From Confusion to Clarity: Generalized mixup

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Abstract

Data augmentation significantly enhances the ability of machine learning models to generalize on unseen data sets. The traditional mixup technique, which linearly interpolates between training examples and their labels, has been effective in increasing model robustness but lacks focus on specific learning challenges. In this work, we introduce a novel adaptation of mixup that integrates a dynamic, confusion matrix-based selection strategy for pairing examples. This method prioritizes frequently misclassified combinations, thereby targeting critical areas where the model underperforms. Our proposed approach, tested extensively on CIFAR-10 and CIFAR-100 datasets with ResNet18, shows that adaptive interpolation based on the confusion matrix notably improves model accuracy. Results demonstrate that lower γ values, which adjust the influence of the confusion matrix, yield the best performance, enhancing generalization while avoiding underexposure to pairs of images from specific classes. Our method, a generalization of mixup, addresses current challenges in machine learning and makes strides in both theoretical and practical aspects of model training.

1 Introduction

Data augmentation is a critical technique in machine learning employed to enhance model robustness. Introduced by Zhang et al. (2017), mixup creates new training examples by computing linear

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interpolations of pairs of examples and their corresponding labels. This technique prevents overfitting and promotes smoother decision boundaries between data points.

The core idea behind mixup is Vicinal Risk Minimization (VRM). Unlike Empirical Risk Minimization (ERM), which aims to minimize errors on the only training data and can lead to overfitting, VRM focuses on reducing errors in the neighborhood of the training examples. Under *mixup*, the model is trained on convex combinations of training examples.

While *mixup* has been successful, its indiscriminate approach to selecting pairs for interpolation does not consider the underlying structure or specific characteristics of the data. Other approaches, namely DMix, (Sawhney et al., 2022), and CoMixup, (Kim et al., 2021), seek to exploit innate traits of a dataset to more efficiently apply standard *mixup*. Building on these advancements, this paper introduces a novel approach that utilizes a variant of the confusion matrix to guide the selection of pairs for *mixup*. Our method targets misclassifications during training by upsampling the pairs of classes that are often mistaken for each other. Our approach aims to utilize *mixup* to smooth the decision boundary between classes that a model finds difficult to distinguish. Our strategy of adaptive sampling leads to faster convergence and improved test accuracy. We show that standard *mixup* is a special case of our method; thus, our approach is a generalization of *mixup*. The code used to run our experiments can be found here or at the following link:

In this paper, we present a comprehensive description of our method, including its theoretical framework, implementation details, and empirical evaluation. By synthesizing insights from prior *mixup* variations and incorporating a mechanism to adapt based on error analysis, we contribute a novel perspective to the field of data augmentation, aiming to provide a more targeted and effective approach to enhancing model generalization.

2 Preliminaries

The original mixup algorithm involves linearly interpolating the features of two training examples and their labels. This process prevents models with high Vapnik-Chervonenkis complexity from memorizing features. The degree to which the mixed example resembles the first example in its pair is controlled by λ , a value between 0 and 1 drawn from the beta distribution. Zhang et al. (2017) derives a new, mixed data point \hat{x} and its label \hat{y} :

$$\hat{x} = \lambda x_i + (1 - \lambda) x_i$$

$$\hat{y} = \lambda y_i + (1 - \lambda)y_i$$

where x_i and x_j are raw input vectors and y_i and y_j are their corresponding labels.

For each instance where a pair of inputs is mixed, λ is selected from the distribution $\beta(\alpha, \alpha)$, where $\alpha \in (0, \infty)$. When $\alpha = 0$, the distribution only takes the values 0 and 1, and as $\alpha \to \infty$, the distribution only takes the value 0.5. At $\alpha = 1$, the distribution is uniform between 0 and 1.

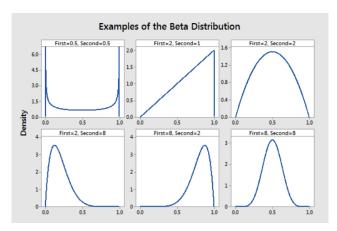


Figure 1: This image shows different variations of the beta distribution.

The original mixup algorithm combines data points indiscriminately, ignoring any trends in the data. There have been attempts to improve mixup's performance by being more selective about which pair of inputs is linearly interpolated; for example, the aforementioned DMix (Sawhney et al., 2022) combines data points only if the hyperbolic tangential distance from each other is significantly high.

The model introduced in this paper selects which data points are mixed together using a different criterion. After each epoch of training, we use a variant of the confusion matrix to upsample examples from classes C_i and C_j if examples from C_i are often attributed to C_j . Thus, we do not modify how a pair of inputs is mixed, but hypothesize that changing how the pair of inputs is selected will decrease the time to convergence and improve accuracy.

3 Proposed Method

We propose a method that generalizes mixup. Zhang et al. (2017) shows that mixup smooths the decision boundary between data points. We hypothesize that a model can benefit from mixup between some pairs of data points more than others. Specifically, it could be especially helpful to perform mixup on data points from pairs of classes that a model often mistakes for one another. Our method follows this logic, upsampling pairs of data points belonging to pairs of classes that the model often confuses.

Standard mixup pairs examples by mixing two copies of the dataset: the first copy is the dataset in its original order, and the second copy is a permutation of the dataset chosen uniformly at random.

Our version of generalized mixup creates a permutation of the dataset using the confusion matrix. For each class C with n examples, we sample without replacement n examples from the dataset to mix with the examples of C via a probability distribution P_C over all the classes, where $P_C(C')$ is relatively high when the model often mislabels examples of class C as C'. The probability distributions P_C can each be represented as a vector of length C, and there are C total P_C . This construction naturally lends itself to a $C \times C$ matrix M. We organize M such that each P_C is a row in M. Because the rows of M each represent a probability distribution, each row must sum to 1. Each column must also sum to 1 so that the probability that two examples are mixed is independent of the sampling order. P_C

The confusion matrix is a matrix representation of the predictions of a multi-class classification model. For each prediction that the model makes, exactly one element of the confusion matrix is incremented, namely the element in the row of the true class and column of the predicted class of the data point. The mixup algorithm turns a multi-class task into a multi-label task: two one-hot labels are interpolated into a vector that generally has two non-zero elements. There is not a standard way to construct a two-dimensional confusion matrix for a multi-label task, so we do the following: for our interpolated example $\hat{x} = \lambda x_i + (1 - \lambda) x_j$ and interpolated label vector $\hat{y} = \lambda y_i + (1 - \lambda) y_j$, where x_i is from class C_a and x_j is from class C_b , we distribute the predicted label vector \hat{y}_p by incrementing the a^{th} row in the confusion matrix by $\lambda \hat{y}_p$ and incrementing the b_{th} row by $(1 - \lambda)\hat{y}_p$. Equivalently, for each true label vector \hat{y} and predicted label vector \hat{y}_p , we increment the confusion matrix by the vector outer product $\hat{y}\hat{y}_p^T$.

At the model's initialization, by random chance, examples of C_a could often be mislabeled as C_b (assume $i \neq j$). This would then cause upsampling of examples from C_a and C_b , which would then likely lead to an increase in the four cells in rows a and b and columns a and b. These start conditions ultimately cause more upsampling between classes C_a and C_b , and so on. To prevent this feedback loop, we modify the result of our vector outer product such that for an example mixed from examples from classes C_a and C_b , we set all values in columns a and b to 0. In other words, our confusion matrix only contains the values attributed to incorrect labels.

Now, we must modify our confusion matrix so that it is doubly stochastic, satisfying the criteria of M. By excluding in the confusion matrix the predicted value of the true classes, the diagonal of our confusion matrix only contains values of 0. It is beneficial to mix between examples of the same class, as Zhang et al. (2017) showed that mixing between same classes alone beats ERM. Thus, we first scale each row such that the sum of all values equals $\frac{c-1}{c}$, where c is the number of classes. We

 $^{^{1}}$ Consider an alternative. Assume that the first row sampled is coincidentally all zeros, except for a value of 1 for class C. Therefore, all examples of C will be sampled before we sample for any subsequent row. If any later rows have a nonzero value for class C, there are no examples of class C to sample, and thus sampling is impacted by row order.

then set each element along the diagonal of the confusion matrix to $\frac{1}{c}$. Therefore, each row of our confusion matrix now gives us a probability distribution from which we can sample examples—a probability distribution that places increased importance on the classes that the model often mislabels.

To make the matrix doubly stochastic, we use the Sinkhorn-Knopp algorithm, which alternates between normalizing the rows and columns. Empirically, we find that this process does not significantly impact our matrix. For $\gamma=1$, the average difference between each matrix element before and after Sinkhorn-Knopp is roughly 0.017.

We then iterate through the rows of the confusion matrix, sampling without replacement from the training data. At each row a, we sample n examples to be mixed with the examples of class C_i . We define a parameter γ that amplifies or reduces the effects of the confusion matrix on the sampling. Before we make our matrix doubly stochastic, we raise each element to the power of γ . As $\gamma \to \infty$, the largest elements dominate. As $\gamma \to 0$, all elements of the confusion matrix approach $\frac{1}{c}$. In this case, when we sample from a row a, each example in the dataset is equally likely to be sampled. Therefore, the permutation is completely random. Thus, as $\gamma \to 0$, we recover standard mixup.

This reasoning justifies our choice to initialize our matrix such that every element is $\frac{1}{c}$. We compute our matrix after each training epoch using the training predictions and exponential averaging of the confusion matrix with momentum 0.5. In practice, Zhang et al. (2017) used batching and see no detriments in performance, so we do the same. Because sampling from our doubly stochastic matrix relies on having an equal number of examples from each class, we use stratified sampling for each batch.

4 Experiments

4.1 Dataset

For our experiments, we utilize datasets specifically designed for benchmarking image classification models (Krizhevsky, 2009). The CIFAR-10 and CIFAR-100 datasets comprise 60,000 color images, each measuring 32×32 pixels, distributed across 10 and 100 classes, respectively. Each dataset is split into 50,000 training images and 10,000 testing images. These datasets contain images from various natural categories, making them ideal for evaluating the performance of deep learning models in recognizing and differentiating between diverse visual patterns. Detailed characteristics of these datasets can be found on the CIFAR dataset website².

²https://www.cs.toronto.edu/~kriz/cifar.html

4.2 Results

We conduct experiments on γ to evaluate the effect of γ on model performance. As γ increases, pairs of examples from classes that the model confuses are more likely to be mixed. We perform the γ experiments on ResNet18 with a learning rate of 0.1. We decrease the learning rate to 0.01 after 50 epochs and 0.001 after 75 epochs. We train for 100 total epochs and use a weight decay of 0.0001. Our mixup parameter α is set to 1. For CIFAR-10, we use a batch size of 250, and for CIFAR-100, we use a batch size of 1000. Results are captured in Table 1 and Figure 2.

γ	Test error: CIFAR-10	Test error: CIFAR-100)
0.063	0.064	0.277
0.125	0.062	0.271
0.25	0.059	0.273
0.5	0.063	0.276
1	0.062	0.276
2	0.068	0.305
Standard mixup	0.065	0.276

Table 1: Test accuracies on CIFAR10 and CIFAR100 for varying γ values.

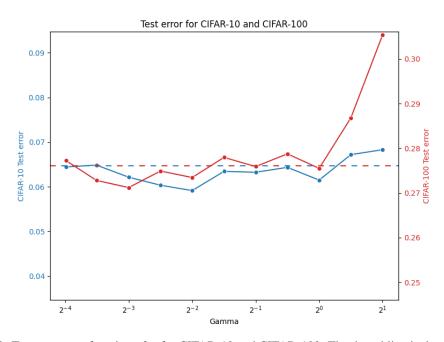


Figure 2: Test error as a function of γ for CIFAR-10 and CIFAR-100. The dotted line is the test error of standard mixup.

Figure 3 shows heatmaps of the average confusion matrix for $\gamma=0.5$ and $\gamma=2$. For high values of γ , pairs of classes are more likely to contain classes that a model often confuses. For example,

automobiles and trucks are often sampled as pairs. The same can be said for airplanes and ships and dogs and cats. For $\gamma=2$, this effect is amplified compared to $\gamma=0.5$.

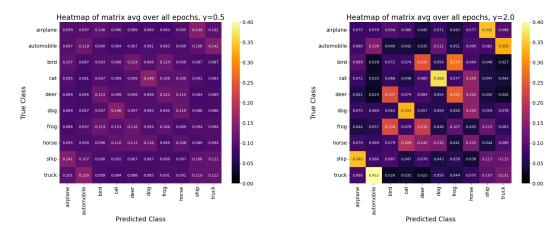


Figure 3: A heatmap of the confusion matrix for $\gamma = 1$ for CIFAR-10, averaged over all epochs.

We show how the standard deviation of the confusion matrix evolves over epochs in Figure 4. Upon initialization, every value in the confusion matrix is $\frac{1}{c}$, where c is the number of classes. The model is initially a poor classifier, so the standard deviation of the confusion matrix increases quickly, only hindered by the exponential averaging momentum value of 0.5. As model performance improves throughout training, we assume that the model mislabels examples of a class to another class less frequently, so the standard deviation slowly decreases. This could be compounded by the effect of our method. Because we are intentionally upsampling pairs of classes that are often confused, the model creates a more linear decision boundary between such pairs. As training continues, the model is less likely to continue making the same mistakes. The average standard deviation for each value of γ is smaller for CIFAR-100 than for CIFAR-10, but the general trend is the same.

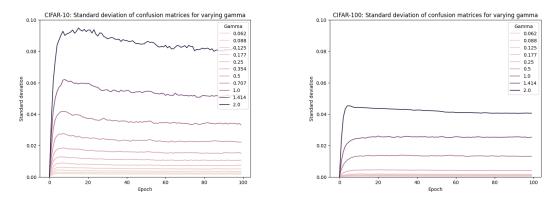


Figure 4: The standard deviation of the confusion matrix as a function of epoch for varying values of γ for both CIFAR-10 and CIFAR-100.

5 Related Work

Our method is inspired by previous scholarship. Since the original mixup paper was published in 2018, work has focused on improving the implementation and adapting it to modality specific tasks.

5.1 Augmentation based on Input Saliency

Although the original *mixup* algorithm is highly effective as a regularizer, many other approaches have made improvements by exploiting the relationships between data inputs. RICAP, presented in Takahashi et al. (2018), samples four random inputs from a dataset, randomly crops them, and then forms a new image from four crops. SaliencyMix, introduced by Uddin et al. (2020), uses a saliency map to crop "important" crops from paired images. It seeks to improve upon previous approaches by pasting the most relevant patch of the second image to the first. They argue this new method is better than other random cut and mix strategies because the augmented image better reflects the intrinsically meaningful information from both inputs.

Similarly, Attentive Cut-Mix, introduced by Walawalkar et al. (2020), uses a feature extractor based on an attention maps of a transformer model. After finding an input's most "descriptive" aspects, it implements Cut-Mix Yun et al. (2019), improving upon that model's random cut and paste between the input pair. In this example, the resulting augmented image of a dog and cat could include the body of a dog with the eyes, nose, and ears of a cat. Co-mixup strategically blends features from different samples, emphasizing saliency and diversity through an optimization framework involving submodular and supermodular functions (Kim et al., 2021).

Finally, CowMask utilizes on the filtering found in most CNNs to augment photos (French et al., 2020). It randomly applies a series of masking filters over a given image, preserving the overall image structure. This pattern of masking resembles the spots on a cow, hence the approach's name.

5.2 Applying mixup based on Input Saliency

The previous approaches diverge sharply from our method. For one, most of them augment based on varying implementations of Cut-Mix (Yun et al., 2019). However, other algorithms seek to improve the original *mixup* algorithm by changing which images are mixed. For example, Recursive-mix (Yang et al., 2022) mixes pairs of inputs, similar to the original implementation of *mixup*. However, mixes are also used as input to later mixes, making the algorithm recursive. MixStyle seeks to mix inputs, specifically images, with different styles (Zhou et al., 2021). For example, it would iterate through a set of paintings and form a feature map identifying the Mona Lisa, Sistine Chapel, and the Birth of Venus as 'Renaissance Art.' Afterward, the algorithm mixes the style features of images and uses the mixed style statistics to reconstruct new images.

AugMix abandons mixing based on a permutation of the input set and instead performs a series of transformations on a given input and then mixes it with the original image (Hendrycks et al., 2019). In this approach, all inputs are mixed with variations of themselves, rather than other members of the input set. Finally, ReMix, proposed by Chou et al. (2020), operates in a similarly to CoMix, introduced in Kim et al. (2021). It mixes the most important parts of two inputs using a saliency map; however, unlike regular *mixup* and CoMix, it decouples the mixing of features and labels. While the inputs are mixed, the labels are set with a bias toward the minority class. This small alteration improves the model's performance on classes with a smaller number of inputs, which improves generalization by eliminating the larger class's influence on the model's output.

6 Conclusion

Standard mixup mixes the list of training examples with a random permutation of itself. We have empirically found that our method improves upon standard mixup. Specifically, standard mixup is a special case of our method when $\gamma=0$. We show that there exist non-zero values of γ that improve upon standard mixup. For CIFAR-10, $\gamma=0.25$ improves upon standard mixup by 0.6%. For CIFAR-100, $\gamma=0.125$ improves upon standard mixup by 0.5%.

We find that the model confuses intuitively similar classes of images like trucks and automobiles. We upsample the pairs of such similar classes to make the decision boundary between them more linear. This claim is supported by the decrease in standard deviation over epochs and our performance improvement over standard mixup. This defends our hypothesis that some pairs of classes can benefit from mixing more than others, and that our method of upsampling is one effective method of doing so.

The results indicate upsampling can be overdone. For larger values of γ , the model likely sees a much smaller range of class combinations, leading to decreased robustness. Our proposed method represents a step forward in the field of data augmentation. It not only uses the principles of Vicinal Risk Minimization but also introduces an adaptive approach that is absent in standard mixup. The ability to integrate error analysis directly into the augmentation process opens new avenues for research and application, particularly in domains where data is limited or highly complex. Future work should focus on expanding this method's applicability to other forms of data beyond images. Work could also be done to find general rules of which value of γ most improves model performance given the dataset and model architecture.

7 Division of Work

- 1. David C. Mason: I completed a comprehensive overview of twelve different papers on differing implementations of *mixup*. From this research, I wrote the related works section, edited the introduction, and aided in the preliminaries section. Afterward, I co-developed the proposed method, and supported the completion of the experiment. Finally, I wrote the conclusion, analyzing our results and evaluating the success of the thesis.
- 2. Harrison F. Stropkay: I performed an initial literature review. I adapted the code from the original *mixup* paper and implemented our method with Tucker. I ran the experiments and created some of the analysis figures. I wrote the proposed method and parts of other sections.
- 3. Tucker C. Simpson: I worked with Harrison to implement our version of *mixup* based on the code from the original *mixup* paper and extended the code to the CIFAR-100 dataset. I worked with Harrison to decide what experiments to run. I wrote some of the analysis and created some of the figures in the experiments section.
- 4. Anastasia C. Johnson: I read through the original MixUp paper and wrote up the preliminaries section using the information from that paper, along with an explanation of confusion matrices, to give context for our method.
- 5. Abdullah Al Maruf: I performed a literature survey on the original *mixup* and related papers, analyzed and plotted some of the results for comparative analysis between different experiments, and initially wrote part of the experiment result subsection along with plots and tables. I wrote the abstract and introduction and made contribution to related works, conclusion etc. I reviewed/revised the entire manuscript for technical accuracy, coherency, and formatting check. I also performed initial experiment with non mix-up data augmentation in CNN to verify that the loss-function cannot be further minimized, thus necessity of *mixup* and further development of augmentation.

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