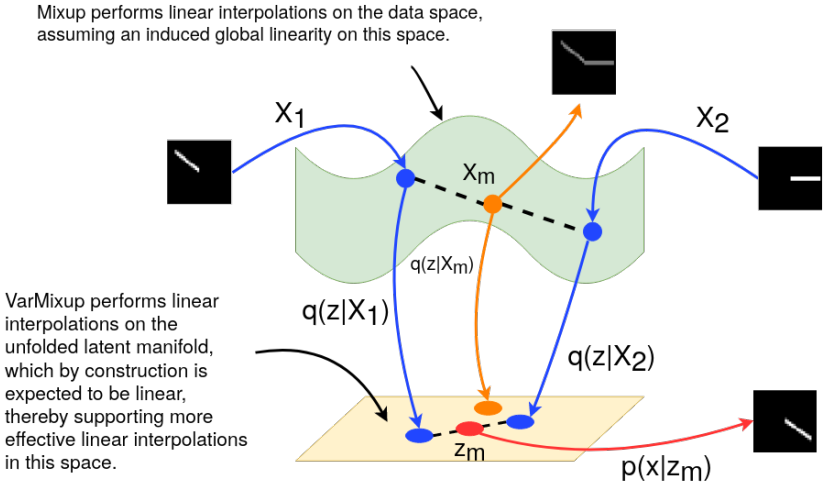


Figure 1. Illustration of conceptual idea behind VarMixup. We interpolate on the unfolded manifold, as defined by a generative model (VAE, in our case).

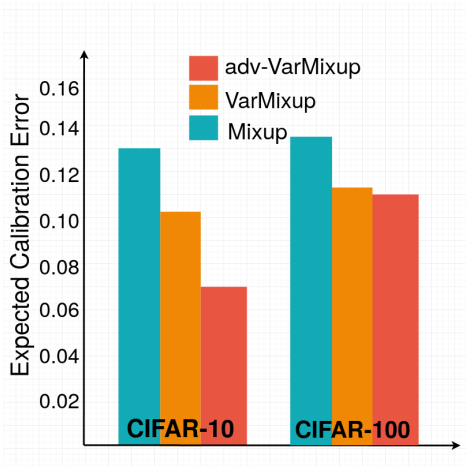


Figure 2. Expected Calibration Error (ECE) [8] of Mixup, VarMixup and adv-VarMixup trained models.

tive:

$$\mathcal{L}_{MMD-VAE} = \gamma \cdot MMD(q_\phi(z)\|p(z)) + \mathbb{E}_{x\sim p_{actual}}\mathbb{E}_{z\sim q_\phi(z|x)}[\log(p_\theta(x|z))] \quad (2)$$

A MMD-VAE doesn't suffer from the aforementioned shortcomings [36], as it maximizes mutual information between $x$ and $z$ by matching the distribution over encodings $q_\phi(z)$ with prior $p(z)$ only in expectation, rather than for every input. We hence train an MMD-VAE to characterize the training distribution more effectively. We now define a Mixup vicinal distribution in the latent space of the trained VAE as $v_{VarMixup}(z, y|x_i, y_i)$

$$= \frac{1}{n}\cdot\sum_{j=1}^{N}\mathbb{E}_\lambda[\delta(z = \lambda\cdot\mathbb{E}_z[q_\phi(z|x_i)] + (1-\lambda)\cdot\mathbb{E}_z[q_\phi(z|x_j)], y = \lambda\cdot y_i + (1-\lambda)\cdot y_j)]$$

where $\lambda \sim \beta(\eta, \eta)$ and $\eta > 0$. Using the above vicinal distribution, $v_{VarMixup}$ and the MMD-VAE decoder, $p_\theta(x|z)$, we construct VarMixup samples as:

$$x' = \mathbb{E}_x[p_\theta(x|\lambda\cdot\mathbb{E}_z[q_\phi(z|x_i)] + (1-\lambda)\cdot\mathbb{E}_z[q_\phi(z|x_j)])]$$
$$y' = \lambda\cdot y_i + (1-\lambda)\cdot y_j$$

From another perspective, one could view our new sampling technique as performing Manifold Mixup [29], however over the latent space of an MMD-VAE (instead of the neural network feature space) and using it for sample reconstruction. We compare against Manifold Mixup in our results to show the improved performance of the learned generative latent space in our VarMixup. Figure 1 illustrates the conceptual idea behind VarMixup.

## 4. Experiments and Results

We now present our experimental studies and results using our method, VarMixup where we focus explicitly on the usefulness of our approach on out-of-distribution test data and addressing predictive uncertainty. We also perform several ablation studies in Appendix A.3 to analyze our approach.

**Implementation Details:** It has been shown [14] that adversarial training removes irrelevant biases (e.g. texture biases) in their hidden representations, thus making them more informative. We hence hypothesize that the considered VAE, if trained adversarially, will have more informative latent encoding than its regular equivalent. This would hence help improve the vicinal distributions like VarMixup. Empirically, we validate this hypothesis in our subsequent experiments and use prefix *adv-* (eg: *adv*-VarMixup) to distinguish them from their regular variants. All models are trained using the Resnet-34 [10] backbone across all datasets.

**Baseline Models:** We compare our method, VarMixup, against Vanilla ERM, Vanilla Mixup [34], Manifold Mixup [29], $l_\infty$ PGD/TRADES adversarial training [18, 35] and $l_\infty$ Interpolated adversarial training [16]. These choice of baselines include non-VRM variants, mixup variants and state-of-the-art adversarial techniques. We also compare against a variant of mixup, which we call Mixup-R where mixup training is done on MMD-VAE's reconstructed image space rather than actual image space. Please refer to Appendix A.2 for more details on training of these baselines.

**Generalization Performance and Robustness to Out-of-Distribution shifts** We first evaluate the trained models on their robustness to various common input corruptions [11], along with their generalization performance on "clean data"

Table 1. Robustness to common input corruptions on CIFAR-10-C, CIFAR-100-C and Tiny-Imagenet-C [11] datasets. Best results in **bold** and second best underlined. Clean accuracy is reported in parentheses using gray colour. Standard deviations are reported over 10 trials.

| Method | CIFAR-10-C | CIFAR-100-C | Tiny-Imagenet-C |
|---|---|---|---|
| AT [18] | 73.12 ± 0.31 (85.58 ± 0.14) | 45.09 ± 0.31 (60.28 ± 0.13) | 15.74 ± 0.36 (22.33 ± 0.16) |
| TRADES [18] | 75.46 ± 0.21 (88.11 ± 0.43) | 45.98 ± 0.41 (63.3 ± 0.32) | 16.20 ± 0.23 (26.12 ± 0.38) |
| IAT [16] | 81.05 ± 0.42 (89.7 ± 0.33) | 50.71 ± 0.25 (62.7 ± 0.21) | 18.69 ± 0.45 (18.08 ± 0.34 ) |
| ERM | 69.29 ± 0.21 (94.5 ± 0.14) | 47.3 ± 0.32 (64.5 ± 0.10) | 17.34 ± 0.27 (49.96 ± 0.12) |
| Mixup | 74.74 ± 0.34 (95.5 ± 0.35 ) | 52.13 ± 0.43 (76.8 ± 0.41) | 21.55 ± 0.37 (53.83 ± 0.17) |
| Mixup-R | 74.27 ± 0.22 (89.88 ± 0.11) | 43.54 ± 0.15 (62.24 ± 0.21) | 21.34 ± 0.32 (53.5 ± 0.28) |
| Manifold-Mixup | 72.54 ± 0.14 (95.2 ± 0.18) | 41.42 ± 0.23 (75.3 ± 0.48) | - |
| VarMixup | **82.57 ± 0.42** (93.91 ± 0.45 ) | 52.57 ± 0.39 (73.2 ± 0.44 ) | 24.87 ± 0.32 (50.98 ± 0.11) |
| *adv*-VarMixup | 82.12 ± 0.46 (92.19 ± 0.32 ) | **54.0 ± 0.41** (72.13 ± 0.34) | **25.36 ± 0.21** (50.58 ± 0.23) |

(test data without corruptions). We evaluate their robustness on the newer CIFAR-10-C, CIFAR-100-C and Tiny-Imagenet-C datasets [11]. These datasets contain images, corrupted with 15 different distortions at 5 severity levels. We report the mean classification accuracy over all distortions on aforementioned corrupted datasets in Table 1. The results show that our method - VarMixup/*adv*-VarMixup achieves superior performance by a margin of $\sim 2-4\%$ consistently across the datasets. The slight drop in the clean accuracy of VarMixup models (shown in parentheses in Table 1) is due to the tradeoff between robustness and clean accuracy, which is a common trend observed in robustness literature.

**Calibration:** A recent study [26] showed that DNNs trained with Mixup are significantly better calibrated than DNNs trained in a regular fashion. Calibration [8] measures how good softmax scores are as indicators of the actual likelihood of a correct prediction. We measure the *Expected Calibration Error (ECE)* [26, 8] of the proposed method, following [26]. Figure 2 shows the calibration error on CIFAR-10 and CIFAR-100 datasets using Mixup, VarMixup and adv-VarMixup. The figure illustrates that our VarMixup models are also better calibrated than regular Mixup.

**Local linearity on loss landscapes:** [21] showed that the local linearity of loss landscapes of neural networks is related to model robustness. The more the loss landscapes are linear, the more the robustness. To further study this observation using our method, we analyze the local linearity of loss landscapes of VarMixup and regular mixup trained models. Qin et al. [21] defines local linearity at a data-point $x$ within a neighbourhood $B(\epsilon)$ as $\gamma(\epsilon, x, y) =$

$$\max_{\delta \in B(\epsilon)} |\mathcal{L}(F_w(x+\delta), y) - \mathcal{L}(F_w(x), y) - \delta^T \nabla_x \mathcal{L}(F_w(x), y)|$$

Figure 3 shows the average local linear error (over test set) with increasing $L_\infty$ max-perturbation $\epsilon$ on CIFAR-10 and CIFAR-100 datasets. As can be seen, VarMixup/*adv*-VarMixup makes the local linear error significantly ($\times$ 2) lesser as compared to regular mixup, thus inducing robustness.

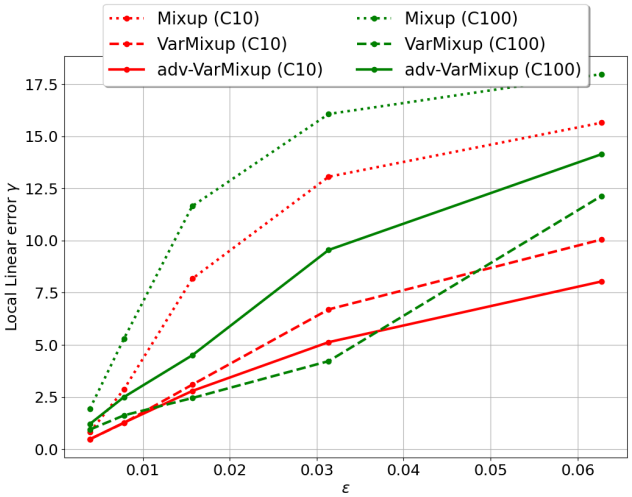


Figure 3. Local linear error of loss landscapes of models trained on CIFAR-10/-100 (denoted as C10 and C100)

## 5. Conclusions

In this work, we proposed a Mixup-based vicinal distribution, VarMixup, which performs linear interpolation on an unfolded latent manifold where linearity in between training examples is likely to be preserved by construction. We show that VarMixup trained models are more robust to common input corruptions and are better calibrated. Our work highlights the efficacy of defining vicinal distributions by using neighbors on unfolded latent manifold rather than data manifold and we believe that our work can open a discussion around this notion of robustness and choice of vicinal distributions on generative latent spaces.

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# A. Appendix

## A.1. Related work on Mixup

[34] proposed Mixup, a method to train models on the convex combination of pairs of examples and their labels. In other words, it constructs virtual training examples as: $x' = \lambda \cdot x_i + (1-\lambda) \cdot x_j; y' = \lambda \cdot y_i + (1-\lambda) \cdot y_j$, where $x_i$, $x_j$ are input vectors; $y_i$, $y_j$ are one-hot label encodings and $\lambda$ is a mixup coefficient, usually sampled from a $\beta(\eta, \eta)$ distribution. By doing so, it regularizes the network to behave linearly in between training examples, thus inducing global linearity between them. A recent variant, Manifold Mixup [29], exploits interpolations at hidden representations, thereby obtaining neural networks with smoother decision boundaries at different levels of hidden representations. AugMix [12] mixes up multiple augmented images and uses a Jensen-Shannon Divergence consistency loss on them to achieve better robustness to common input corruptions [11]. In semi-supervised learning, MixMatch [2] obtains state-of-the-art results by guessing low-entropy labels for data-augmented unlabeled examples and mixes labeled and unlabeled data using Mixup. It has been shown that apart from better generalization, Mixup also improves the robustness of models to adversarial perturbations as well. To further boost this robustness at inference time, Pang et al. [20] recently proposed a Mixup Inference technique which performs a mixup of input $x$ with a clean sample $x_s$ and passes the corresponding mixup sample $(\lambda \cdot x + (1-\lambda) \cdot x_s)$ into the classifier as the processed input. Other efforts related to Mixup [26] have shown that Mixup-trained networks are better calibrated i.e., the predicted softmax scores are better indicators of the actual likelihood of a correct prediction than DNNs trained in the regular fashion. Additionally, they also observed that mixup-trained DNNs are less prone to over-confident predictions on out-of-distribution and random-noise data. None of these efforts however address Mixup from a generative latent space, which is the focus of this work. Efforts such as [20] and [26], in fact, have inferences that motivate the need to consider a latent Mixup space to address a model's robustness and predictive uncertainty.

From a different perspective, Xu et al. [30] used domain mixup to improve the generalization ability of models in domain adaptation. Adversarial Mixup Resynthesis [1] attempted mixing latent codes used by autoencoders through an arbitrary mixing mechanism that can recombine codes from different inputs to produce novel examples. This work however has a different objective and focuses on generative models in a GAN-like setting, while our work focuses on robustness and predictive uncertainty. The work by Liu et al. [17] may be closest to ours in terms of approach as they use an adversarial autoencoder (AAE) to impose a uniform distribution on the feature representations. However, their work deals with improving generalization performance, while ours looks at robustness and predictive uncertainty, as already stated. Furthermore, we propose a new method, VarMixup, which focuses on directly exploiting the manifold learned by a Variational Autoencoder (VAE) (and do not regularize it unlike previous work) during Mixup and report improved adversarial robustness. We also present useful insights into the working of VarMixup (which is lacking in earlier work including [17]), thus making our contributions unique and more complete.

## A.2. Baseline Training Details

Here, we report the training details of baselines used for comparing out approach in Table 1.

1. *ERM* - Vanilla Empirical Risk Minimization using Adam optimizer ($lr = 1e-3$) for 100 epochs on all datasets.

2. *Mixup* - Vanilla Mixup training [34] using Adam optimizer ($lr = 1e-3$) for 150 epochs on all datasets. Mixup coefficient is sampled from $\beta(1, 1)$.

3. *Mixup-R* - Mixup training on MMD-VAE's reconstructed image space [34] using Adam optimizer ($lr = 1e-3$) for 150 epochs on all datasets. Mixup coefficient is sampled from $\beta(1, 1)$.

4. *Manifold Mixup* - Manifold Mixup training [29] using Adam optimizer ($lr = 1e-3$) for 150 epochs on all

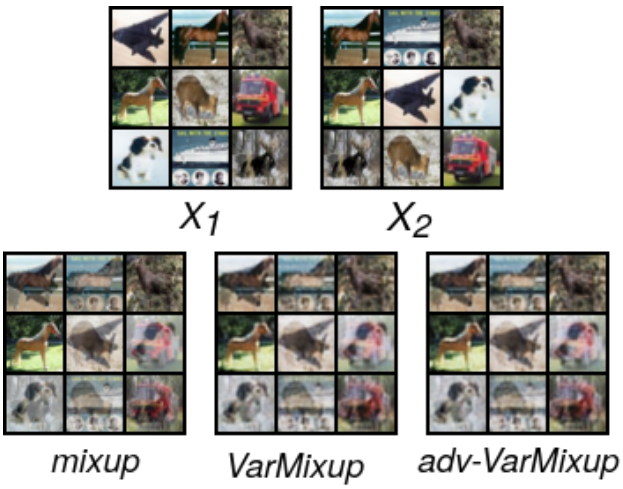


Figure 4. Samples generated by mixup, VarMixup and *adv*-VarMixup on CIFAR-10 (Mixup coefficient $\lambda = 0.5$).

datasets. Mixup coefficient is sampled from $\beta(2, 2)$.

5. *AT and TRADES* - $l_\infty$ PGD/TRADES adversarial training [18, 35] with $\epsilon = 8/255$ and step-size $\alpha = 2/255$. Models are trained using Adam optimizer ($lr = 1e-3$) for 250 epochs on all datasets.

6. *IAT* - $l_\infty$ Interpolated adversarial training [16] with $\epsilon = 8/255$ and step-size $\alpha = 2/255$. Interpolation coefficient is sampled from $\beta(1, 1)$. Models are trained using Adam optimizer ($lr = 1e-3$) for 350 epochs on all datasets.

### A.3. Ablation Studies

**Analyzing VarMixup samples:** Figure 4 shows sample data generated by regular Mixup, VarMixup, and *adv*-VarMixup on two images. Although mixup or VarMixup samples look perceptually similar, they are quite different at a statistical level. We measure the Frechet Inception Distance (FID) [13] and Kernel Inception Distance [3] between regular training data and training data generated by mixup/VarMixup/ *adv*-VarMixup. These scores summarize how similar the two groups are in terms of statistics on computer vision features of the raw images calculated using the Inceptionv3 model used for image classification. Lower scores indicate the two groups of images are more similar, or have more similar statistics, with a perfect score being 0.0 indicating that the two groups of images are identical. Figure 5 reports these metrics on CIFAR-10 and CIFAR-100 respectively. The greater FID and KID scores indicate that we are adding off-manifold samples (w.r.t. the manifold characterized by training data) to the training using our approach.

**Computational Overhead:** We compare the computational time of our trained models using VarMixup/*adv*-

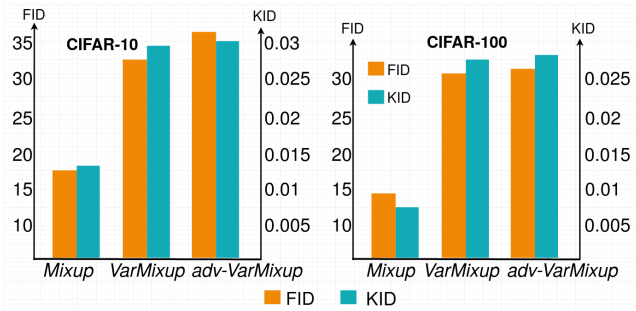


Figure 5. FID and KID scores between training set and mixup/VarMixup generated samples on CIFAR-10 and CIFAR-100

VarMixup with commonly used adversarial training techniques, AT and TRADES. VarMixup, *adv*-VarMixup, AT and TRADES take around 3, 5, 8.8 and 15 hours respectively for training. The training time of the MMD-VAE was also considered here. While already significantly faster than AT and TRADES, the proposed method will be more scalable and time-efficient, if a VAE trained on a dataset such as ImageNet can be directly used to generate VarMixup samples for other datasets. This is a typical transfer learning setting, and we hence study the performance of training VarMixup models on CIFAR-10 and CIFAR-100 datasets using MMD-VAE trained on the Tiny-Imagenet dataset. Respectively, VarMixup obtained mean corruption accuracy of 82.0 % and 53.25 % on CIFAR-10-C and CIFAR-100-C benchmarks, thus making our approach time-efficient and also scalable.