Squared $\ell_2$ Norm as Consistency Loss for Leveraging Augmented Data to Learn Robust and Invariant Representations

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Abstract

Data augmentation is one of the most popular techniques for improving the robustness of neural networks. In addition to directly training the model with original samples and augmented samples, a torrent of methods regularizing the distance between embeddings/representations of the original samples and their augmented counterparts have been introduced. In this paper, we explore these various regularization choices, seeking to provide a general understanding of how we should regularize the embeddings. Our analysis suggests the ideal choices of regularization correspond to various assumptions. With an invariance test, we argue that regularization is important if the model is to be used in a broader context than accuracy-driven setting because non-regularized approaches are limited in learning the concept of invariance, despite equally high accuracy. Finally, we also show that the generic approach we identified (squared $\ell_2$ norm regularized augmentation) outperforms several recent methods, which are each specially designed for one task and significantly more complicated than ours, over three different tasks.

1 Introduction

Recent advances in deep learning has delivered remarkable empirical performance over i.i.d test data, and the community continues to investigate the more challenging and realistic scenario when models are tested in robustness over non-i.i.d data (e.g., Ben-David et al., 2010; Szegedy et al., 2013). Recent studies suggest that one challenge is the model’s tendency in capturing undesired signals (Geirhos et al., 2019; Wang et al., 2020), thus combating this tendency may be a key to robust models.

To help models ignore the undesired signals, data augmentation (i.e., diluting the undesired signals of training samples by applying transformations to existing examples) is often used. Given its widely usage, we seek to answer the question: how should we train with augmented samples so that the assistance of augmentation can be taken to the fullest extent to learn robust and invariant models?

In this paper, We analyze the generalization behaviors of models trained with augmented data and associated regularization techniques. We investigate a set of assumptions and compare the worst-case expected risk over unseen data when i.i.d samples are allowed to be transformed according to a function belonging to a family. We bound the expected risk with terms that can be computed during training, so that our analysis can inspire how to regularize the training procedure. While all the derived methods have an upper bound of the expected risk, with progressively stronger assumptions, we have progressively simpler regularization, allowing practical choices to be made according to the understanding of the application. Our contributions of this paper are as follows:

- We offer analyses of the generalization behaviors of augmented models trained with different regularizations: these regularizations require progressively stronger assumptions of the data and the augmentation functions, but progressively less computational efforts. For example, with assumptions pertaining to augmentation transformation functions, the Wasserstein distance over the original and augmented empirical distributions can be calculated through simple $\ell_1$ norm distance.

- We test and compare these methods and offer practical guidance on how to choose regularizations in practice. In short, regularizing the squared $\ell_2$ distance of logits between the augmented samples and original samples is a favorable method, suggested by both theoretical and empirical evidence.
• With an invariance test, we argue that vanilla augmentation does not utilize the augmented samples to the fullest extent, especially in learning invariant representations, thus may not be ideal unless the only goal of augmentation is to improve the accuracy over a specific setting.

2 Related Work & Key Differences

Data augmentation has been used effectively for years. Tracing back to the earliest convolutional neural networks, we notice that even the LeNet applied on MNIST dataset has been boosted by mixing the distorted images to the original ones (LeCun et al., 1998). Later, the rapidly growing machine learning community has seen a proliferate development of data augmentation techniques (e.g., flipping, rotation, blurring etc.) that have helped models climb the ladder of the state-of-the-art (one may refer to relevant survey (Shorten and Khoshgoftaar, 2019) for details). Recent advances expanded the conventional concept of data augmentation and invented several new approaches, such as leveraging the information in unlabelled data (Xie et al., 2019), automatically learning augmentation functions (Ho et al., 2019; Hu et al., 2019; Wang et al., 2019; Zhang et al., 2020; Zoph et al., 2019), and generating the samples (with constraint) that maximize the training loss along training (Fawzi et al., 2016), which is later widely accepted as adversarial training (Madry et al., 2018).

While the above works mainly discuss how to generate the augmented samples, in this paper, we mainly answer the question about how to train the models with augmented samples. For example, instead of directly mixing augmented samples with the original samples, one can consider regularizing the representations (or outputs) of original samples and augmented samples to be close under a distance metric (also known as a consistency loss). Many concrete ideas have been explored in different contexts. For example, $\ell_2$ distance and cosine similarities between internal representations in speech recognition (Liang et al., 2018), squared $\ell_2$ distance between logsits (Kannan et al., 2018), or KL divergence between softmax outputs (Zhang et al., 2019a) in adversarially robust vision models, Jensen–Shannon divergence (of three distributions) between embeddings for texture invariant image classification (Hendrycks et al., 2020). These are but a few examples of the concrete and successful implementations for different applications out of a huge collection (e.g., (Wu et al., 2019; Guo et al., 2019; Zhang et al., 2019b; Shah et al., 2019; Asai and Hajishirzi, 2020; Sajjadi et al., 2016; Zheng et al., 2016; Xie et al., 2015)), and one can easily imagine methods permuting these three elements (distance metrics, representation or outputs, and applications) to be invented. Even further, although we are not aware of the following methods in the context of data augmentation, given the popularity of GAN (Goodfellow, 2016) and domain adversarial neural network (Ganin et al., 2016), one can also expect the distance metric generalizes to a specialized discriminator (i.e. a classifier), which can be intuitively understood as a calculated (usually maximized) distance measure, Wasserstein-1 metric as an example (Arjovsky et al., 2017; Gulrajani et al., 2017).

Key Differences: With this rich collection of regularizing choices, which one method should we consider in general? More importantly, do we actually need the regularization at all? These questions are important for multiple reasons, especially considering that there are paper suggesting that these regularizations may lead to worse results (Jeong et al., 2019). In this paper, we answer the first question with a proved upper bound of the worst case generalization error, and our upper bound explicitly describes what regularizations are needed. For the second question, we will show that regularizations can help the model to learn the concept of invariance.

There are also several previous discussions regarding the detailed understandings of data augmentation (Yang et al., 2019; Chen et al., 2019; Hernández-García and König, 2018; Rajput et al., 2019; Dao et al., 2019), among which, (Yang et al., 2019) is probably the most relevant as it also defends the usage of regularizations. However, we believe our discussions are more comprehensive and supported theoretically, since our analysis directly suggests the ideal regularization. Also, empirically, we design an invariance test in addition to the worst-case accuracy used in the preceding work.

3 Training Strategies with Augmented Data

Notations $(X, Y)$ denotes the data, where $X \in \mathcal{R}^{n \times p}$ and $Y \in \{0, 1\}^{n \times k}$ (one-hot vectors for $k$ classes), and $f(\cdot; \theta)$ denotes the model, which takes in the data and outputs the softmax (probabilities of the prediction) and $\theta$ denotes the corresponding parameters. $g(\cdot)$ completes the prediction (i.e., mapping softmax to one-hot prediction). $l(\cdot, \cdot)$ denotes a generic loss function. $a(\cdot)$ denotes a transformation that alters the undesired signals of a sample, i.e., the data augmentation method. $a \in \mathcal{A}$, which is the set of transformation functions. $P$ denotes the distribution of $(x, y)$. For any sampled $(x, y)$, we have
\((a(x), y)\), and we use \(P_a\) to denote the distribution of these transformed samples. \(r(\cdot; \theta)\) denotes the risk of model \(\theta\). \(\hat{\cdot}\) denotes the estimated term \(\cdot\).

### 3.1 Well-behaved Data Transformation Function

Despite the strong empirical performance data augmentation has demonstrated, it should be intuitively expected that the performance can only be improved when the augmentation is chosen wisely. Therefore, before we proceed to analyze the behaviors of training with data augmentations, we need first regulate some basic properties of the data transformation functions used. Intuitively, we will consider the following three properties.

- “Dependence-preservation” with two perspectives: Label-wise, the transformation cannot alter the label of the data, which is a central requirement of almost all the data augmentation practice. Feature-wise, the transformation will not introduce new dependencies between the samples. Notice that this dependence-preservation assumption appears strong, but it is one of the central assumptions required to derive the generalization bounds.

- “Efficiency”: the augmentation should only generate new samples of the same label as minor perturbations of the original one. If a transformation violates this property, there should exist other simpler transformations that can generate the same target sample.

- “Vertices”: There are extreme cases of the transformations. For example, if one needs the model to be invariant to rotations from 0° to 60°, we consider the vertices to be 0° rotation function (thus identity map) and 60° rotation function. In practice, one usually selects the transformation vertices with intuitions and domain knowledge.

We now formally define these three properties. The definition will depend on the model, thus these properties are not only regulating the transformation functions, but also the model. We introduce the Assumptions A1-A3 corresponding to the properties.

**A1:** Dependence-preservation: the transformation function will not alter the dependency regarding the label (i.e., for any \(a() \in A\), \(a(x)\) will have the same label as \(x\)) or the features (i.e., for any \(a_1(), a_2() \in A\), \(a_1(x_1) \perp a_2(x_2)\) for any \(x_1, x_2 \in X\) that \(x_1 \neq x_2\), in other words, \(a_1(x_1)\) and \(a_2(x_2)\) are independent if \(x_1\) and \(x_2\) are independent).

**A2:** Efficiency: for \(\tilde{\theta}\) and any \(a() \in A\), \(f(a(x); \tilde{\theta})\) is closer to \(x\) than any other samples under a distance metric \(d_x(\cdot, \cdot)\), i.e.,

\[
d_x(f(a(x); \tilde{\theta}), f(x; \tilde{\theta})) \leq \min_{x' \in X} \, d_x(f(a(x); \tilde{\theta}), f(x'; \tilde{\theta})).
\]

**A3:** Vertices: For a model \(\tilde{\theta}\) and a transformation \(a()\), we use \(P_{a, \tilde{\theta}}\) to denote the distribution of \(f(a(x); \tilde{\theta})\) for \((x, y) \sim P\). “Vertices” argues that exists two extreme elements in \(A\), namely \(a^+\) and \(a^-\), with certain metric \(d_x(\cdot, \cdot)\), we have

\[
d_x(P_{a^+, \tilde{\theta}}, P_{a^-, \tilde{\theta}}) = \sup_{a_1, a_2 \in A} \, d_x(P_{a_1, \tilde{\theta}}, P_{a_2, \tilde{\theta}})
\]

Note that \(d_x(\cdot, \cdot)\) is a metric over two distributions and \(d_x(\cdot, \cdot)\) is a metric over two samples. Also, slightly different from the intuitive understanding of “vertices” above, **A3** regulates the behavior of embedding instead of raw data. All of our follow-up analysis will require **A1** to hold, but with more assumptions held, we can get computationally lighter methods with bounded error.

### 3.2 Background, Robustness, and Invariance

One central goal of machine learning is to understand the generalization error. When the test data and train data are from the same distribution, many previous analyses can be sketched as:

\[
r_P(\tilde{\theta}) \leq \hat{r}_P(\tilde{\theta}) + \phi(||\Theta||, n, \delta)
\]

which states that the expected risk can be bounded by the empirical risk and a function of hypothesis space \(||\Theta||\) and number of samples \(n\); \(\delta\) accounts for the probability when the bound holds. \(\phi()\) is a function of these three terms. Depending on the details of different analyses, different concrete examples of this generic term will need different assumptions. We use a generic assumption **A4** to denote the assumptions required for each example. More concrete discussions are in Appendix A.
Robustness. In addition to the generalization error above, we also study the robustness by following the established definition as in the worst case expected risk when the test data is allowed to be shifted to some other distributions by transformation functions in $\mathcal{A}$. Formally, we study

$$r_{\mathcal{P}}(\hat{\theta}) = \mathbb{E}_{(x,y) \sim \mathcal{P}} \max_{a \sim \mathcal{A}} I(g(f(a(x);\hat{\theta})) \neq y)$$

As $r_{\mathcal{P}}(\hat{\theta}) \leq r_{\mathcal{P}}(\hat{\theta})$, we only need to study (3). We will analyze (3) in different scenarios involving different assumptions and offer formalizations of the generalization bounds under each scenario. Our bounds shall also immediately inspire the development of methods in each scenario as the terms involved in our bound are all computable within reasonable computational loads.

Invariance. In addition to robustness, we are also interested in whether the model learns to be invariant to the undesired signals. Intuitively, if data augmentation is used to help dilute the undesired signals from data by altering the undesired signals with $a() \in \mathcal{A}$, a successfully trained model with augmented data will map the raw data with various undesired signals to the same embedding. Thus, we study the following metric to quantify the model’s ability in learning invariant representations:

$$I(\hat{\theta}, \mathcal{P}) = \sup_{a_1, a_2 \in \mathcal{A}} d_2(\mathcal{P}_{a_1, \hat{\theta}}, \mathcal{P}_{a_2, \hat{\theta}}),$$

where $\mathcal{P}_{a, \hat{\theta}}$ to denote the distribution of $f(a(x); \hat{\theta})$ for $(x, y) \sim \mathcal{P}$. $d_2()$ is a distance over two distributions, and we suggest to use Wasserstein metric given its favorable properties (e.g., see practical examples in Figure 1 of (Cuturi and Doucet, 2014) or theoretical discussions in (Villani, 2008)). Due to the difficulties in assessing $f(a(x); \hat{\theta})$ (as it depends on $\hat{\theta}$), we mainly study (4) empirically, and argue that models trained with explicit regularization of the empirical counterpart of (4) will have favorable invariance property.

3.3 Worst-case Augmentation (Adversarial Training)

We consider robustness first. (3) can be written equivalently into the expected risk over a pseudo distribution $\mathcal{P}'$ (see Lemma 1 in (Tu et al., 2019)), which is the distribution that can sample the data leading to the worst expected risk. Thus, equivalently, we can consider $\sup_{\mathcal{P}' \in T(\mathcal{P}, \mathcal{A})} r_{\mathcal{P}'}(\hat{\theta})$. With an assumption relating the worst distribution of expected risk and the worst distribution of the empirical risk (namely, A5, in Appendix A), the bound of our interest (i.e., $\sup_{\mathcal{P}' \in T(\mathcal{P}, \mathcal{A})} r_{\mathcal{P}'}(\hat{\theta})$) can be analogously analyzed through $\sup_{\mathcal{P}' \in T(\mathcal{P}, \mathcal{A})} \hat{r}_{\mathcal{P}'}(\hat{\theta})$. By the definition of $\mathcal{P}'$, we can have:

**Lemma 3.1.** With Assumptions A1, A4, and A5, with probability at least $1 - \delta$, we have

$$\sup_{\mathcal{P}' \in T(\mathcal{P}, \mathcal{A})} r_{\mathcal{P}'}(\hat{\theta}) \leq \frac{1}{n} \sum_{(x,y) \sim \mathcal{P}} I(g(f(a(x);\hat{\theta})) \neq y) + \phi(|\theta|, n, \delta)$$

This result is a straightforward follow-up of the preceding discussions. In practice, it aligns with the adversarial training (Madry et al., 2018), a method that has demonstrated impressive empirical successes in the robust machine learning community.

While the adversarial training has been valued by its empirical superiorities, it may still have the following two directions that can be improved: firstly, it lacks an explicit enforcement of the concept of invariance between the original sample and the transformed sample; secondly, it assumes that elements of $\mathcal{A}$ are enumerable, thus $\frac{1}{n} \sum_{(x,y) \sim \mathcal{P}} \sup_{a \in \mathcal{A}} I(g(f(a(x);\hat{\theta})) \neq y)$ is computable. The remaining discussions expand along these two directions.

3.4 Regularized Worst-case Augmentation

To force the concept of invariance, the immediate solution might be to apply some regularizations to minimize the distance between the embeddings learned from the original sample and the ones learned from the transformed samples. We have offered a summary of these methods in Section 2.

To have a model with small invariance score, the direct approach will be regularizing the empirical counterpart of (4). We notice that existing methods barely consider this regularization, probably because of the computational difficulty of Wasserstein distance. Conveniently, we have the following result that links the $\ell_1$ regularization to the Wasserstein-1 metric in the context of data augmentation.
Proposition 3.2. With Assumption \( A2 \), and \( d_e(\cdot, \cdot) \) in \( A2 \) chosen to be \( \ell_1 \) norm, for any \( a \in A \), we have

\[
\sum_i ||f(x_i; \tilde{\theta}) - f(a(x_i); \tilde{\theta})||_1 = W_1(f(x; \tilde{\theta}), f(a(x); \tilde{\theta}))
\]

This result conveniently allows us to use \( \ell_1 \) norm distance to replace Wasserstein metric, integrating the advantages of Wasserstein metric while avoiding practical issues such as computational complexity and difficulty to pass the gradient back during backpropagation.

We continue to discuss the generalization behaviors. Our analysis remains in the scope of multi-class classification, where the risk is evaluated as misclassification rate, and the model is optimized with cross-entropy loss (with the base chosen to be log base in cross-entropy loss). This setup aligns with \( A4 \), and should represent the modern neural network studies well enough.

Before we proceed, we need another technical assumption \( A6 \) (details in Appendix A), which can be intuitively considered as a tool that allows us to relax classification error into cross-entropy error, so that we can bound the generalization error with the terms we can directly optimize during training.

We can now offer another technical result:

Theorem 3.3. With Assumptions \( A1, A2, A4, A5 \), and \( d_e(\cdot, \cdot) \) in \( A2 \) is \( \ell_1 \) norm, with probability at least \( 1 - \delta \), the worst case generalization risk will be bounded as

\[
\sup_{P' \in T(P, A)} r_{P'}(\tilde{\theta}) \leq \hat{r}_{P}(\tilde{\theta}) + \sum_i ||f(x_i; \tilde{\theta}) - f(x_i'; \tilde{\theta})||_1 + \phi(||\theta||, n, \delta)
\]

and \( x' = a(x) \), where \( a = \arg \min_{a \in A} y^T f(a(x); \tilde{\theta}) \).

This technical result also immediately inspires the method to guarantee worst case performance, as well as to explicitly enforce the concept of invariance. Notice that \( a = \arg \max_{a \in A} y^T f(a(x); \tilde{\theta}) \) is simply selecting the augmentation function maximizing the cross-entropy loss, a standard used by many worst case augmenting method (e.g., Madry et al., 2018).

3.5 Regularized Training with Vertices

As \( A \) in practice is usually a set with a large number of (and possibly infinite) elements, we may not always be able to identify the worst case transformation function with reasonable computational efforts. This limitation also prevents us from effective estimating the generalization error as the bound requires the identification of the worst case transformation.

Our final discussion is to leverage the vertex property of the transformation function to bound the worst case generalization error:

Lemma 3.4. With Assumptions \( A1-A6 \), and \( d_e(\cdot, \cdot) \) in \( A2 \) chosen as \( \ell_1 \) norm distance, \( d_e(\cdot, \cdot) \) in \( A3 \) chosen as Wasserstein-1 metric, assuming there is a \( a' \in A \) where \( \hat{r}_{P_{a'}}(\tilde{\theta}) = \frac{1}{2}(\hat{r}_{P_{a'+}}(\tilde{\theta}) + \hat{r}_{P_{a'-}}(\tilde{\theta})) \), with probability at least \( 1 - \delta \), we have:

\[
\sup_{P' \in T(P, A)} r_{P'}(\tilde{\theta}) \leq \frac{1}{2}(\hat{r}_{P_{a'+}}(\tilde{\theta}) + \hat{r}_{P_{a'-}}(\tilde{\theta})) + \sum_i ||f(a^+(x_i); \tilde{\theta}) - f(a^-(x_i); \tilde{\theta})||_1 + \phi(||\theta||, n, \delta)
\]

This result inspires the method that can directly guarantee the worst case generalization risk and can be optimized conveniently without searching for the worst-case transformations. However, this method requires a good domain knowledge of the vertices of the transformation functions.

3.6 Engineering Specification of Relevant Methods

Our theoretical analysis has lead to a line of methods, however, not every method can be effectively implemented, especially due to the difficulties of passing gradient back for optimizations. Therefore, to boost the influence of the loss function through backpropagation, we recommend to adapt the methods with the following two changes: 1) the regularization is enforced on logits instead of softmax; 2) we use squared \( \ell_2 \) norm instead of \( \ell_1 \) norm because \( \ell_1 \) norm is not differentiable everywhere. We discuss the effects of these compromises in ablation studies in Appendix E.

Also, in the cases where we need to identify the worst case transformation functions, we iterate through all the transformation functions and identify the function with the maximum loss.

Overall, our analysis leads to the following main training strategies:
VA (vanilla augmentation): mix the augmented samples of a vertex function to the original ones for training (original samples are considered as from another vertex in following experiments).

VWA (vanilla worst-case augmentation): at each iteration, identify the worst-case transformation functions and train with samples generated by them (also known as adversarial training).

RA (regularized augmentation): regularizing the squared $\ell_2$ distance over logits between the original samples and the augmented samples of a fixed vertex transformation function.

RWA (regularized worst-case augmentation): regularizing the squared $\ell_2$ distance over logits between the original samples and the worst-case augmented samples identified at each iteration.

4 Experiments

We first use some synthetic experiments to verify our assumptions and inspect the consequences when the assumptions are not met (in Appendix C). Then, in the following paragraphs, we test the methods discussed to support our arguments in learning robustness and invariance. Finally, we show the power of our discussions by competing with advanced methods designed for specific tasks.

4.1 Experiments for Learning Robust & Invariant Representation

Experiment Setup: We first test our arguments with two data sets and three different sets of the augmentations. We study MNIST dataset with LeNet architecture, and CIFAR10 dataset with ResNet18 architecture. To examine the effects of the augmentation strategies, we disable all the heuristics that are frequently used to boost the test accuracy of models, such as the default augmentation many models trained for CIFAR10 adopted, and the BatchNorm (also due to the recent arguments against the effects of BatchNorm in learning robust features (Wang et al., 2020)), although forgoing these heuristics will result in a lower overall performance than one usually expects.

We consider three different sets of transformation functions:

- Texture: we use Fourier transform to perturb the texture of the data by discarding the high-frequency components of the given a radius $r$. The smaller $r$ is, the less high-frequency components the image has. We consider $A = \{a(), a_{12}(), a_{10}(), a_5(), a_6()\}$, where $a()$ is the identity map. Thus, vertexes are $a()$ and $a_6$.

- Rotation: we rotate the images clockwise $r$ degrees. We consider $A = \{a(), a_{15}(), a_{30}(), a_{45}(), a_{60}()\}$, where $a()$ is the identity map. Thus, vertexes are $a()$ and $a_{60}$.

- Contrast: we create the images depicting the same semantic information, but with different scales of the pixels, including the negative color representation. Therefore, we have $A = \{a(x) = x, a_1(x) = x/2, a_2(x) = x/4, a_3(x) = 1 - x, a_4(x) = (1 - x)/2, a_5(x) = (1 - x)/4, \}$ where $x$ stands for the image whose pixel values have been normalized to be between 0 and 1. We consider $a()$ and $a_3()$ as vertexes.

We first train the baseline models to get reasonably high performance, and then train other augmented models with the same hyperparameters. VA and RA are augmented with vertexes, while VWA and RWA are augmented with $A$. For methods with a regularizer, we run the experiments with 9 hyperparameters evenly split in the logspace from $10^{-4}$ to $10^4$, and we report the methods with the best worst-case accuracy.

Evaluation Metrics: We consider three different evaluation metrics:

- Clean: test accuracy on the original test data, mainly reported as a reference for other metrics.

- Robustness: the worst accuracy when each sample can be transformed with $a \in A$.

- Invariance: A metric to test whether the models learns the concept of invariance (details to follow).

Invariance-test: To test whether a model can truly learns the concept of invariance within $A = \{a_1(), a_2(), \ldots , a_t()\}$ of $t$ elements, we design a new evaluation metric: for a sampled collection of data of the sample label $i$, denoted as $X^{(i)}$, we generate the transformed copies of it with $A$, resulting in
Table 1: Results of MNIST data (“C” stands for clean accuracy, “R” stands for robustness, and “I” stands for invariance score): invariance score shows big differences while accuracy does not.

| Texture | Rotation | Pixel-value |
|---------|----------|-------------|
| C       | R        | I           |
| Base    | 0.9290   | 0.9843      | 0.9236      |
| VA      | 0.9923   | 0.9902      | 0.9916      |
| RA      | 0.9908   | 0.9905      | 1.0000      |
| VWA     | 0.9919   | 0.9900      | 0.9976      |
| RWA     | 0.9911   | 0.9909      | 1.0000      |

\(X^{(i)}_{a_1}, X^{(i)}_{a_2}, \ldots, X^{(i)}_{a_t}\). We combined these copies into a dataset, denoted as \(X^{(i)}\). For every sample \(x\) in \(X^{(i)}\), we retrieve its \(t\) nearest neighbors of other samples in \(X^{(i)}\), and calculate the overlap of the retrieved samples and \(\{a_1(x), a_2(x), \ldots, a_t(x)\}\). Since the identity map is in \(A\), so the calculated overlap score will be in \([1/t, 1]\). The distance used is \(d(\cdot, \cdot) = ||f(\cdot; \theta) - f(\cdot; \tilde{\theta})||_1\), where \(\tilde{\theta}\) is the model we are interested to examine. Finally, we report the averaged score for every label. Thus, a high overlap score indicates the prediction of model \(\tilde{\theta}\) is invariant to the augmentation functions in \(A\). If we use other distance functions, the reported values may differ, but we notice that the rank of the methods compared in terms of this test barely changes.

**Results:** We show the results in Table 1 and Table 6 (in Appendix) for MNIST and CIFAR10 respectively. Table 1 shows that RWA is generally a superior method, in terms of all the metrics, especially the invariance evaluation as it shows a much higher invariance score than competing methods. We believe this advantage of invariance comes from two sources: regularizations and the fact that RWA has seen all the augmentation functions in \(A\). In comparison, RA also has regularization but only sees the vertices in \(A\), so the invariance score of RA is not compatible to RWA, although better than VA. Table 6 roughly tells the same story. More discussions are in Appendix D.

**Other results (Appendix E):** The strength of RWA can also be shown in several other different scenarios, even in the out-of-domain test scenario where the transformation functions are not in \(A\). RWA generally performs the best, although not the best in every single test. We also perform ablation test to validate the choice of squared \(\ell_2\) norm over logits in contrast to other distance metrics. Our choice performs the best in the worst-case performance. This advantage is expected as our choice is validated by theoretical arguments as well as consideration of engineering convenience.

Overall, the empirical performances align with our expectation from the theoretical discussion: while all methods discussed have a bounded worst case performance, we do not intend to compare the upper bounds because smaller upper bounds do not necessarily guarantee a smaller risk. However, worst case augmentation methods tend to show a better worst case performances because they have been augmented with all the elements in \(A\). Also, there is no clear evidence suggesting the difference between augmentation methods and its regularized versions in terms of the worst case performance, but it is clear that regularization helps to learn the concept of invariance.

### 4.2 Comparison to Advanced Methods

Finally, we also compete our generic data augmentation methods against several specifically designed methods in different applications. We use the four generic methods (VA, RA, VWA, and RWA) with generic transformation functions (\(A\) of “rotation”, “contrast”, or “texture” used in the synthetic experiments). We compare our methods with techniques invented for three different topics of study (rotation invariant, texture perturbation, and cross-domain generalization), and each of these topics has seen a long line of method development. We follow each own tradition (e.g., rotation methods are usually tested in CIFAR10 dataset, seemingly due to the methods’ computational requirements), test over each own most challenging dataset (e.g., ImageNet-Sketch is the most recent and challenging dataset in domain generalization, although less studied), and report each own evaluation metric (e.g., methods tested with ImageNet-C are usually evaluated with mCE).

Overall, the performances of our generic methods outperform these advanced SOTA techniques. Thus, the main conclusion, as validated by these challenging scenarios, are (1) usage of data augmentation can outperform carefully designed methods; (2) usage of the consistency loss can further improve the performances; (3) regularized worst-case augmentation generally works the best.
### Table 2: Comparison to advanced rotation-invariant models. We report the test accuracy on the test sets clockwise rotated, $0^\circ-60^\circ$ and $300^\circ-360^\circ$. Average accuracy is also reported. Augmentation methods only consider $0^\circ-60^\circ$ clockwise rotations during training.

|          | Base | ST  | GC  | ETN | VA  | RA  | VWA | RWA |
|----------|------|-----|-----|-----|-----|-----|-----|-----|
| Clean    | 23.9 | 24.5| 22.8| 23  | 27.2| 22.4| 23  | 23  |
| mCE      | 80.6 | 74.3| 72.7| 73.4| 68.4| 64.9| 76.3| 75.6| 74.8|

### Table 3: Summary comparison to advanced models over ImageNet-C data. Performance reported (mCE) follows the standard in ImageNet-C data: clean error and mCE are both the smaller the better.

|          | Base | InfoDrop | HEX | PAR | VA | RA | VWA | RWA |
|----------|------|----------|-----|-----|----|----|-----|-----|
| Top-1    | 0.1204| 0.1224   | 0.1292| 0.1306| 0.1362| 0.1405| 0.1432| 0.1486|
| Top-5    | 0.2408| 0.2564   | 0.2627| 0.2715| 0.2793| 0.2846| 0.2933|

### Table 4: Comparison to advanced cross-domain image classification models, over ImageNet-Sketch dataset. We report top-1 and top-5 accuracy following standards on ImageNet related experiments.

**Rotation-invariant Image Classification** We compare our results with specifically designed rotation-invariant models, mainly Spatial Transformer (ST) (Jaderberg et al., 2015), Group Convolution (GC) (Cohen and Welling, 2016), and Equivariant Transformer Network (ETN) (Tai et al., 2019). We also attempted to run CGNet (Kondor et al., 2018), but the procedure does not scale to the CIFAR10 and ResNet level. The results are reported in Table 2, where most methods use the same architecture (ResNet34 with most performance boosting heuristics enabled), except that GC uses ResNet18 because ResNet34 with GC runs 100 times slower than others, thus not practical. We test the models with nine different rotations including $0^\circ$ degree rotation. Augmentation related methods are using the $A$ of “rotation” in synthetic experiments, so the testing scenario goes beyond what the augmentation methods have seen during training. The results in Table 2 strongly endorse the efficacy of augmentation-based methods. Interestingly, regularized augmentation methods, with the benefit of learning the concept of invariance, tend to behave well in the transformations not considered during training. As we can see, RA outperforms VWA on average.

**Texture-perturbed ImageNet classification** We also test the performance on the image classification over multiple perturbations. We train the model over standard ImageNet training set and test the model with ImageNet-C data (Hendrycks and Dietterich, 2019), which is a perturbed version of ImageNet by corrupting the original ImageNet validation set with a collection of noises. Following the standard, the reported performance is mCE, which is the smaller the better. We compare with several methods tested on this dataset, including Patch Uniform (PU) (Lopes et al., 2019), AutoAugment (AA) (Cubuk et al., 2019), MaxBlur pool (MBP) (Zhang, 2019), Stylized ImageNet (SIN) (Hendrycks and Dietterich, 2019), AugMix (AM) (Hendrycks et al., 2020), AugMix w. SIN (AMS) (Hendrycks et al., 2020). We use the performance reported in (Hendrycks et al., 2020). Again, our augmentation only uses the generic texture with perturbation (the $A$ in our texture synthetic experiments with radius changed to 20, 25, 30, 35, 40). The results are reported in Table 3 (with more details in Table 13), which shows that our generic method outperform the current SOTA methods after a continued finetuning process with reducing learning rates.

**Cross-domain ImageNet-Sketch Classification** We also compare to the methods used for cross-domain evaluation. We follow the set-up advocated by (Wang et al., 2019b) for domain-agnostic cross-domain prediction, which is training the model on one or multiple domains without domain identifiers and test the model on an unseen domain. We use the most challenging setup in this scenario: train the models
with standard ImageNet training data, and test the model over ImageNet-Sketch data (Wang et al., 2019a), which is a collection of sketches following the structure ImageNet validation set. We compare with previous methods with reported performance on this dataset, such as InfoDrop (Achille and Soatto, 2018), HEX (Wang et al., 2019b), and PAR (Wang et al., 2019a), and report the performances in Table 4. Notice that, our data augmentation also follows the requirement that the characteristics of the test domain cannot be utilized during training. Thus, we only augment the samples with a generic augmentation set (.4 of “contrast” in synthetic experiments). The results again support the strength of the correct usage of data augmentation.

5 Conclusion

In this paper, we conducted a systematic inspection to study the proper regularization techniques that are provably related to the generalization error of a machine learning model, when the test distribution are allowed to be perturbed by a family of transformation functions. With progressively more specific assumptions, we identified progressively simpler methods that can bound the worst case risk. We summarize the main take-home messages below:

- Regularizing a norm distance between the logits of the originals samples and the logits of the augmented samples enjoys several merits: the trained model tend to have good worst cast performance, and can learn the concept of invariance (as shown in our invariance test). Although our theory suggests ℓ₁ norm, but we recommend squared ℓ₂ norm in practice considering the difficulties of passing the (sub)gradient of ℓ₁ norm in backpropagation.

- With the vertex assumption held (it usually requires domain knowledge to choose the vertex functions), one can use “regularized training with vertices” method and get good empirical performance in both accuracy and invariance, and the method is at the same complexity order of vanilla training without data augmentation. When we do not have the domain knowledge (thus are not confident in the vertex assumption), we recommend “regularized worst-case augmentation”, which has the best performance overall, but requires extra computations to identify the worst-case augmented samples at each iteration.

References

A. Achille and S. Soatto. Information dropout: Learning optimal representations through noisy computation. IEEE transactions on pattern analysis and machine intelligence, 40(12):2897–2905, 2018.

M. Arjovsky, S. Chintala, and L. Bottou. Wasserstein gan, 2017.

A. Asai and H. Hajishirzi. Logic-guided data augmentation and regularization for consistent question answering, 2020.

S. Ben-David, J. Blitzer, K. Crammer, A. Kulesza, F. Pereira, and J. W. Vaughan. A theory of learning from different domains. Machine learning, 79(1-2):151–175, 2010.

S. Bobkov and M. Ledoux. One-dimensional empirical measures, order statistics, and Kantorovich transport distances, volume 261. American Mathematical Society, 2019.

O. Bousquet, S. Boucheron, and G. Lugosi. Introduction to statistical learning theory. In Summer School on Machine Learning, pages 169–207. Springer, 2003.

S. Chen, E. Dobriban, and J. H. Lee. A group-theoretic framework for data augmentation, 2019.

T. Cohen and M. Welling. Group equivariant convolutional networks. In International conference on machine learning, pages 2990–2999, 2016.

E. D. Cubuk, B. Zoph, D. Mane, V. Vasudevan, and Q. V. Le. Autoaugment: Learning augmentation strategies from data. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 113–123, 2019.

M. Cuturi and A. Doucet. Fast computation of wasserstein barycenters. 2014.

T. Dao, A. Gu, A. Ratner, V. Smith, C. D. Sa, and C. Ré. A kernel theory of modern data augmentation. In K. Chaudhuri and R. Salakhutdinov, editors, Proceedings of the 36th International Conference
A. Fawzi, H. Samulowitz, D. S. Turaga, and P. Frossard. Adaptive data augmentation for image classification. In 2016 IEEE International Conference on Image Processing, ICIP 2016, Phoenix, AZ, USA, September 25-28, 2016, pages 3688–3692. IEEE, 2016.

Y. Ganin, E. Ustinova, H. Ajakan, P. Germain, H. Larochelle, F. Laviolette, M. Marchand, and V. Lempitsky. Domain-adversarial training of neural networks. The Journal of Machine Learning Research, 17(1):2096–2030, 2016.

R. Geirhos, P. Rubisch, C. Michaelis, M. Bethge, F. A. Wichmann, and W. Brendel. Imagenet-trained CNNs are biased towards texture; increasing shape bias improves accuracy and robustness. In International Conference on Learning Representations, 2019.

I. Goodfellow. Nips 2016 tutorial: Generative adversarial networks. arXiv preprint arXiv:1701.00160, 2016.

I. Gulrajani, F. Ahmed, M. Arjovsky, V. Dumoulin, and A. Courville. Improved training of wasserstein gans, 2017.

H. Guo, K. Zheng, X. Fan, H. Yu, and S. Wang. Visual attention consistency under image transforms for multi-label image classification. In IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2019, Long Beach, CA, USA, June 16-20, 2019, pages 729–739. Computer Vision Foundation / IEEE, 2019.

D. Hendrycks and T. Dietterich. Benchmarking neural network robustness to common corruptions and perturbations. Proceedings of the International Conference on Learning Representations, 2019.

D. Hendrycks, N. Mu, E. D. Cubuk, B. Zoph, J. Gilmer, and B. Lakshminarayanan. Augmix: A simple data processing method to improve robustness and uncertainty. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020. OpenReview.net, 2020.

A. Hernández-García and P. König. Data augmentation instead of explicit regularization, 2018.

D. Ho, E. Liang, X. Chen, I. Stoica, and P. Abbeel. Population based augmentation: Efficient learning of augmentation policy schedules. In K. Chaudhuri and R. Salakhutdinov, editors, Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA, volume 97 of Proceedings of Machine Learning Research, pages 2731–2741. PMLR, 2019.

Z. Hu, B. Tan, R. R. Salakhutdinov, T. M. Mitchell, and E. P. Xing. Learning data manipulation for augmentation and weighting. In Advances in Neural Information Processing Systems, pages 15738–15749, 2019.

M. Jaderberg, K. Simonyan, A. Zisserman, et al. Spatial transformer networks. In Advances in neural information processing systems, pages 2017–2025, 2015.

J. Jeong, S. Lee, J. Kim, and N. Kwak. Consistency-based semi-supervised learning for object detection. In Advances in Neural Information Processing Systems, pages 10758–10767, 2019.

H. Kannan, A. Kurakin, and I. Goodfellow. Adversarial logit pairing, 2018.

R. Kondor, Z. Lin, and S. Trivedi. Clebsch–gordan nets: a fully fourier space spherical convolutional neural network. In Advances in Neural Information Processing Systems, pages 10117–10126, 2018.

Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. Proceedings of the IEEE, 86(11):2278–2324, 1998.

D. Liang, Z. Huang, and Z. C. Lipton. Learning noise-invariant representations for robust speech recognition. In 2018 IEEE Spoken Language Technology Workshop (SLT), pages 56–63. IEEE, 2018.

P. Liang. Cs229t/stat231: Statistical learning theory (winter 2016), 2016.

R. G. Lopes, D. Yin, B. Poole, J. Gilmer, and E. D. Cubuk. Improving robustness without sacrificing accuracy with patch gaussian augmentation. arXiv preprint arXiv:1906.02611, 2019.

A. Madry, A. Makelov, L. Schmidt, D. Tsipras, and A. Vladu. Towards deep learning models resistant to adversarial attacks. In 6th International Conference on Learning Representations, ICLR 2018,
S. Rajput, Z. Feng, Z. Charles, P.-L. Loh, and D. Papailiopoulos. Does data augmentation lead to positive margin? In International Conference on Machine Learning, pages 5321–5330, 2019.

M. Sajjadi, M. Javanmardi, and T. Tasdizen. Regularization with stochastic transformations and perturbations for deep semi-supervised learning. In Advances in neural information processing systems, pages 1163–1171, 2016.

M. Shah, X. Chen, M. Rohrbach, and D. Parikh. Cycle-consistency for robust visual question answering. In The IEEE Conference on Computer Vision and Pattern Recognition (CVPR), June 2019.

C. Shorten and T. M. Khoshgoftaar. A survey on image data augmentation for deep learning. Journal of Big Data, 6(1):60, 2019.

C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus. Intriguing properties of neural networks. arXiv preprint arXiv:1312.6199, 2013.

K. S. Tai, P. Ballis, and G. Valaint. Equivariant transformer networks. arXiv preprint arXiv:1901.11399, 2019.

Z. Tu, J. Zhang, and D. Tao. Theoretical analysis of adversarial learning: A minimax approach. In Advances in Neural Information Processing Systems, pages 12259–12269, 2019.

C. Villani. Topics in optimal transportation. Number 58. American Mathematical Soc., 2003.

C. Villani. Optimal transport: old and new, volume 338. Springer Science & Business Media, 2008.

H. Wang, S. Ge, E. P. Xing, and Z. C. Lipton. Learning robust global representations by penalizing local predicitive power, 2019a.

H. Wang, Z. He, Z. C. Lipton, and E. P. Xing. Learning robust representations by projecting superficial statistics out. In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6–9, 2019. OpenReview.net, 2019b.

H. Wang, X. Wu, Z. Huang, and E. P. Xing. High frequency component helps explain the generalization of convolutional neural networks. In Computer Vision and Pattern Recognition (CVPR), 2020.

Y. Wang, X. Pan, S. Song, H. Zhang, G. Huang, and C. Wu. Implicit semantic data augmentation for deep networks. In Advances in Neural Information Processing Systems, pages 12614–12623, 2019c.

X. Wu, Y. Mao, H. Wang, X. Zeng, X. Gao, E. P. Xing, and M. Xu. Regularized adversarial training (RAT) for robust cellular electron cryo tomograms classification. In I. Yoo, J. Bi, and X. Hu, editors, 2019 IEEE International Conference on Bioinformatics and Biomedicine, BIBM 2019, San Diego, CA, USA, November 18-21, 2019, pages 1–6. IEEE, 2019.

Q. Xie, Z. Dai, E. Hovy, M.-T. Luong, and Q. V. Le. Unsupervised data augmentation. arXiv preprint arXiv:1904.12848, 2019.

S. Xie, T. Yang, X. Wang, and Y. Lin. Hyper-class augmented and regularized deep learning for fine-grained image classification. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 2645–2654, 2015.

F. Yang, Z. Wang, and C. Heinze-Deml. Invariance-inducing regularization using worst-case transformations suffices to boost accuracy and spatial robustness. In Advances in Neural Information Processing Systems, pages 14757–14768, 2019.

H. Zhang, Y. Yu, J. Jiao, E. P. Xing, L. E. Ghaoui, and M. I. Jordan. Theoretically principled trade-off between robustness and accuracy. In K. Chaudhuri and R. Salakhutdinov, editors, Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA, volume 97 of Proceedings of Machine Learning Research, pages 7472–7482. PMLR, 2019a.

R. Zhang. Making convolutional networks shift-invariant again. arXiv preprint arXiv:1904.11186, 2019.

X. Zhang, Q. Wang, J. Zhang, and Z. Zhong. Adversarial autoaugment. In International Conference on Learning Representations, 2020.

Z. Zhang, S. Wu, S. Liu, M. Li, M. Zhou, and T. Xu. Regularizing neural machine translation by target-
bidirectional agreement. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 443–450, 2019b.

S. Zheng, Y. Song, T. Leung, and I. Goodfellow. Improving the robustness of deep neural networks via stability training. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 4480–4488, 2016.

B. Zoph, E. D. Cubuk, G. Ghiasi, T.-Y. Lin, J. Shlens, and Q. V. Le. Learning data augmentation strategies for object detection, 2019.
A Additional Assumptions

A4: We list two classical examples here:

– when $A4$ is “$\Theta$ is finite, $l(\cdot, \cdot)$ is a zero-one loss, samples are i.i.d”, $\phi(|\Theta|, n, \delta) = \sqrt{(\log(|\Theta|) + \log(1/\delta))/2n}$

– when $A4$ is “samples are i.i.d”, $\phi(|\Theta|, n, \delta) = 2R(L) + \sqrt{(\log 1/\delta)}/2n$, where $R(L)$ stands for Rademacher complexity and $L = \{l_\theta | \theta \in \Theta\}$, where $l_\theta$ is the loss function corresponding to $\theta$.

For more information or more concrete examples of the generic term, one can refer to relevant textbooks such as (Bousquet et al., 2003).

A5: the worst distribution for expected risk equals the worst distribution for empirical risk, i.e.,

$$\arg \max_{P \in T(P, A)} r_P(\hat{\theta}) = \arg \max_{P' \in T(P, A)} \hat{r}_{P'}(\hat{\theta})$$

where $T(P, A)$ is the collection of distributions created by elements in $A$ over samples from $P$.

Assumption A5 appears very strong, however, the successes of methods like adversarial training (Madry et al., 2018) suggest that, in practice, A5 might be much weaker than it appears.

A6: With $(x, y) \in (X, Y)$, the worst case sample in terms of maximizing cross-entropy loss and worst case sample in terms of maximizing classification error for model $\hat{\theta}$ follows:

$$\forall x, \frac{y^T f(x; \hat{\theta})}{\inf_{a \in A} y^T f(a(x); \hat{\theta})} \geq \exp \left( I(g(f(x; \hat{\theta})) \neq g(f(x'; \hat{\theta})) \right) \tag{8}$$

where $x'$ stands for the worst case sample in terms of maximizing classification error, i.e.,

$$x' = \arg \min_x y^T g(f(x; \hat{\theta}))$$

Also,

$$\forall x, \inf_{a \in A} y^T f(a(x); \hat{\theta}) \geq 1 \tag{9}$$

Although Assumption A6 appears complicated, it describes simple situations that we will unveil in two scenarios:

- If $g(f(x; \hat{\theta})) = g(f(x'; \hat{\theta}))$, which means either the sample is misclassified by $\hat{\theta}$ or the adversary is incompetent to find a worst case transformation that alters the prediction, the RHS of Eq. 8 is 1, thus Eq. 8 always holds (because $A$ has the identity map as one of its elements).

- If $g(f(x; \hat{\theta})) \neq g(f(x'; \hat{\theta}))$, which means the adversary finds a transformation that alters the prediction. In this case, A2 intuitively states that the $A$ is reasonably rich and the adversary is reasonably powerful to create a gap of the probability for the correct class between the original sample and the transformed sample. The ratio is described as the ratio of the prediction confidence from the original sample over the prediction confidence from the transformed sample is greater than $e$.

We inspect Assumption A6 by directly calculating the frequencies out of all the samples when it holds. Given a vanilla model (Base), we notice that over 74% samples out of 50000 samples fit this assumption.
B Proof of Theoretical Results

B.1 Proof of Lemma 3.1

Lemma. With Assumptions A1, A4, and A5, with probability at least $1 - \delta$, we have

$$\sup_{P' \in T(P, A)} r_{P'}(\bar{\theta}) \leq \frac{1}{n} \sum_{(x,y) \sim P} \sup_{a \in A} l(g(f(a(x); \bar{\theta})) \neq y) + \phi(|\Theta|, n, \delta)$$

(10)

Proof. With Assumption A5, we simply say

$$\arg \max_{P' \in T(P, A)} r_{P'}(\bar{\theta}) = \arg \max_{P' \in T(P, A)} \bar{r}_{P'}(\bar{\theta}) = P_w$$

we can simply analyze the expected risk following the standard classical techniques since both expected risk and empirical risk are studied over distribution $P_w$.

Now we only need to make sure the classical analyses (as discussed in A4) are still valid over distribution $P_w$:

- when $A4$ is “$\Theta$ is finite, $l(\cdot, \cdot)$ is a zero-one loss, samples are i.i.d, $\phi(|\Theta|, n, \delta) = \sqrt{\log(|\Theta|) + \log(1/\delta)}/2n$.

The proof of this result uses Hoeffding’s inequality, which only requires independence of random variables. One can refer to Section 3.6 in Liang (2016) for the detailed proof.

- when $A4$ is “samples are i.i.d, $\phi(|\Theta|, n, \delta) = 2R(\mathcal{L}) + \sqrt{\log 1/\delta}/2n$. The proof of this result relies on McDiarmid’s inequality, which also only requires independence of random variables. One can refer to Section 3.8 in Liang (2016) for the detailed proof.

Assumption A1 guarantees the samples from distribution $P_w$ are still independent, thus the generic term holds for at least these two concrete examples, thus the claim is proved.

B.2 Proof of Proposition 3.2

Proposition. With $A2$, and $d_\ast(\cdot, \cdot)$ in $A2$ chosen to be $\ell_1$ norm, for any $a \in A$, we have

$$\sum_i ||f(x_i; \tilde{\theta}) - f(a(x_i); \tilde{\theta})||_1 = W_1(f(x; \tilde{\theta}), f(a(x); \tilde{\theta}))$$

(11)

Proof. We leverage the order statistics representation of Wasserstein metric over empirical distributions (e.g., see Section 4 in Bobkov and Ledoux (2019))

$$W_1(f(x; \tilde{\theta}), f(a(x); \tilde{\theta})) = \inf_\sigma \sum_i ||f(x_i; \tilde{\theta}) - f(a(x_{\sigma(i)}); \tilde{\theta})||_1$$

where $\sigma$ stands for a permutation of the index, thus the infimum is taken over all possible permutations. With Assumption A2, when $d_\ast(\cdot, \cdot)$ in $A2$ chosen to be $\ell_1$ norm, we have:

$$||f(x_i; \tilde{\theta}) - f(a(x_i); \tilde{\theta})||_1 \leq \min_{j \neq i} ||f(x_i; \tilde{\theta}) - f(a(x_j); \tilde{\theta})||_1$$

Thus, the infimum is taken when $\sigma$ is the natural order of the samples, which leads to the claim.

B.3 Proof of Theorem 3.3

Theorem. With Assumptions A1, A2, A4, A5, and A6, and $d_\ast(\cdot, \cdot)$ in $A2$ is $\ell_1$ norm, with probability at least $1 - \delta$, the worst case generalization risk will be bounded as

$$\sup_{P' \in T(P, A)} r_{P'}(\bar{\theta}) \leq \bar{r}_{P'}(\bar{\theta}) + \sum_i ||f(x_i; \tilde{\theta}) - f(x'_i; \tilde{\theta})||_1 + \phi(|\Theta|, n, \delta)$$

(12)

and $x' = a(x)$, where $a = \arg \max_{a \in A} \mathbf{y}^\top f(a(x); \tilde{\theta})$. 

14
Proof. First of all, in the context of multiclass classification, where \( g(f(x; \theta)) \) predicts a label with one-hot representation, and \( y \) is also represented with one-hot representation, we can have the empirical risk written as:

\[
\hat{r}_P(x; \hat{\theta}) = 1 - \frac{1}{n} \sum_{(x,y) \sim P} y^\top g(f(x; \hat{\theta}))
\]

Thus,

\[
\sup_{P' \in T(P,A)} \hat{r}_{P'}(x; \hat{\theta}) = \hat{r}_P(x; \hat{\theta}) + \sup_{P' \in T(P,A)} \hat{r}_{P'}(x; \hat{\theta}) - \hat{r}_P(x; \hat{\theta})
\]

\[
= \hat{r}_P(x; \hat{\theta}) + \frac{1}{n} \sup_{P' \in T(P,A)} \left( \sum_{(x,y) \sim P} y^\top g(f(x; \hat{\theta})) - \sum_{(x,y) \sim P'} y^\top g(f(x; \hat{\theta})) \right)
\]

With A6, we can continue with:

\[
\sup_{P' \in T(P,A)} \hat{r}_{P'}(x; \hat{\theta}) \leq \hat{r}_P(x; \hat{\theta}) + \frac{1}{n} \sup_{P' \in T(P,A)} \left( \sum_{(x,y) \sim P} y^\top \log(f(x; \hat{\theta})) - \sum_{(x,y) \sim P'} y^\top \log(f(x; \hat{\theta})) \right)
\]

If we use \( e(\cdot) = -y^\top \log(\cdot) \) to replace the cross-entropy loss, we simply have:

\[
\sup_{P' \in T(P,A)} \hat{r}_{P'}(x; \hat{\theta}) \leq \hat{r}_P(x; \hat{\theta}) + \frac{1}{n} \sup_{P' \in T(P,A)} \left( \sum_{(x,y) \sim P} e(f(x; \hat{\theta})) - \sum_{(x,y) \sim P'} e(f(x; \hat{\theta})) \right)
\]

Since \( e(\cdot) \) is a Lipschitz function with constant \( \leq 1 \) (because of A6, Eq.(9)) and together with the dual representation of Wasserstein metric (See e.g., Villani (2003)), we have

\[
\sup_{P' \in T(P,A)} \hat{r}_{P'}(x; \hat{\theta}) \leq \hat{r}_P(x; \hat{\theta}) + W_1(f(x, \hat{\theta}), f(x', \hat{\theta}))
\]

where \( x' = a(x) \), where \( a = \arg \max_{a \in \mathcal{A}} y^\top f(a(x); \hat{\theta}) \).

Further, we can use the help of Proposition 3.2 to replace Wasserstein metric with \( \ell_1 \) distance. Finally, we can conclude the proof with Assumption A5 as how we did in the proof of Lemma 3.1. \( \square \)

B.4 Proof of Lemma 3.4

Lemma. With Assumptions A1-A6, and \( d_z(\cdot, \cdot) \) in A2 chosen as \( \ell_1 \) norm distance, \( d_z(\cdot, \cdot) \) in A3 chosen as Wasserstein-1 metric, assuming there is a \( a'() \in \mathcal{A} \) where \( \hat{r}_{P_{a'}}(\hat{\theta}) = \frac{1}{2}(\hat{r}_{P_{a'}}(\hat{\theta}) + \hat{r}_{P_{a'}}(\hat{\theta})) \), with probability at least \( 1 - \delta \), we have:

\[
\sup_{P' \in T(P,A)} r_{P'}(\hat{\theta}) \leq \frac{1}{2}(\hat{r}_{P_{a'}}(\hat{\theta}) + \hat{r}_{P_{a'}}(\hat{\theta})) + \sum_i ||f(a^+(x_i); \hat{\theta}) - f(a^-(x'_i); \hat{\theta})||_1 + \phi(|\theta|, n, \delta) \quad (13)
\]

Proof. We can continue with

\[
\sup_{P' \in T(P,A)} \hat{r}_{P'}(x; \hat{\theta}) \leq \hat{r}_P(x; \hat{\theta}) + W_1(f(x, \hat{\theta}), f(x', \hat{\theta}))
\]

from the proof of Lemma 3.3. With the help of Assumption A3, we have:

\[
d_z(f(a^+(x), \hat{\theta}), f(a^-(x), \hat{\theta})) \geq d_z(f(x, \hat{\theta}), f(x', \hat{\theta}))
\]

When \( d_z(\cdot, \cdot) \) is chosen as Wasserstein-1 metric, we have:

\[
\sup_{P' \in T(P,A)} \hat{r}_{P'}(x; \hat{\theta}) \leq \hat{r}_P(x; \hat{\theta}) + W_1(f(a^+(x), \hat{\theta}), f(a^-(x), \hat{\theta}))
\]

Further, as the LHS is the worst case risk generated by the transformation functions within \( \mathcal{A} \), and \( \hat{r}_P(x; \hat{\theta}) \) is independent of the term \( W_1(f(a^+(x), \hat{\theta}), f(a^-(x), \hat{\theta})) \), WLOG, we can replace \( \hat{r}_P(x; \hat{\theta}) \) with the risk of an arbitrary distribution generated by the transformation function in \( \mathcal{A} \). If we choose to use \( \hat{r}_{P_{a'}}(\hat{\theta}) = \frac{1}{2}(\hat{r}_{P_{a'}}(\hat{\theta}) + \hat{r}_{P_{a'}}(\hat{\theta})) \), we can conclude the proof, with help from Proposition 3.2 and Assumption A5 as how we did in the proof of Lemma 3.3. \( \square \)
C Synthetic Results to Validate Assumptions

We test the assumptions introduced in this paper over MNIST data and rotations as the variation of the data.

**Assumption A2:** We first inspect Assumption A2, which essentially states the distance \(d_e(\cdot, \cdot)\) is the smaller between a sample and its augmented copy (60° rotation) than the sample and the augmented copy from any other samples. We take 1000 training examples and calculate the \(\ell_1\) pair-wise distances between the samples and its augmented copies, then we calculated the frequencies when the A2 hold for one example. We repeat this for three different models, the vanilla model, the model trained with augmented data, and the model trained with regularized adversarial training. The results are shown in the Table 5 and suggest that, although the A2 does not hold in general, it holds for regularized adversarial training case, where A2 is used. Further, we test the assumption in a more challenging case, where half of the training samples are 15° rotations of the other half, thus we may expect the A2 violated for every sample. Finally, as A2 is essentially introduced to replace the empirical Wasserstein distance with \(\ell_1\) distances of the samples and the augmented copies, we directly compare these metrics. However, as the empirical Wasserstein distance is forbiddingly hard to calculate (as it involves permutation statistics), we use a greedy heuristic to calculate by iteratively picking the nearest neighbor of a sample and then remove the neighbor from the pool for the next sample. Our inspection suggests that, even in the challenging scenario, the paired distance is a reasonably good representative of Wasserstein distance for regularized adversarial training method.

**Assumption A3:** Whether Assumption A3 hold will depend on the application and the domain knowledge of vertices, thus here we only discuss the general performances if we assume A3 hold. Conveniently, this can be shown by comparing the performances of RA and the rest methods in the experiments reported in Section 4.1: out of six total scenarios (\{texture, rotation, contrast\} × \{MNIST, CIFAR10\}), there are four scenarios where RA outperforms VWA, this suggests that the domain-knowledge of vertices can actually help in most cases, although not guaranteed in every case.

**Assumption A6:** We inspect Assumption A6 by directly calculating the frequencies out of all the samples when it holds. Given a vanilla model (Base), we notice that over 74% samples fit this assumption.
Table 6: Results of CIFAR10 data. (“C” stands for clean accuracy, “R” stands for robustness, and “I” stands for invariance score): invariance score shows big differences while accuracy does not.

### D Additional Details of Synthetic Experiments Setup

**Results Discussion** Table 6 tells roughly the same story with Table 1. The invariance score of the worst case methods in Table 6 behave lower than we expected, we conjecture this is mainly because some elements in $A$ of “contrast” will transform the data into samples inherently hard to predict (e.g. $a(x) = x/4$ will squeeze the pixel values together, so the images look blurry in general and hard to recognize), the model repeatedly identifies these case as the worst case and ignores the others. As a result, RWA effectively degrades to RA yet is inferior to RA because it does not have the explicit vertex information. To verify the conjecture, we count how often each augmented sample to be considered as the worst case: for “texture” and “rotation”, each augmented sample generated by $A$ are picked up with an almost equal frequency, while for “contrast”, $x/2$ and $(1-x)/2$ are identified only 10%-15% of the time $x/4$ and $(1-x)/4$ are identified as the worst case.
Table 7: More methods tested with more comprehensive metrics over MNIST on texture

|      | Worst | Clean | Vertex | All   | Beyond | Invariance |
|------|-------|-------|--------|-------|--------|------------|
| Base | 0.9860| 0.9921| 0.9911 | 0.9463| 0.9236 |
| VA   | 0.9906| **0.9928** | **0.9925** | **0.9927** | 0.9650 | 0.9876     |
| RA   | 0.9904| 0.9909 | 0.9910 | 0.9909 | 0.9747 | 1          |
| VWA  | 0.9903| 0.9922 | 0.9923 | 0.9696 | 0.9940 |
| RWA  | **0.9911** | 0.9915 | 0.9915 | **0.9773** | 1     |
| RA-\(\ell_1\) | 0.9897| 0.9904 | 0.9901 | 0.9903 | 0.9728 | 1          |
| RA-W | 0.9858| 0.9888 | 0.9902 | 0.9893 | 0.9433 | 0.6428     |
| RA-D | 0.9892| 0.9921 | 0.9912 | 0.9919 | 0.9373 | 0.2588     |
| RA-KL | 0.9980| 0.9980 | 0.9980 | 0.9980 | 0.9980 | 0.9980     |
| RAsmax | 0.9898| 0.9917 | 0.9919 | 0.9920 | 0.9633 | 0.9928     |
| RAsmax-\(\ell_1\) | 0.9904| 0.9925 | 0.9918 | 0.9925 | 0.9672 | 0.9960     |

Table 8: More methods tested with more comprehensive metrics over MNIST on rotation.

|      | Worst | Clean | Vertex | All   | Beyond | Invariance |
|------|-------|-------|--------|-------|--------|------------|
| Base | 0.2960| 0.9921| 0.7410 | 0.8914| 0.2056 |
| VA   | 0.9336| 0.9884 | 0.9886 | 0.9775 | 0.8711 | 0.5628     |
| RA   | 0.9525| 0.9930 | 0.9919 | 0.9829 | 0.9201 | 0.6044     |
| VWA  | 0.9408| 0.9466 | 0.9827 | 0.5979 | 0.6284 |
| RWA  | **0.9882** | 0.9934 | **0.9934** | **0.9417** | **0.8856** |
| RA-\(\ell_1\) | 0.9532| 0.9913 | 0.9916 | 0.9824 | 0.9145 | 0.5912     |
| RA-W | 0.9274| 0.9882 | 0.9875 | 0.9757 | 0.8514 | 0.4600     |
| RA-D | 0.9368| 0.9895 | 0.989  | 0.9782 | 0.8431 | 0.4132     |
| RA-KL | 0.9424| 0.9875 | 0.9872 | 0.9762 | 0.9194 | 0.6800     |
| RAsmax | 0.9389| 0.9900 | 0.9901 | 0.9792 | 0.8631 | 0.6060     |
| RAsmax-\(\ell_1\) | 0.9424| 0.9913 | 0.9901 | 0.9804 | 0.8663 | 0.5864     |

E More Synthetic Results

E.1 Experiment Setup

To understand these methods, we introduce a more comprehensive test of these methods, including the five methods discussed in the main paper, and multiple ablation test methods, including

- RA-\(\ell_1\): when squared \(\ell_2\) norm of RA is replaced by \(\ell_1\) norm.
- RA-W: when the norm distance of RA is replaced by Wasserstein distance, enabled by the implementation of Wasserstein GAN Arjovsky et al. (2017); Gulrajani et al. (2017).
- RA-D: when the norm distance of RA is replaced by a discriminator. Our implementation uses a one-layer neural network.
- RA-KL: when the norm distance of RA is replaced by KL divergence.
- RAsoftmax: when the regularization of RA is applied to softmax instead of logits.
- RAsoftmax-\(\ell_1\): when the regularization of RA is applied to softmax instead of logits, and the squared \(\ell_2\) norm is replaced by \(\ell_1\) norm. This is the method suggested by pure theoretical discussion if we do not concern with the difficulties of passing gradient through backpropagation.

And we test these methods in the three scenarios mentioned in the previous section: texture, rotation, and contrast. The overall test follows the same regime as the one reported in the main manuscript, with additional tests:

- Vertex: average test performance on the perturbed samples with the vertex function from \(A\). Models with worst case augmentation are not tested with vertex as these models do not have the specific concept of vertex.
- All: average test performance on all the samples perturbed by all the elements in \(A\).
Table 9: More methods tested with more comprehensive metrics over MNIST on contrast.

| Method          | Worst | Clean | Vertex | All   | Beyond | Invariance |
|-----------------|-------|-------|--------|-------|--------|------------|
| Base            | 0.2699| 0.9921| 0.6377 | 0.2988| 0.2003 |
| VA              | 0.9837| 0.9922| 0.9917 | 0.6044| 0.4153 |
| RA              | 0.9823| 0.9936| 0.9930 | 0.6512| 0.4166 |
| VWA             | 0.4470| 0.5360| 0.7515 | 0.4649| 0.2210 |
| RWA             | 0.9893| 0.9940| 0.9930 | 0.4841| 0.8786 |
| RA-ℓ₁          | 0.9776| 0.9935| 0.9932 | 0.6251| 0.4176 |
| RA-W           | 0.7357| 0.9867| 0.9865 | 0.6044| 0.4153 |
| RA-D           | 0.9833| 0.9913| 0.9921 | 0.9909| 0.6199 |
| RA-KL          | 0.9105| 0.9894| 0.9882 | 0.6512| 0.4166 |
| RA_{softmax}   | 0.9839| 0.9916| 0.9910 | 0.5843| 0.4236 |
| RA_{softmax-ℓ₁}| 0.9844| 0.9920| 0.9918 | 0.5843| 0.4236 |

Table 10: More methods tested with more comprehensive metrics over CIFAR10 on texture

| Method          | Worst | Clean | Vertex | All   | Beyond | Invariance |
|-----------------|-------|-------|--------|-------|--------|------------|
| Base            | 0.3219| 0.7013| 0.5997 | 0.3084| 0.7140 |
| VA              | 0.5949| 0.6601| 0.6394 | 0.6530| 0.5583 |
| RA              | 0.6259| 0.6571| 0.6485 | 0.6553| 0.5826 |
| VWA             | 0.5814| 0.6049| 0.6024 | 0.5213| 0.1160 |
| RWA             | 0.6358| 0.6630| 0.6612 | 0.5892| 1      |
| RA-ℓ₁          | 0.6230| 0.6609| 0.6511 | 0.6578| 0.5775 |
| RA-W           | 0.6140| 0.6860| 0.6578 | 0.6783| 0.5801 |
| RA-D           | 0.5794| 0.7663| 0.6734 | 0.7288| 0.5632 |
| RA-KL          | 0.5866| 0.5873| 0.5868 | 0.5870| 0.5804 |
| RA_{softmax}   | 0.6197| 0.6263| 0.6268 | 0.6266| 0.5831 |
| RA_{softmax-ℓ₁}| 0.6319| 0.653 | 0.6480 | 0.6516| 0.5830 |

• Beyond: To have some sense of how well the methods can perform in the setting that follows the same concept, but not considered in A, and not (intuitively) limited by the vertices of A, we also test the accuracy of the models with some transformations related to the elements in A, but not in A. To be specific:
  - Texture: \( A_{\text{beyond}} = \{a_5(), a_4()\} \).
  - Rotation: \( A_{\text{beyond}} = \{a_330(), a_345()\} \).
  - Contrast: \( A_{\text{beyond}} = \{a(x) = x/2 + 0.5, a(x) = x/4 + 0.75, a(x) = (1 - x)/2 + 0.5, a(x) = (1 - x)/4 + 0.75\} \)

We report the average test accuracy of the samples tested all the elements in \( A_{\text{beyond}} \).

E.2 Results

We report the results in Table 7-12.

Ablation Study First we consider the ablation study to validate our choice as the squared \( \ell_2 \) norm regularization, particularly because our choice considers both the theoretical arguments and practical arguments regarding gradients. In case of worst-case prediction, we can see the other RA variants can barely outperform RA, even not the one that our theoretical arguments directly suggest (RA_{\text{softmax-ℓ₁}} or RA-W). We believe this is mostly due to the challenges of passing the gradient with \( \ell_1 \) norm and softmax, or through a classifier.

We also test the performances of other regularizations that are irrelevant to our theoretical studies, but are popular choices in general (RA-D and RA-KL). These methods in general perform badly, can barely match RA in terms of the worst-case performance. Further, when some cases when RA-D and RA-KL can outperform RA in other accuracy-wise testing, these methods tend to behave terribly in invariance test, which suggests these regularizations are not effective. In the cases when RA-D and RA-KL can match RA in invariance test, these methods can barely compete with RA.
| Method     | Worst | Clean | Vertex | All    | Beyond | Invariance |
|------------|-------|-------|--------|--------|--------|------------|
| Base       | 0.0871| 0.7013| 0.4061 | 0.4634 | 0.5016 |            |
| VA         | 0.4399| 0.7378| 0.7199 | 0.6835 | 0.5096 | 0.6168     |
| RA         | 0.5166| 0.6815| 0.6741 | 0.6452 | 0.4408 | 0.8520     |
| VWA        | 0.6099| 0.7140| 0.7406 | 0.4446 | 0.9172 |            |
| RWA        | 0.6486| 0.7606| 0.7507 | 0.4614 | 0.9244 |            |

Table 11: More methods tested with more comprehensive metrics over CIFAR10 on rotation.

| Method     | Worst | Clean | Vertex | All    | Beyond | Invariance |
|------------|-------|-------|--------|--------|--------|------------|
| RA-$\ell_1$| 0.4685| 0.7505| 0.7290 | 0.6852 | 0.4878 | 0.6248     |
| RA-W       | 0.4228| 0.7468| 0.7287 | 0.6822 | 0.4753 | 0.6072     |
| RA-D       | 0.4298| 0.7752| 0.7456 | 0.6941 | 0.4662 | 0.2664     |
| RA-KL      | 0.5848| 0.4241| 0.4221 | 0.4211 | 0.3946 | 0.9200     |
| RA$_{softmax}$ | 0.5143| 0.7187| 0.7175 | 0.6851 | 0.4694 | 0.8188     |
| RA$_{softmax}$-$\ell_1$ | 0.4779| 0.7341| 0.725  | 0.6911 | 0.4944 | 0.7288     |

Table 12: More methods tested with more comprehensive metrics over CIFAR10 on contrast.

**Broader Test** We also test our methods in the broader test. As we can see, RWA behaves the best in most of the cases. In three out of these six test scenarios, RWA lost to three other different methods in the “beyond” case. However, we believe, in general, this is still a strong evidence to show that RWA is a generally preferable method.

Also, comparing the methods of RA vs. VA, and RWA vs. VWA, we can see that regularization helps mostly in the cases of “beyond” in addition to “invariance” test. This result again suggests the importance of regularizations, as in practice, training phase is not always aware of all the transformation functions during test phase.
Table 13: Comparison to advanced models over ImageNet-C data. Performance reported (mCE) follows the standard in ImageNet-C data: mCE is the smaller the better.

F Additional Discussions for Comparisons with Advanced Methods

Cross-domain ImageNet-Sketch Classification