On the Benefits of Defining Vicinal Distributions in Latent Space [1]

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[1]Acknowledging DST, Govt of India (IMPRINT program) for funding; IIT-Hyderabad and JICA for provision of GPU servers .

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Drawback: Overparametrized NNs suffer from memorization → leads to undesirable behavior of network outside the training distribution.

Vicinal Risk Minimization

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→ define a vicinity or neighbourhood around each training example (eg. in terms of brightness, contrast, imperceptible noise, etc.)

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

, 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).

Vicinal Risk Minimization

Expected Vicinal Risk is given by

$$w^* = arg \min_w \int \mathcal{L}(F_w(x), y) \cdot dp_v(x, y) = \frac{1}{N} \cdot \sum_{i=1}^{N} g(F_w, \mathcal{L}, x_i, y_i)$$

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where $g(F_w, \mathcal{L}, x_i, y_i) = \int \mathcal{L}(F_w(x), y) \cdot dv(x, y|x_i, y_i)$.
$\rightarrow$ *Gaussian* and *Mixup* are few popular examples of vicinal distributions.

Mixup

Mixup is a popular technique to train models for better generalisation

[2] Pang et al., Mixup inference: Better exploiting mixup to defend adversarial attacks, ICLR 2020

[3] Hendrycks et al., Augmix: A simple method to improve robustness and uncertainty under data shift, ICLR 2020

[4] Lamb et al., Interpolated adversarial training : Achieving robust neural networks without sacrificing too much accuracy. AISec'19

[5] Thulasidasan et al., On mixup training: Improved calibration and predictive uncertainty for deep neural networks. NeurIPS 2019

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- Pang et al., 2020 [2]; Hendrycks et al., 2020 [3]; Lamb et al., 2019 [4] - Mixup to improve the robustness of models.
- Thulasidasan et al., 2019 [5] - Mixup-trained networks are significantly better calibrated.

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- Experiments shows that VarMixup boosts the robustness to out-of-distribution shifts as well calibration.
- Additional analysis show that VarMixup significantly decreases the local linearity error of the neural network.

Motivation

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- linearity in between training examples is more readily observed.

- Leverage such latent to capture the induced global linearity in between examples, and define Mixup.

Details

- We opt for an MMD-VAE [6] because of its advantage over vanilla KL based VAE [7]:

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

[6] Zhao et al., Infovae: Information maximizing variational autoencoder, 2017
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- Mixup vicinal distribution in the latent space of the trained VAE as $v_{VarMixup}(z, y | x_i, y_i) =$

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

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- Equivalent to constructing VarMixup samples as:

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

$$y' = \lambda \cdot y_i + (1 - \lambda) \cdot y_j$$

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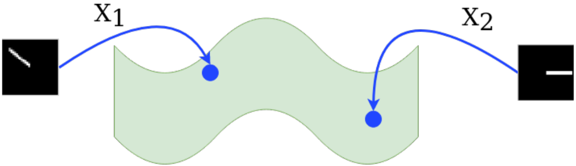
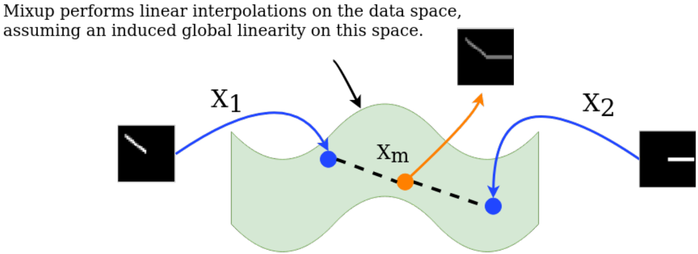
Illustration



Illustration



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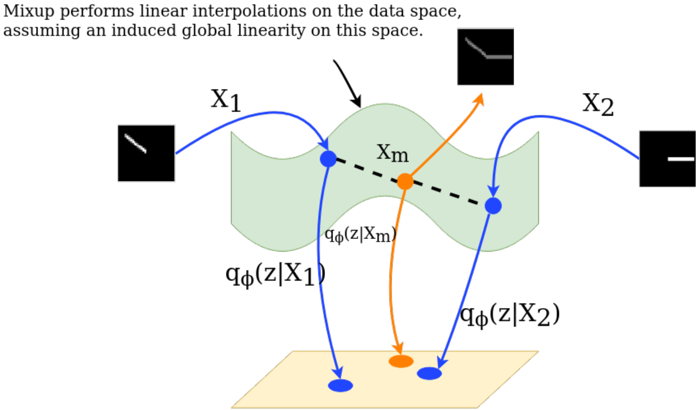
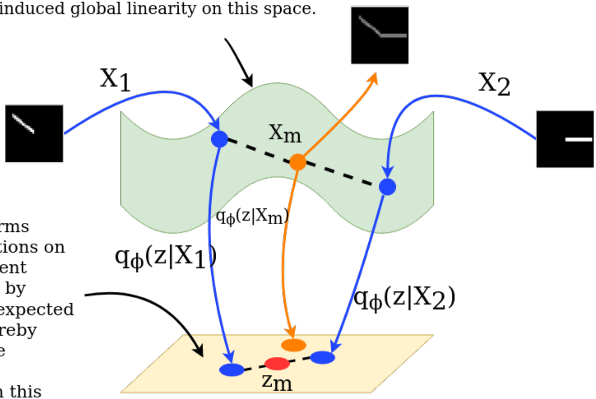


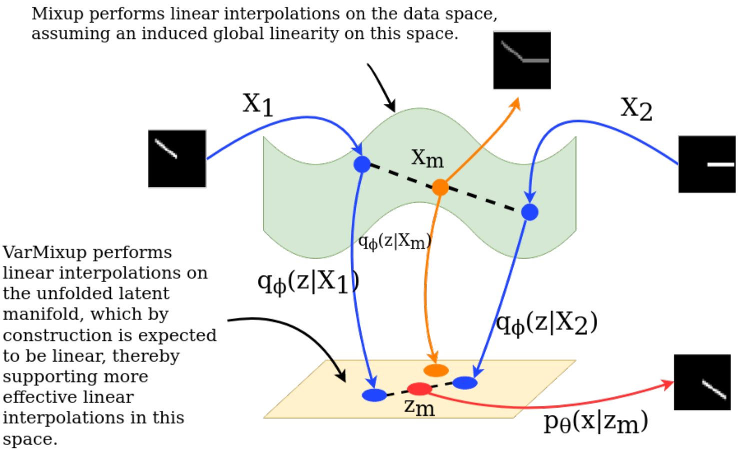
Illustration

Mixup performs linear interpolations on the data space, assuming an induced global linearity on this space.



VarMixup performs linear interpolations on the unfolded latent manifold, which by construction is expected to be linear, thereby supporting more effective linear interpolations in this space.

Illustration



Out-of-Distribution Generalization

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Figure 2: Example ImageNet-C corruptions. These corruptions are encountered only at test time and not

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- Robustness to common input corruptions on CIFAR-10-C, CIFAR-100-C and Tiny-Imagenet-C
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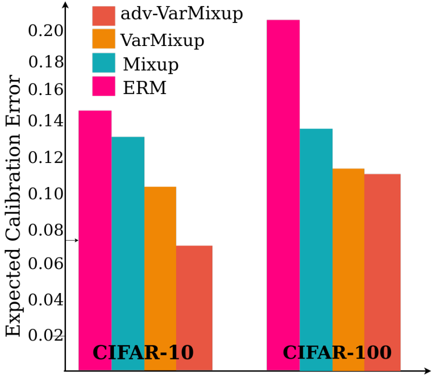
Method	CIFAR-10-C	CIFAR-100-C	Tiny-Imagenet-C
AT (Madry et al., 2018)	73.12 ± 0.31 (85.58 ± 0.14)	45.09 ± 0.31 (60.28 ± 0.13)	15.74 ± 0.36 (22.33 ± 0.16)
TRADES (Zhang et al., 2019)	75.46 ± 0.21 (88.11 ± 0.43)	45.98 ± 0.41 (63.3 ± 0.32)	16.20 ± 0.23 (26.12 ± 0.38)
IAT (Lamb et al., 2019)	81.05 ± 0.42 (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)	<u>52.57 ± 0.39</u> (73.2 ± 0.44)	<u>24.87 ± 0.32</u> (50.98 ± 0.11)
adv-VarMixup	<u>82.12 ± 0.46</u> (92.19 ± 0.32)	**54.0 ± 0.41** (72.13 ± 0.34)	**25.36 ± 0.21** (50.58 ± 0.23)

Calibration

- measures how good softmax scores are as indicators of the actual likelihood of a correct prediction.
- We measure the *Expected Calibration Error (ECE, lower the better)* [9]



[9] Guo et al., On calibration of modern neural networks , 2017

Local Linearity of Loss Surfaces

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[10] Qin et al., Adversarial robustness through local linearization, NeurIPS 2019

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- Local linearity at a data-point x within a neighbourhood $B(\epsilon)$ as $\gamma(\epsilon, x, y) =$

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

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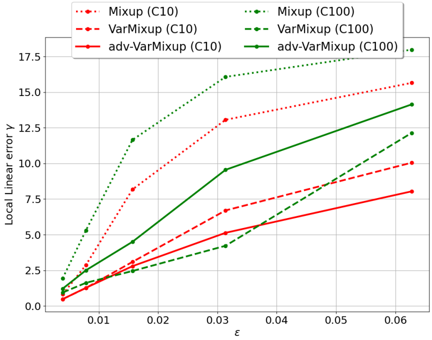

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- VarMixup trained models are more robust to corruptions and are better calibrated.

- Highlights the efficacy of defining vicinal distributions by using neighbors on unfolded latent manifold rather than data manifold.