Preventing Manifold Intrusion with Locality: Local Mixup

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Abstract

Mixup is a data-dependent regularization technique that consists in linearly interpolating input samples and associated outputs. It has been shown to improve accuracy when used to train on standard machine learning datasets. However, authors have pointed out that Mixup can produce out-of-distribution virtual samples and even contradictions in the augmented training set, potentially resulting in adversarial effects. In this paper, we introduce Local Mixup in which distant input samples are weighted down when computing the loss. In constrained settings we demonstrate that Local Mixup can create a trade-off between bias and variance, with the extreme cases reducing to vanilla training and classical Mixup. Using standardized computer vision benchmarks, we also show that Local Mixup can improve test accuracy.

1 Introduction

Deep Learning has become the golden standard for many tasks in the fields of machine learning and signal processing. Using a large number of tunable parameters, Deep Neural Networks (DNNs) are able to identify subtle dependencies in large training datasets to be later leveraged to perform accurate predictions on previously unseen data. Without constraints or enough samples, many models can fit the training data (high variance) and it is difficult to find the ones that would generalize correctly (low bias).

Regularization techniques have been deployed with the aim of improving generalization (Goodfellow et al., 2016). In (Guo et al., 2019), the authors categorize these techniques into data-independent or data-dependent ones. For example some data-independent regularization techniques constrain the model by penalizing the norm of the parameters, for instance through weight decay (Loshchilov and Hutter, 2017). A popular data-dependent regularization technique consists of artificially increasing the size of the training set, which is referred to as data augmentation (Simard et al., 2001). In the field of computer vision, for example, it is very common to generate new samples using basic class-invariant transformations (Krizhevsky et al., 2012; He et al., 2016a).

In (Zhang et al., 2017), the authors introduce Mixup, a data augmentation technique in which artificial training samples (\(\tilde{x}, \tilde{y}\)), called virtual samples, are generated through linear interpolations between two training samples (\(x_i, y_i\)) and (\(x_j, y_j\)). The associated output is computed as the corresponding linear interpolation on the respective outputs. Mixup improves generalization error of state-of-the-art models on ImageNet, CIFAR, speech, and tabular datasets (Zhang et al., 2017). This method is also used in the context of few shot learning (Mangla et al., 2020; Dhillon et al., 2019).

By using linear interpolation, virtual samples can in some cases contradict each other, or even generate out-of-distribution inputs. This phenomenon has been recently described in (Guo et al., 2019) where the authors use the term manifold intrusion. As such, it is not clear if Mixup is always desirable. More generally, the question arises of whether Mixup could be constrained to reduce the risk of generating such spurious interpolations. In this paper we introduce Local Mixup, where virtual samples are weighted in the training loss. The weight of each possible virtual sample depends on the distance between the endpoints of the corresponding segment (\(x_i, x_j\)). In particular, this method can be implemented to forbid interpolations between samples that are too distant from each other in the input domain, reducing the risk of generating spurious virtual samples.

Here are our main contributions:

- We introduce Local Mixup, a mixup method de-
pending on a single parameter whose extremes correspond to classical Mixup and Vanilla.

- In dimension one, we prove that Local Mixup allows to select a bias/variance trade-off.
- In higher dimensions, we show that Local Mixup can help achieve more accurate models than classical Mixup using standard vision datasets.
- Our work contributes more broadly to better understanding the impact of Mixup during training.

2 Related Work

Introducing notations: In Machine or Deep Learning, a training dataset $D_{\text{train}}$ is used to learn the model’s parameters, and a test one $D_{\text{test}}$ is used to evaluate the performance of the model on previously unseen inputs (Bishop, 2006). We also consider that both input and output data lie in metric spaces $(\mathcal{X}, d_X)$ and $(\mathcal{Y}, d_Y)$. Typically, $\mathcal{X}$ and $\mathcal{Y}$ are assumed to be Euclidean spaces with the usual metrics. We denote by $f : \mathcal{X} \rightarrow \mathcal{Y}$ the parametric model to be trained and by $\mathcal{F}$ the hypothesis set, i.e. the set containing all candidate parametrizations of the model $f \in \mathcal{F}$.

To train our model, we use an error function $L$ that measures the discrepancy between the model outputs and expected ones. Training the model amounts to minimizing the training loss while generalization may be quantitatively evaluated by the test loss:

$$L_{\text{vanilla}} = \sum_{(x,y) \in D} L(f(x), y).$$

Data augmentation and mixup: To improve generalization one can use regularization techniques (Goodfellow et al., 2016). Among them, data augmentation is a form of data-dependent regularization (Guo et al., 2019). It artificially generates new samples, resulting in increasing $D_{\text{train}}$ (Simard et al., 2001), and can apply on the outputs $y$ (Sukhbaatar et al., 2014) or on the inputs $x$ (Zhang et al., 2016; DeVries and Taylor, 2017; Yun et al., 2019; Cukur et al., 2018; Krizhevsky et al., 2012; He et al., 2016a). The use of data-dependent methods relying on some sort of mixing has recently emerged (Zhang et al., 2017; Verma et al., 2019; Yun et al., 2019; DeVries and Taylor, 2017; Hendrycks et al., 2019; Kim et al., 2020; Chou et al., 2020; Liu et al., 2021; Chen et al., 2020; Yin et al., 2021). They usually mix two or more inputs and the corresponding labels.

The pioneering mixing method is Mixup (Zhang et al., 2017), whose mixed samples $(\tilde{x}, \tilde{y})$ are generated by linear interpolations between pairs of samples, i.e. $\tilde{x}_{i,j,\lambda} = \lambda x_i + (1 - \lambda) x_j$ and $\tilde{y}_{i,j,\lambda} = \lambda y_i + (1 - \lambda) y_j$ for some training samples $(x_i, y_i)$ and $(x_j, y_j)$ and some $\lambda \in [0, 1]$. The Mixup training criterion is defined as:

**Definition 2.1 (Mixup Criterion).** Let $\lambda \sim \text{Beta}(\alpha, \beta)$, $i, j$ discrete variables uniformly drawn with repetitions in $\{0, \ldots, n-1\}$. $f^*$ minimizes the Mixup criterion if:

$$f^* = \arg\min_{f \in \mathcal{F}} \frac{1}{n^2} \sum_{D_{\text{train}}^2} \sum_{(\tilde{y}_{i,j,\lambda}, f(\tilde{x}_{i,j,\lambda})) \in L_{\text{mixup}}} L(\tilde{y}_{i,j,\lambda}, f(\tilde{x}_{i,j,\lambda})).$$

In other words, Mixup encourages the model $f$ to associate linearly interpolated inputs with the corresponding linearly interpolated outputs (Zhang et al., 2017). The positive effect of this linear behavior in between samples questioned several authors who aimed at explaining theoretically and empirically Mixup. Carratino et al. (2020) shows that Mixup can be interpreted as the combination of a data transformation and a data perturbation. A first transform shrinks both inputs and outputs towards their mean. The
second proof is given by reformulating the Mixup loss. Guwali et al. (2020) highlight that Mixup impacts the Lipschitz constant $L$ of the gradient of the network.

**Improvements over mixup:** In other works, authors propose to improve Mixup using various approaches. For example in (Chou et al. 2020), the idea is to use different $\lambda_i, \lambda_j$ to mix the input and the outputs, in (Liu et al. 2021; Rame et al. 2021; Yun et al. 2019), the authors explore using other (i.e. nonlinear) interpolation methods. in (Yin et al.; Greenwald et al. 2021; Chen et al. 2020) the authors extend the mixing to more than two elements.

**Our proposed approach:** In this paper, we aim at avoiding the phenomenon described as manifold intrusion, and introduced in (Guo et al. 2019). This phenomenon is depicted in Figure 1 on the right, where we see that virtual samples created through mixup between distant red samples lie outside the manifold domain for the red class. As we do not have access to the underlying manifold domains when we train a model, the rationale of our contribution is to favor interpolations between samples that are close enough in the input domain. Where the method described in (Guo et al. 2019) learns which interpolations should be kept through training, we advocate in this paper for a purely geometric approach where a decreasing weight is applied when computing the loss depending on the distance between interpolated samples.

### 3 Mixup in dimension 1

Let us consider the simple case where our model $f$ is defined on $\mathbb{R}$. Without loss of generality, let us consider that the training set $D_{\text{train}} = \{x_i, y_i\}$ is ordered by increasing input, i.e., $x_i \leq x_{i+1}$.

For a given $\tilde{x}$, Mixup’s loss implies that the output $f^*(\tilde{x})$ of the model is determined by the set $E(\tilde{x})$ of all convex combinations that can be obtain $\tilde{x}$ from two training inputs $x_i$ and $x_j$: $E(\tilde{x}) = \{i, j, \lambda_{i,j} \mid \tilde{x} = \lambda_{i,j} x_i + (1 - \lambda_{i,j}) x_j\}$. It is clear that for any $\tilde{x} \in [x_0, x_{n-1}]$, $E(\tilde{x})$ is non empty and finite. In practice, the distribution of $\lambda$ can be uniform (Zhang et al., 2017; Verma et al., 2019) $\sim Beta(\alpha = 1, \beta = 1) = U(0, 1)$. In this case, we show that the output $f^*(\tilde{x})$ of an input $x \in [x_0, x_n]$ is the barycenter of the target values corresponding to the points of $E(\tilde{x})$.

**Lemma 3.1.** $\forall \tilde{x} \in [x_0, x_{n-1}]$,

$$f^*(\tilde{x}) = \frac{1}{\text{card}(E(\tilde{x}))} \sum_{(i, j, \lambda_{i,j}) \in E(\tilde{x})} \lambda_{i,j} y_i + (1 - \lambda_{i,j}) y_j,$$

(1)

**Proof.** Let $\tilde{x} \in [x_0, x_{n-1}]$ and $0 \leq \lambda \leq 1$. For a given triplet $(i, j, \lambda) \in E(\tilde{x})$. We have $E[L(y_i, j, \lambda_{i,j}, f^*(\tilde{x}))|\tilde{x}, i, j, \lambda_{ij}] = L(y_i, j, \lambda_{i,j}, f^*(\tilde{x}))$ as the value of $y_i, j, \lambda_{i,j}$ and $\tilde{x}$ are known. Then we minimize the error for all $y_i, j, \lambda_{i,j}$ given by $E(\tilde{x})$. Then the value of $f^*(x)$ is only determined by the sum of the losses over $E(\tilde{x})$ since the elements of $E(\tilde{x})$ are equally probable (distributions of $i, j, \lambda$ are uniform).

$$E[L(f^*(\tilde{x}), y_{i,j}, \lambda_{i,j})] = \sum_{\tilde{x} \in E(\tilde{x})} E[L(f^*(\tilde{x}), y_{i,j}, \lambda_{i,j})|\tilde{x}, i, j, \lambda_{ij}]$$

$$= \sum_{\tilde{x} \in E(\tilde{x})} E[L(f^*(\tilde{x}), y_{i,j}, \lambda_{i,j})]$$

(2)

We assume $L$ to be either the cross entropy or the squared L2 loss. In either case, by nulling the derivative of Equation (2) w.r.t. the value $f^*(\tilde{x})$, we get:

$$f^*(\tilde{x}) = \frac{1}{\text{card}(E(\tilde{x}))} \sum_{E(\tilde{x})} y_{i,j, \lambda_{i,j}}$$

A consequence of this lemma is the following theorem:

**Theorem 3.2.** The function $f^*$ that minimizes the loss on the training set is piecewise linear on $[x_0, x_{n-1}]$, linear on each segment $[x_i, x_{i+1}]$ and defined by Equation (1).

When $\tilde{x}$ varies in $[x_i, x_{i+1}]$, the set of possible combinations (between training samples) leading to $\tilde{x}$ does not change, only the corresponding coefficients $\lambda$ vary linearly. Since the expression of Equation (1) is linear in each of those coefficients, $f^*$ is itself linear as a function of $\tilde{x}$. The set of possible combinations will change whenever $\tilde{x}$ switches to another interval, e.g. $[x_{i-1}, x_i]$. In this case new combinations are possible and others may disappear, leading to another linear function. $f^*$ is still continuous everywhere because new or disappearing combinations are associated either to $\lambda = 0$ or $\lambda = 1$ for $\tilde{x} = x_j$ and $j \in \{1, \cdots, n\}$.

In practice inferring a function $f^*$ that minimizes that the Mixup Criterion is usually not desired in machine learning, and one looks for $f$ with a sufficiently small loss to have a regularizing effect. Indeed $f^*$ is not likely to generalize well. Still, we note that it tends to an average of convex combinations and thus leads to a model with a low variance.

### 4 Local Mixup

#### 4.1 Locality graphs

Consider a (training) dataset $D$ made of pairs $(x, y)$. We propose to build a graph from $D$ as follows. We
define \(G_D = \langle V, W \rangle\) where \(V = \{x \mid \exists y, (x, y) \in D\}\). The symmetric real matrix \(W\) is based on \(D\), where \(D\) is the pairwise distance matrix \(D_{i,j} = d_X(x_i, x_j)\).

In this work, we consider various ways to obtain \(W\), but the rationale is always the same: to obtain a similarity matrix where large weights correspond to closest pairs of samples. Namely, we consider \(K\)-nearest neighbors graphs, where we set to 1 weights of target vertices corresponding to the \(K\) closest samples for a given source vertex and 0 otherwise; thresholded graphs where \(W_{i,j} = \phi(D_{i,j})\) and \(\phi(d) = 1_{d \leq \varepsilon}\); smooth decreasing exponential graphs where \(W_{i,j} = \exp(-\alpha D_{i,j})\). The loss is then weighted using \(W\):

\[
L_{\text{local mixup}} = \sum_{D_{i,j} \neq 0} W_{i,j} \mathcal{L}(\tilde{y}_{i,j,\lambda}, f(\tilde{x}_{i,j,\lambda})).
\tag{3}
\]

For computational cost considerations, we compute a graph for each batch (random subset) of samples during stochastic gradient descent. As such, the weights associating two samples can vary depending on the chosen graph and random batch.

In the extreme case where some weights are 0, the corresponding virtual samples are discarded during gradient descent, resulting in only considering local interpolations of samples, hence the name \textit{Local Mixup}.

### 4.2 Low dimension

In this section, we are interested in proving that \textit{Local Mixup} allows to tune a trade-off between bias and variance on trained models. For this purpose, we simplify the problem to dimension 1 and only consider \(K\)-nearest neighbor graphs.

In this case, note that varying \(K\) can create a range of settings where \(K = 0\) boils down to vanilla training and \(K > n\) where \(n\) is the number of training samples boils down to classical Mixup.

#### 4.2.1 Local Mixup and the bias/variance trade-off

Let us first recall the definitions of the bias and variance in the context of a machine learning problem.

**Definition 4.1 (Bias and Variance).** Let us consider a training set \(D_{\text{train}}\) and a function \(f\) from \(X\) to \(Y\). We define Bias and Variance as follow:

- **Bias:** \(\text{Bias}(f)^2 = \mathbb{E}_{\text{train}}[(f(x) - y)^2]\).
- **Variance:** \(\text{Var}(f) = \mathbb{E}_{\text{train}}[(f - \mathbb{E}_{\text{train}}[f])^2]\).

We consider two settings. In the first one, the input domain \(\mathbb{Z}/n\mathbb{Z}\) is periodic and thus the number of samples is finite. In the second one, the input domain \(\mathbb{Z}\) is infinite and outputs are independent and identically (i.i.d) generated using a random variable.

**Periodic setting**

Let us consider that the training set \(D_{\text{train}}\) is made of pairs \((x, y)\), where \(\{x \mid \exists y, (x, y) \in D_{\text{train}}\} = \mathbb{Z}/n\mathbb{Z}\). We also consider \(d_X(x, x') = |x - x'| \in \{0, \ldots, n-1\}\).

In this case, we can write explicit formulations of \(f_K^*(x_i)\), the function that minimizes the \textit{Local Mixup} criterion for \(K\)-nearest neighbors graphs. Following similar arguments to those used to obtain Equation (1): for a given \(x_i\) we know that the optimal value for \(f_K^*(x_i)\), would be an average of the \(\tilde{y}\) that correspond to the possible interpolations. we obtain:

\[
\forall x_i \in \mathbb{Z}/n\mathbb{Z}, f_K^*(x_i) = \frac{1}{K(K+1)/2} (2K y_i + S_K(x_i)),
\tag{4}
\]

where \(S_K(x_i)\) is defined recursively as follows:

\[
S_{K+1} = \begin{cases} 0 & \text{if } K = 0 \\ S_K(x_i) + A_{K+1}(x_i) & \forall K \geq 1 \end{cases}
\tag{5}
\]

and:

\[
A_K(x_i) = \frac{1}{K} \sum_{k=1}^{K-1} (K-k) \cdot y_{i-k} + k \cdot y_{i+k-k}.
\]

On Figure 2 we depicted for a given \(x_i\) the different interpolations and \(\tilde{y}\) that contribute to \(f_K^*(x_i)\). In blue the interpolation between \(x_i\) and its direct neighbors, in red the interpolation between points other than \(x_i\) that happen to intersect \(x_i\). As we increase \(K\), the influence of \(S_K\) (red points) increases.

We obtain the following Lemma, showing that the expected value of \(f_K^*\) is invariant with respect to \(K\):

**Lemma 4.1.** Expected value of \(f_K^*\) For any \(K\), the expected value of \(f_K^*\) is

\[
\mathbb{E}_{\text{train}}[f_K^*] = \mathbb{E}_{\text{train}}[y].
\tag{6}
\]
Proof.
\[ E_{\text{train}}[f_K^r] = \frac{1}{n} \sum_{i=1}^{n} f_K^r(x_i) \]
\[ = \frac{2}{nK(K + 3)} (2nK E_{\text{train}}[y] + \sum_{i=1}^{n} \sum_{k=1}^{K} A_k(x_i)) \]
and using the fact that \( y_{i+n} = y_i \):
\[ \sum_{i=1}^{n} \sum_{k=1}^{K} A_k(x_i) = \sum_{i=1}^{n} \sum_{k=1}^{K} \frac{k-1}{k} y_{i-l} + \frac{l}{k} y_{i+k-l} \]
\[ = \sum_{i=1}^{n} y_i \sum_{k=1}^{K} \frac{k-1}{k} 1 = n E_{\text{train}}[y] \frac{K(K-1)}{2}. \]
then \( E_{\text{train}}[f_K^r] = E_{\text{train}}[y] \).

We obtain the following theorem:

**Theorem 4.2** (Convergence of \( f_K^r \) in the periodic setting). As \( K \) grows, it holds that:

\[ \forall x_i \in \mathbb{Z}/n\mathbb{Z}, \]
\[ f_K^r(x_i) \to E_{\text{train}}[y], \]
\[ \text{Bias}^2(f_K^r) \to E_{\text{train}}[(y_i - E_{\text{train}}[y])^2], \]
\[ \text{Var}(f_K^r) = E_{\text{train}}[(f_K^r(x_i) - E_{\text{train}}[f_K^r(x_i)])^2] \to 0, \]
\[ \text{Var}(f_K^r) \text{ is eventually nonincreasing.} \]

Proof. We can explicitly write the limit of \( S_K \). We first prove this lemma (the proof is omitted here but available as supplementary material):

**Lemma 4.3.** Let \( K = Mn + r, M \in \mathbb{N}^* \) and \( 0 \leq r < n-1 \). We assume \( E_{\text{train}}[y] \geq 0 \), then:

\[ (M+1)n \cdot E_{\text{train}}[y] + \eta \geq AK \geq Mn \cdot E_{\text{train}}[y] - \eta, \]
with \( \eta = O(K E_{\text{train}}[y]) \).

Then combined with Equation [3] we can demonstrate the convergence of the sum \( S_K \) and find its limit:

**Corollary 4.3.1.** For \( K = NM \to \infty \)
\[ S_K \to \frac{1}{2} \sum_{i=1}^{n} y_i M^2 n = \frac{1}{2} E_{\text{train}}[y] K^2. \]

As a result, given Equation [4], the limit of \( f_K^r \) is \( E_{\text{train}}[y] \).

To prove the monotonicity of the variance we want to show: \( \text{Var}(f_K^r+1) \leq \text{Var}(f_K^r) \) for \( K \) large enough.

We use the König-Huygens theorem and Lemma 4.1 to compute the difference between the two variances:
\[ \text{Var}(f_K+1) - \text{Var}(f_K) \]
\[ = E_{\text{train}}[(f_{K+1}(x))^2] - E_{\text{train}}[(f_K(x))^2] \]
\[ = E_{\text{train}}[(f_{K+1}(x))^2] - (f_K(x))^2]. \]

We then show that for any \( x \in [x_0, x_{n-1}] \) and \( K \) large enough, \((f_{K+1}(x))^2 \leq (f_K(x))^2 \). To do so we get an asymptotic equivalent:
\[ (f_{K+1}(x))^2 - (f_K(x))^2 \sim \frac{K}{C} E_{\text{train}}[y], \]
where \( C \) is a positive constant.

This theorem states two main results: 1) in the case of Mixup the function that minimize the loss \( f^* \) has zero variance and converges to \( E_{\text{train}}[y] \). 2) Eventually the variance of the function that minimizes the Local Mixup criterion is decreasing, showing that the proposed Local Mixup can indeed trade the trade-off between the bias and variance.

**i.i.d random output setting**

Let us now consider that the training set is made of inputs \( \{x \mid y, (x, y) \in \mathcal{D}_{\text{train}}\} = \mathbb{Z} \) and \( y_i \) are i.i.d. according to a random variable \( R \) of variance \( \sigma^2 \).

**Theorem 4.4.** For a signal with i.i.d outputs, the variance is eventually bounded by:
\[ \frac{4^2 \sigma^2}{K^2} \leq \text{Var}(f_K(x_i)) \leq 8 \sigma^2. \]

Proof. Let us choose \( x_i \) and \( K > 1 \). First observe that \( f_K^r(x_i) \) is a sum of random variables. We rewrite \( S_K \) with the coefficients \( a_k^r = \sum_{i=k+1}^{K} \frac{1}{k} \):
\[ S_K = \sum_{k=1}^{K-1} (y_{i-k} + y_{i+k}) a_k^r. \]
We obtain:
\[ \text{Var}(f_K^r(x_i)) = \text{Var} \left( \frac{2 \cdot (2K y_i + S_K)}{K(K+3)} \right) \]
leading to:
\[ \text{Var}(f_K^r(x_i)) = 4^2 \left( \frac{K}{K(K+3)} \right)^2 \text{Var}(y_i) \]
\[ + \sum_{k=1}^{K-1} \left( \frac{2a_k^r}{K(K+3)} \right)^2 (\text{Var}(y_{i-k}) + \text{Var}(y_{i+k})). \]
We use the fact that \( \frac{1}{K} \leq a_k^r \leq K. \)
Then when \( K \to \infty \):
\[ \frac{4^2 \sigma^2}{K^2} \leq \text{Var}(f_K(x_i)) \leq \frac{8 \sigma^2}{K}. \]
4.2.2 Invariance of linear models

Interestingly, we can show that both Mixup and Local Mixup lead to the same optimal linear models, as stated in the following theorem:

**Theorem 4.5.** For a linear model: \( f(x) = ax + b \), \( a, b \in \mathbb{R} \), the function \( f^* \) that minimizes the loss of Mixup and Local Mixup is the same.

**Proof.** For mixup, we showed with Equation (1) the function \( f^* \) is a piecewise linear function. The same equation applies for Local Mixup except that the set \( E_x \) is smaller for Local Mixup as the number of endpoints is restricted. As a piecewise linear function, linear on each segment \([x_i, x_{i+1}]\): \( f^* \) can be written as \( f^* = a_i x + b_i \) where each \((a_i, b_i)\) are defined on \([x_i, x_{i+1}]\). Let us consider \( F \) to be restricted to linear functions, then the coefficients \( a, b \) are the averages of the \((a_i, b_i)\).

4.3 High Dimension and Lipschitz constraint

The proofs given in low dimension have some limitations. Basically, the averaging effect happens since any point \( x \) within the interval \([x_1, x_n]\) can be written as at least one convex combination of pairs from the training set. Contradictions may occur as illustrated above when several combinations corresponds to \( x \). In higher dimension such explicit contradictions are not necessarily expected. Still, we show that Local Mixup has an impact on the Lipschitz constant of the networks.

First recall the definition of a \( q \)-Lipschitz function:

**Definition 4.2 (Lipschitz Continuous and Lipschitz Constant).** Given two metric spaces \((\mathcal{X}, d_X), (\mathcal{Y}, d_Y)\) and a function \( f : \mathcal{X} \rightarrow \mathcal{Y} \), \( f \) is Lipschitz continuous if there exists a real constant \( q \geq 0 \) s.t for all \( x_i \) and \( x_j \) in \( \mathcal{X} \),

\[
d_Y(f(x_i), f(x_j)) \leq q d_X(x_i, x_j). \tag{13}
\]

If \( f \) is \( q \)-Lipschitz continuous, we define the optimal Lipschitz constant \( Q_{sup} \) as

\[
Q_{sup} = \sup_{x_i, x_j \in \mathcal{X}, x_i \neq x_j} \frac{d_Y(f(x_i), f(x_j))}{d_X(x_i, x_j)}. \tag{14}
\]

For simplicity, let us consider a classification problem where \( d_Y \) is 0 if the two considered samples are of the same class and 1 otherwise.

Then the training set imposes a lower bound on the optimal Lipschitz constant:

\[
Q_{sup} \geq \min_{x_i, x_j \in D, y_i \neq y_j} \left( d_X(x_i, x_j) \right)^{-1}. \tag{15}
\]

For Mixup and Local Mixup, the virtual samples increase the size of the training set, resulting in stronger constraints on the optimal Lipschitz constant.

In more details, consider the case of a thresholded graph with parameter \( \varepsilon \) when using Local Mixup. In this case, the increased training set for each class \( y \) can be written as \( S_\varepsilon(y) = \{ \lambda x_i + (1 - \lambda) x_j, 0 \leq \lambda \leq 1 \mid y_i = y_j = y \} \), \( d_X(x_i, x_j) \leq \varepsilon \), the set of all segments constructed from two samples that are close enough in the input domain and sharing the same label \( y \). We then obtain the following theorem:

**Theorem 4.6.** The lower bound \( Q(D) \) is increasing with \( \varepsilon \).

**Proof.** We directly use the inclusion \( S_\varepsilon(y) \subset S_{\varepsilon'}(y), \forall \varepsilon \leq \varepsilon' \).

We shall show in the experiments that \( \varepsilon \) can indeed impact \( Q(D) \) on standard vision datasets.

5 Experiments

5.1 Low dimension

As stated in the introduction and [Guo et al., 2019], Mixup leads to interpolations that may be misleading for the model. To illustrate this effect, we consider a 2d toy dataset of two coiling spirals where such interpolations occur frequently. The two coiling spirals is a binary classification dataset: each spiral corresponds to a different class. We expect to retrieve better performance for Local Mixup compared to Mixup: local interpolations are likely to stay in the same spiral and therefore avoid manifold intrusion. For this experiment we use a thresholded graph with parameter \( \varepsilon \).

To carry out this experiment, we generate 1000 samples for each class and add a Gaussian noise with standard deviation \( \sigma = 1.5 \) (controlling the spirals’ thickness). A typical draw is depicted in Figure 3. We use a large value of \( \sigma \) to avoid trivial solutions to the problem. Once the dataset is generated we split it randomly into two parts: a training set containing 80% of the samples and a test set containing the remaining 20% (used to compute the error rates). We then use a fully connected neural network made of two hidden layers with 100 neurons and use the ReLU function as non linearity. We average the test errors over 1000 runs. For small values of \( \varepsilon \) many weights of the graph are zero and thus the corresponding interpolations are disregarded into the loss. This means that for a given batch only a small proportion of samples are regarded to compute the loss. Without any correction, different values of \( \varepsilon \) lead to different batch sizes. To avoid side
effects, we vary the batch size so that in average the same number of samples are used to update the loss.

To select an appropriate value of $\varepsilon$, we first looked at the distribution of distances between pairs of inputs in the training set. This distribution is depicted in Figure 4. We observe that the distribution is relatively uniform between 0 and 4, and as such in our experiments we vary $\varepsilon$ between 0 and 4 using steps of 0.5.

In Figure 5, we depict the evolution of the average error rate as a function of the parameter $\varepsilon$. Recall that the extremes for $\varepsilon = 0$ and $\varepsilon = 4$ correspond respectively to Vanilla and Mixup. One can note the significant benefit of Mixup and Local Mixup over Vanilla. As expected, Local Mixup presents a minimum error rate which is significantly smaller than Mixup’s error rate. We can note that the minimum is reached with a value of $\varepsilon$ smaller than the first quantile. This means that for this dataset Mixup interpolations given above this threshold are either useless or misleading for the network’s training.

It is worth pointing out that this toy dataset is particularly suitable to generate contradictory virtual samples. We delve into more complex and real world datasets in the following subsection.

**5.2 High dimension**

**5.2.1 Lipschitz lower bound**

To illustrate the impact of $\varepsilon$ on the optimal Lipschitz constant, we use the dataset CIFAR-10 [Krizhevsky, 2012] which is made of small images of size 32x32 pixels and 3 colors. There are 50,000 images in the training set corresponding to 10 classes.

We are interested in showcasing the evolution of $Q(D)$ when varying $\varepsilon$. The results are depicted in Figure 6.

For classical Mixup we obtained $Q(D) = 0.11$ and for Vanilla $Q(D) = 0.073$. Note that these two extremes are reached with Local Mixup when $\varepsilon = 0$ and $\varepsilon \geq 50$.

We observe that $\varepsilon$ can be used to smoothly tune the lower bound $Q(D)$. In practice, a lower $Q(D)$ is preferable, but this only accounts for the optimal Lipschitz constant. Larger values of $\varepsilon$ lead to larger training sets and thus potentially better generalization.
We now test our proposition on different classification datasets and architectures. We consider the datasets CIFAR10 (Krizhevsky, 2012), Fashion-MNIST (Xiao et al., 2017) and SVHN (Netzer et al., 2011). Fashion-MNIST is composed of clothes images of size 28x28 pixels (grayscale). There are 60,000 images in the training set corresponding to 10 classes. SVHN is a real-world image dataset made of small cropped digits of size 32x32 pixels and 3 colors. There are 73257 digits in the training set corresponding to 10 classes. For these tests, we use a smooth decreasing exponential graph parametrized by $\alpha$.

For CIFAR10, we implement a ResNet18 (He et al., 2016) as in (Zhang et al., 2017), and average the error rates over 100 runs. We report the mean and confidence interval at 95%. We observed that Local Mixup with a value of $\alpha = 0.003$ showed a smaller error rate than the Vanilla network and Mixup, with disjoint confidence intervals. For Fashion-MNIST, we implement a DenseNet (Huang et al., 2017) and average the error rates over 10 runs. We also report the mean and confidence intervals at 95%. Again, Local Mixup with a value of $\alpha = 1e - 3$ presents a smaller error rate than both the baseline and Mixup. Note that for this dataset and this network architecture Mixup impacts negatively the error rate, suggesting that on this dataset Mixup creates spurious interpolations as discussed in (Guo et al., 2015). For SVHN we implement a LeNet-5 (LeCun et al., 1998) architecture (3 convolution layers). Again, Local Mixup performs better than both Vanilla and Mixup.

For these experiments, we also tried to use a $K$-nearest neighbor graph or a thresholded graph but without being able to achieve smaller error rates compared to Mixup or even Vanilla. This may indicate that some segments generated by Mixup are important to act as a regularizer during training even if some of them may generate manifold intrusions. By tuning $\alpha$, we weigh the importance of this regularization.

5.2.3 Discussion

Experiments in both low and high dimensions demonstrated the capacity of Local Mixup to outperform Mixup thanks to the use of locality. Still, the choice of the added hyper-parameter ($\alpha$, $\varepsilon$ or $K$) is essential and data dependent. For now, we reported results selecting the parameter leading to the best test error rate among a small number of possibilities. In future work we would like to rely on quantitative information given on the topology such as the histogram of the distance or persistence diagrams (Wasserman, 2018) to tune these hyper-parameters.

Note also that to embed the notion of locality we decided to use the Euclidean metric, although in general datasets lie in nonlinear manifolds. On CIFAR10 for example, in (Abouelnaga et al., 2016) the authors show that it is possible to achieve classification scores significantly better than the chance level using the Euclidean metric, but very far from state-of-the-art. There would be many possibilities to improve over using the Euclidean metric, including using pullback metrics (Jost and Jost, 2008; Kalatzis et al., 2020) given by the euclidean distance between the samples once in the feature space corresponding to the penultimate layer.

6 Conclusion

In this paper, we introduced a methodology called Local Mixup, in which pairs of samples are interpolated and weighted in the loss depending on the distance between them in the input domain. This methodology comes with a hyper-parameter that allows to provide a continuous range of solutions between Vanilla and classical Mixup. Using a simple framework, we showed that Local Mixup can control the bias/variance trade-off of trained models. In more general settings, we showed that Local Mixup can tune a lower bound on the Lipschitz constant of the trained model. We used real world datasets to prove the ability of Local Mixup to achieve better generalization, as measured using the test error rate, than Vanilla and classical Mixup.

Overall, our methodology introduces a simple way to incorporate locality notions into Mixup. We believe that such a notion of locality is beneficial and could be leveraged to a greater level in future work, or could be incorporated to the various Mixup extensions that
have been proposed in the community. In future work, we would like to investigate further the choice of the graph, the choice of the hyper-parameter that comes with it, and trainable versions of Local Mixup. Extending the theoretical results to more general contexts would definitely allow to gain further intuition on the effect of locality on Mixup.

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