On the Separability of Classes with the Cross-Entropy Loss Function

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Abstract

In this paper, we focus on the separability of classes with the cross-entropy loss function for classification problems by theoretically analyzing the intra-class distance and inter-class distance (i.e. the distance between any two points belonging to the same class and different classes, respectively) in the feature space, i.e. the space of representations learnt by neural networks. Specifically, we consider an arbitrary network architecture having a fully connected final layer with Softmax activation and trained using the cross-entropy loss. We derive expressions for the value and the distribution of the squared $\ell_2$ norm of the product of a network dependent matrix and a random intra-class and inter-class distance vector (i.e. the vector between any two points belonging to the same class and different classes), respectively, in the learnt feature space (or the transformation of the original data) just before Softmax activation, as a function of the cross-entropy loss value. The main result of our analysis is the derivation of a lower bound for the probability with which the inter-class distance is more than the intra-class distance in this feature space, as a function of the loss value. We do so by leveraging some empirical statistical observations with mild assumptions and sound theoretical analysis. As per intuition, the probability with which the inter-class distance is more than the intra-class distance decreases as the loss value increases, i.e. the classes are better separated when the loss value is low. To the best of our knowledge, this is the first work of theoretical nature trying to explain the separability of classes in the feature space learnt by neural networks trained with the cross-entropy loss function.

1 Introduction

Classification problems are ubiquitous in machine learning. Deep neural networks ([7, 13, 5, 15]) have been immensely successful in solving supervised classification problems. A central part of these networks is the final Softmax layer to obtain the predicted probabilities of belonging to each class. The most commonly used loss function for classification problems is the cross-entropy loss. The cross-entropy loss along with the final Softmax layer try to obtain class-wise linear partitions of the representation/transformation of the original data just before the Softmax layer by maximizing the likelihood of the data with respect to the network parameters.

On the other hand, more conventional techniques such as Fisher Linear Discriminant Analysis (LDA) try to obtain a linear separation of the data by maximizing the separation between the class-means (relative to the sum of the variances of the data in each class). Similarly, in an SVM ([2]) maximum margin (binary) classifier, the goal is to find a linear separation of the data (either in its original space or after using a kernel) by obtaining two parallel hyper-planes that partition the two classes of data such that the distance between them (which is basically the "margin") is as large as possible. Since the cross-entropy loss function is based on the maximum likelihood estimate approach, it does not directly try to maximize the separation between the classes, which LDA and SVM do.

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Two related self-explanatory terms used in the literature are "intra-class compactness" and "inter-class separability". There is no shortage of works ([11, 10, 9, 1, 4, 14, 16]) which point out that the vanilla cross-entropy loss with Softmax does not quite promote high intra-class compactness and inter-class separability and therefore propose modified loss functions/architectures which address this issue. However, there is not much of theoretical justification to properly explain this issue for the cross-entropy loss.

In this work, we provide a probabilistic quantification of the separability of classes attained in the feature space learnt by a network trained with the cross-entropy loss, as a function of the loss value. Our main contributions are as follows. Firstly in Theorem 1, we provide an expression for the value and the complementary cumulative distribution function (ccdf) of the squared $\ell_2$ norm of the product of a network dependent matrix and a random intra-class distance vector (i.e. the vector between any two random data points having the same ground truth class) in the feature space. Secondly in Theorem 2, we provide a lower bound for the value as well as the ccdf of the squared $\ell_2$ norm of the product of a network dependent matrix and a random inter-class distance vector between any two classes (i.e. the vector between any two data points having different ground truth classes) in the feature space. The network dependent matrix is the same for both the aforementioned cases if we consider the intra-class distance in a class say, $c$, and the inter-class distance between the same class $c$ and another class $c' \neq c$. Thereafter in Theorem 3, considering two random points belonging to $c$ and one random point belonging to $c'$, we derive a lower bound on the probability with which the squared $\ell_2$ norm of the product of the previously mentioned network dependent matrix and the inter-class distance vector between the first point belonging to $c$ and the one belonging to $c'$ is more than the squared $\ell_2$ norm of the product of the same matrix and the intra-class distance vector between the two points belonging to $c$, times a certain factor (of our choice) $> 1$. Next, in Theorem 4 (our main result), with some assumptions on the distribution of the entries of the aforementioned matrix, we derive a lower bound on the probability with which the inter-class distance (between the first point in $c$ and the one in $c'$) is more than the intra-class distance (between the two points in $c$) times a certain factor (of our choice) $\geq 1$. Finally, in Theorem 5, we provide an expression for the expected per-class accuracy of the network model in consideration, as a function of the loss value, to relate accuracy with class separability.

To the best of our knowledge, this is the first theoretical attempt at quantifying the separability of classes, attained with the cross-entropy loss function.

2 Problem Description and Preliminaries

Consider a classification problem with $C$ classes, labelled from 0 through to $(C - 1)$. Assume that we have trained a neural network architecture (be it a fully connected network or a convolutional network) having a fully connected final layer with the Softmax activation and using the cross-entropy loss (which is the most common model for classification problems) for the problem in hand. Denote this network by $N_c$. Consider $m$ data points $x_1, x_2, \ldots, x_m$ (which could be 1-D inputs such as vectors or 2-D inputs such as images etc.) whose ground truth classes are $c(x_1), c(x_2), \ldots, c(x_m)$, respectively. Let $y_i^{(j)} = \delta(j - c(x_i))$, where $\delta(z) = 1$ if $z = 0$ and $\delta(z) = 0$ if $z \neq 0$. Finally, let the probability of $x_i$ belonging to class $j$ predicted by our network $N_c$ be denoted by $\hat{y}_i^{(j)}$. Then the cross-entropy loss is given as follows:

$$L = -\frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{C} y_i^{(j)} \log \left( \hat{y}_i^{(j)} \right) \tag{1}$$

Let us denote the transformed points (which are the features or representations learnt by the network) acting as inputs to the final Softmax layer, by $\phi(x)$. These are 1-D vectors of dimension $n$. Thus, $x_1, x_2, \ldots, x_m$ get transformed to $\phi(x_1), \phi(x_2), \ldots, \phi(x_m)$, respectively. Denote the weights and biases of the last layer by $A$ (which is a $C \times n$ matrix) and $b$ (which is a $C \times 1$ vector). Let the $j^{th}$ ($1 \leq j \leq C$) row of $A$ be denoted by $a_j$. Similarly, let the $j^{th}$ ($1 \leq j \leq C$) element of $b$ be denoted by $b_j$. Then we have:

$$\hat{y}_i^{(j)} = \exp \left( a_j^T \phi(x_i) + b_j \right) / \sum_{k=1}^{C} \exp \left( a_k^T \phi(x_i) + b_k \right) \tag{2}$$

Empirically, we observed that $\left( -\log \left( \hat{y}_i^{(c(x_i))} \right) \right)^{1/\beta}$ approximately follows an exponential distribution (say with mean $\mu$) where $\beta$ is a constant depending on the network and dataset properties. For
MNIST and CIFAR-10, $\beta \approx 4$ on the networks that we tried. Refer to Section 4 for more details. So:

$$\mathbb{P} \left( \left( -\log \left( \hat{y}_{c(x_1)} \right) \right)^{1/\beta} < z \right) = 1 - \exp(-z/\mu) \tag{3}$$

The relation between the parameter $\mu$ and the cross-entropy loss value $L$ is given as per Lemma 1.

**Lemma 1.** Assuming that the expected value of $-\log \hat{y}_{c(x)}$ for the model in consideration is approximately equal to the sample average value of this quantity (which is equal to $L$), we have:

$$\mu = \left( L/\Gamma(\beta + 1) \right)^{1/\beta}$$

where $\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}dx$ (the standard Gamma function)

**Proof:** Let us denote the random variable $(-\log \hat{y}_{c(x)}))^{1/\beta}$ by $\hat{Y}$. Then, $\hat{Y} \sim \exp(\mu)$ and $\mathbb{E}[\hat{Y}^\beta] = L$. But:

$$\mathbb{E}[\hat{Y}^\beta] = \int_0^\infty t^\beta (1/\mu)e^{-(t/\mu)} dt = \mu^\beta \Gamma(\beta + 1) = L$$

From this, we get the required result.

In the next section, we derive the probability of the squared inter-class distance being more than the squared intra-class distance times a certain factor $\geq 1$, in the $n$-dimensional feature/representation (i.e. the $\phi$) space (due to $\mathcal{N}_c$) as a function of $L$, to illustrate the separability of the classes.

Throughout the rest of this paper, when we say intra/inter-class distance, we mean intra/inter-class distance in the $\phi$ space. Also, $\|z\|$ refers to the $\ell_2$ norm of the vector $z$ and whenever we say norm, we mean the $\ell_2$ norm. Finally, we shall denote the set $\{0, \ldots, (C-1)\}$ by $[C]$.

### 3 Main Results

The proofs of all the theorems in this section can be found in the supplementary material.

We firstly present a theorem related to the intra-class distance.

**Theorem 1.** Consider a general class, say $c \in [C]$, and two randomly chosen points $x_1$ and $x_2$ (without loss of generality) belonging to class $c$. Then their transformed representations in the $n$-dimensional $\phi$ space are $\phi(x_1)$ and $\phi(x_2)$, respectively. Let $\Delta \phi(x)^{(c)} = \phi(x_1) - \phi(x_2)$. Also, let the probabilities of $x_1$ and $x_2$ belonging to their ground truth class $c$, predicted by the network be denoted by $\hat{y}_1$ and $\hat{y}_2$, respectively. Finally, consider the $(C-1) \times n$ matrix $A_c$ whose rows are given by $(a_j - a_c)$ with $j \in [C] - \{c\}$. Then under the assumption that for each class $j \neq c$, $\hat{y}_1^{(c)} / (1 - \hat{y}_1) = \hat{y}_2^{(c)} / (1 - \hat{y}_2)$ (where $\hat{y}_i^{(c)}$ is the probability of $x_i$ belonging to class $j$ predicted by the network for $i = \{1, 2\}$), we have:

$$\|A_c \Delta \phi(x)^{(c)}\|^2 = (C - 1) \log^2 \left( \frac{1/\hat{y}_1 - 1}{1/\hat{y}_2 - 1} \right)$$

Also, the complementary cumulative distribution function (ccdf) of $\|A_c \Delta \phi(x)^{(c)}\|^2$ turns out to be:

$$\mathbb{P}(\|A_c \Delta \phi(x)^{(c)}\|^2 > \nu (C - 1)) = 1 - \int_0^\infty \left( e^{-h_1(\alpha, -\sqrt{\nu})} - e^{-h_1(\alpha, \sqrt{\nu})} \right) e^{-\alpha \mu} d\alpha$$

for $\nu \geq 0$,

where $h_1(w, z) = \log \left( \frac{1 + e^{(w \mu)^{\beta}}}{\mu} \right)$ (and $\mu$ is obtained from Lemma 1).

Observe that $\Delta \phi(x)^{(c)}$ is a randomly chosen intra-class distance vector for class $c$. So Theorem 1 provides the value as well as the ccdf of the squared norm of the product of the matrix $A_c$ (which is of course network dependent) and a random intra-class distance vector. The assumption mentioned in Theorem 1 can be interpreted as follows - given that $x_1$ and $x_2$ belong to the same class $c$, for each class $j \neq c$, the conditional probability of $x_1$ belonging to class $j$ given that it does not belong to class $c$, predicted by the network, is the same as that for $x_2$. We acknowledge that this might not be valid for all points (such as adversarial examples) but we assume that it holds approximately for a large number of points belonging to the same class. Further, this assumption enables us to do some kind of analysis and without it, the problem becomes completely intractable. Unfortunately, even with this assumption, we could not simplify the ccdf integral further and had to resort to numerical methods to evaluate it.

Next, we present a theorem analogous to Theorem 1 for the inter-class distance.
Theorem 2. Consider two distinct classes, say $c$ and $c' \in [C]$. Also, consider two randomly chosen points $x$ and $x'$ (without loss of generality) belonging to classes $c$ and $c'$, respectively. Their transformed representations in the $n$-dimensional $\phi$ space are $\phi(x)$ and $\phi(x')$, respectively. Let $\Delta \phi(x)^{(c,c')} = \phi(x) - \phi(x')$. Also, let the probabilities of $x$ and $x'$ belonging to their respective ground truth classes $c$ and $c'$, predicted by the network be denoted by $\hat{y}$ and $\hat{y}'$, respectively. Finally, consider the $(C - 1) \times n$ matrix $A_c$ whose rows are given by $(a_j - a_c)$ with $j \in [C] - \{c\}$. Then under the assumption of Theorem 1, for some constant $\kappa_{c,c'} \geq 1$, we have:

$$\|A_c \Delta \phi(x)^{(c,c')}\|^2 \geq (C - 1) \log^2 \left( \frac{((\kappa_{c,c'} - 1)/\hat{y}') + 1}{((1/\hat{y}') - 1))/((1/\hat{y}') - 1)} \right)$$

Also, the ccdf of $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ turns out to be:

$$\mathbb{P} \left( \|A_c \Delta \phi(x)^{(c,c')}\|^2 > \nu(C - 1) \right) \geq 1 - \int_0^\infty (e^{-h_2(\alpha, -\nu \tau)} - e^{-h_2(\alpha, \sqrt{\nu})}) e^{-\alpha} \mu(a) \, da$$

where $h_2(u, z) = \left\{ \log \left( 1 + e^{c \left( \frac{\kappa_{c,c'} - 1}{e(\mu u)^{2/3} - 1} \right) } \right) \right\}^{1/\beta}$ (and $\mu$ is obtained from Lemma 1).

Observe that $\Delta \phi(x)^{(c,c')}$ is a randomly chosen inter-class distance vector between classes $c$ and $c'$. So Theorem 2 provides a lower bound for the value as well as the ccdf of the squared norm of the product of $A_c$ (network dependent and same as in Theorem 1 if $c$ is the same as in Theorem 1) and a random inter-class distance vector. $\kappa_{c,c'}$ turns out to be the inverse of the conditional probability of $x'$ belonging to class $c$ given that it does not belong to class $c'$ (ground truth class of $x'$), predicted by the network. Recall from the assumption of Theorem 1 (and the discussion below it) that $\kappa_{c,c'}$ is assumed to be a constant for all points within $c'$. We further provide a corollary for the special case when all the classes other than the ground truth class are equally similar/dissimilar to each other.

Corollary 1. In Theorem 2, if all classes other than the ground truth class are equally similar/dissimilar to each other, then $\kappa_{c,c'} = (C - 1) \forall c \neq c'$.

Here also, we could not simplify the ccdf integral further and had to resort to numerical methods.

We now show the ccdfs of $\|A_c \Delta \phi(x)^{(c)}\|^2$ and $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ for visual comparison (since it is very difficult to compare them analytically) in Figure 1. Observe that the ccdf of $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ is significantly above that of $\|A_c \Delta \phi(x)^{(c)}\|^2$ which indicates that $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ is more likely to be larger than $\|A_c \Delta \phi(x)^{(c)}\|^2$. Also notice the variation of the ccdfs with respect to $L$. When $L$ increases, the ccdf of $\|A_c \Delta \phi(x)^{(c)}\|^2$ increases while that of $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ decreases. This makes sense intuitively since for higher loss values, we expect the separation of the classes to be worse than that at a lower loss value.

Figure 1: Plots of the ccdf of $\|A_c \Delta \phi(x)^{(c)}\|^2$ and $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ for $L = 0.1, 0.4, 0.7$ and $1.0$ with $\beta = 4, C = 10$ and $\kappa_{c,c'} = C - 1 = 9$.

Theorem 1 and Theorem 2 provide individual results related to the intra-class and inter-class distance vectors. Using these two theorems, we next present a theorem to (probabilistically) compare the values of $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ and $\|A_c \Delta \phi(x)^{(c)}\|^2$.
Theorem 3. Consider a randomly chosen point \( x_1 \) belonging to class \( c \in [C] \). Now consider two points, \( x_2 \) also belonging to class \( c \) and \( x_3 \) belonging to class \( c' \neq c \). Their transformed representations in the \( n \)-dimensional \( \phi \) space are \( \phi(x_1) \), \( \phi(x_2) \) and \( \phi(x_3) \), respectively. Let \( \Delta \phi(x)^{(c)} = \phi(x_1) - \phi(x_2) \) and \( \Delta \phi(x)^{(c,c')} = \phi(x_1) - \phi(x_3) \). Also recall \( A_c \) as defined in Theorem 1 and Theorem 2, the assumption in Theorem 1, \( \kappa_{c,c'} \) in Theorem 2 and \( \mu \) from Lemma 1. Then for any \( \gamma > 1 \):

\[
\mathbb{P} \left( \| A_c \Delta \phi(x)^{(c,c')} \|^2 > \gamma \| A_c \Delta \phi(x)^{(c)} \|^2 \right) \geq \int_{a_1=0}^{\infty} \int_{a_2=0}^{\infty} \left| e^{-h_3(a_1,a_2,\sqrt{\gamma})} - e^{-h_2(a_1,a_2,\sqrt{\gamma})} e^{-\alpha_1} e^{-\alpha_2} da_1 da_2 \right| = b_A(\gamma, L)
\]

where \( h_3(p,q,r) = \mu \left\{ \log \left( 1 + \left( e^{(p+q)\beta} - 1 \right) \right) \right\}^{1/\beta} \). So Theorem 3 provides a lower bound, i.e. \( b_A(\gamma, L) \), on the probability with which the squared norm of the product of the matrix \( A_c \) and a random inter-class distance vector (between one point in \( c \) and another one in \( c' \)) is more than the squared norm of the product of \( A_c \) and a random intra-class distance vector (between the aforementioned point in \( c \) and another point in \( c \) itself), times a certain factor \( \gamma > 1 \). Once again, the double integral in Theorem 3 had to be evaluated numerically.

In Figure 2a, we show the variation of \( b_A(\gamma, L) \) vs. \( L \) for fixed values of \( \beta = 4 \), \( C = 10 \) and \( \kappa_{c,c'} = C - 1 \). Observe that \( b_A(\gamma, L) \) decreases as \( L \) increases which is consistent with our intuition that separability of the classes is more pronounced for smaller loss values. Similarly, in Figure 2b, we show the variation of \( b_A(\gamma, L) \) vs. \( C \) for fixed values of \( \beta = 4 \) and \( L = 0.4 \). We used \( \kappa_{c,c'} = C - 1 \) for all the four values of \( C \). In this case, we observe that \( b_A(\gamma, L) \) increases as \( C \) increases, which is expected since we used \( \kappa_{c,c'} = C - 1 \) (which increases as \( C \) increases).

However, we would like to estimate the probability with which the squared norm of the inter-class distance vector is more than the squared norm of the intra-class distance vector times a certain factor \( \gamma > 1 \). To do this, we shall use Theorem 3 and make the following assumption:

Assumption 1. The entries of the matrix \( A_c \) are zero mean i.i.d Gaussian random variables.

This assumption enables us to bound the squared intra-class and inter-class distances in a small envelope around the suitably re-scaled (by the same constant) value of the squared norm of the product of \( A_c \) and the intra-class and inter-class distance vectors respectively. Although not perfectly valid, similar assumptions have been used in other works (13, 12) too. With the above assumption in mind, we state our main theorem:

Theorem 4. Let \( F_C^\chi(u) \) be the cdf of a chi-squared random variable with \( (C - 1) \) degrees of freedom evaluated at \( (C - 1)u \). Then, under Assumption 1, the same settings as in Theorem 3 and with the function \( b_A \) as defined in Theorem 3, we have for any \( \gamma > 1 \):

\[
\mathbb{P} \left( \| \Delta \phi(x)^{(c,c')} \|^2 > \gamma \| \Delta \phi(x)^{(c)} \|^2 \right) \geq \max_{0 < \epsilon_1, \epsilon_2 < 1} \left( \frac{1 + \epsilon_1}{1 - \epsilon_2} \right) \left( F_C^\chi(1 + \epsilon_1) - F_C^\chi(1 - \epsilon_2) \right) = b(\gamma, L)
\]

Therefore, we can relate the probability with which the squared norm of the inter-class distance vector is more than the squared norm of the intra-class distance vector times a certain factor \( \gamma > 1 \) to the probability with which the squared norm of the inter-class distance vector is more than the squared norm of the intra-class distance vector times a certain factor \( \gamma > 1 \), times the maximum of the cdf of a chi-squared random variable with \( (C - 1) \) degrees of freedom evaluated at \( (C - 1)(1 + \epsilon_1) \) and \( (C - 1)(1 - \epsilon_2) \).
The lower bound provided above holds regardless of the validity of the assumption in Theorem 1. We next provide a theorem on the expected per-class accuracy of the network model in consideration, Theorem 5. (refer to Figure 4 and the discussion above it in Section 4). In this paper, we do not investigate the variation of \( \beta \) or how it affects the obtained expressions. Finally, there is dependence on the number of classes (can be seen in Figure 3) and also on the value of \( \kappa \) (simply assumed to be \( C - 1 \)). We discretized \( \epsilon_1, \epsilon_2 \in (0, 1) \) in steps of 0.1 each to report the approximate values of \( b_c(L) \).

We provide code to compute \( b(\gamma, L) \) (and \( b_A(\gamma, L) \)) in the supplementary material.

Figure 3: Approximate values of \( b_c(L) \) vs. \( L \) for \( C = 10, 20, 30, 40, 50, 60 \) with \( \kappa_{c,c'} = C - 1 \) and \( \beta = 4 \). We discretized \( \epsilon_1, \epsilon_2 \in (0, 1) \) in steps of 0.1 each to report the approximate values of \( b_c(L) \).

We next provide a theorem on the expected per-class accuracy of the network model in consideration, as a function of \( L \), to relate model accuracy with the separability of classes.

**Theorem 5.** Let there be \( N_c \) examples belonging to class \( c \in [C] \). Under the assumption of Theorem 1, define \( \kappa^*_c \triangleq \min_{c'\neq c} \kappa_{c',c} \) (\( \kappa_{c',c} \)'s are the same as in Theorem 2). Then the expected number of examples in class \( c \) correctly classified, say \( N^\text{corr}_c \), is:

\[
N^\text{corr}_c = N_c \left( 1 - \exp \left( - \left( \frac{L}{L} \log(1 + \kappa^*_c) \right)^{1/\beta} \right) \right) \geq N_c \left( 1 - \exp \left( - \left( \frac{L}{L} \log(2) \right)^{1/\beta} \right) \right).
\]

The lower bound provided above holds regardless of the validity of the assumption in Theorem 1.

Observe that the expected per-class accuracy \( (N^\text{corr}_c / N_c) \) is a decreasing function of \( L \) (as expected) and an increasing function of \( \kappa^*_c \) (i.e. classes with higher \( \kappa^*_c \) will have better per-class accuracy).

So we conclude that a lower loss value leads to better separation of the classes (from Figure 3 and Theorem 4) as well as better accuracy (from Theorem 5).

**Dependence of the obtained results on the dataset and network architecture:** All the theorems stated before depend on the properties of the dataset as well as the network. Firstly, all the results are a function of the cross-entropy loss value which depends on the choice of the network (a very simple architecture may not be able to fit the data very well leading to a higher loss value than that obtained using a more complicated architecture) as well as on the dataset (the same network may perform well on one dataset but not too well on another dataset). Secondly, the value of \( \beta \) also plays a critical role in all the obtained expressions and it might depend on the dataset as well as the network architecture (refer to Figure 4 and the discussion above it in Section 4). In this paper, we do not investigate the variation of \( \beta \) or how it affects the obtained expressions. Finally, there is dependence on the number of classes (can be seen in Figure 3) and also on the value of \( \kappa_{c,c'} \) (simply assumed to be \( C - 1 \) in our plots) even though both of them could be thought of as being properties of the dataset itself.
4 Experiments

Due to length constraints on the manuscript, we are able to describe the results of our experiments on only two datasets (CIFAR-10 and MNIST) here. We also performed experiments on two synthetically generated datasets (named SYN-1 and SYN-2) which can be found in the supplementary material.

Firstly, we mention some relevant details for the CIFAR-10 and MNIST experiments.

**CIFAR-10**: We fitted a deep convolutional neural network (the entire architecture can be found in the supplementary material) having a fully connected final layer with Softmax activation and \( n = 512 \). We trained the model for 50 epochs and the corresponding loss value over the test set was \( L = 0.4516 \). For this case, we observed that with \( \beta = 4 \), the distribution of \( \left( -\log (\hat{y}_i^{(c(x_i))}) \right)^{1/\beta} \) closely resembles an exponential distribution.

**MNIST**: In this case, we fitted a shallow convolutional neural network (the entire architecture and some more details are in the supplementary material) having a fully connected final layer with Softmax activation and \( n = 128 \). The test set loss value after training the model for 12 epochs was \( L = 0.0298 \). Just as in the previous case, we observed that even here, \( \beta = 4 \) results in a closely resembling exponential distribution.

Figure 4a and Figure 4b contain the plots of the distribution of \( \left( -\log (\hat{y}_i^{(c(x_i))}) \right)^{1/\beta} \) along with the closest fit exponential distribution for CIFAR-10 and MNIST with \( \beta = 4 \), over the test set (size of which was 10000 for both datasets). The value of \( \beta \) probably depends on the dataset, the network architecture and perhaps even the number of classes. For instance, in the case of SYN-1 and SYN-2 which are similar datasets with 20 classes each and had shallow fully connected neural networks fitted onto them (more details about these datasets can be found in the supplementary material as mentioned earlier), the optimal values of \( \beta \) turned out to be 2 and 1.4, respectively. In Figure 4c and Figure 4d, we show the distribution of \( \left( -\log (\hat{y}_i^{(c(x_i))}) \right)^{1/\beta} \) along with the closest fit exponential distribution for SYN-1 with \( \beta = 2 \) and SYN-2 with \( \beta = 1.4 \), respectively, over the test set (size of which was 4000 and 6000 for SYN-1 and SYN-2, respectively).

| Class 1 \((c_1)\) | Class 2 \((c_2)\) | \(p_1\) | \(p_2\) |
|---|---|---|---|
| 0 | 1 | 0.9902 | 0.9998 |
| 1 | 2 | 0.9990 | 0.9145 |
| 2 | 9 | 0.9660 | 0.9687 |
| 4 | 0 | 0.9816 | 0.9944 |
| 7 | 1 | 0.9529 | 0.9973 |
| 2 | 3 | 0.9836 | 0.9844 |
| 3 | 8 | 0.9890 | 0.9876 |
| 5 | 6 | 0.9735 | 0.9896 |
| 6 | 8 | 0.9835 | 0.9725 |
| 9 | 8 | 0.9875 | 0.9391 |

(a) MNIST

| Class 1 \((c_1)\) | Class 2 \((c_2)\) | \(p_1\) | \(p_2\) |
|---|---|---|---|
| 0 | 2 | 0.8755 | 0.8176 |
| 1 | 9 | 0.7376 | 0.8430 |
| 3 | 4 | 0.7569 | 0.7408 |
| 4 | 7 | 0.8289 | 0.7595 |
| 2 | 6 | 0.7668 | 0.8577 |
| 5 | 6 | 0.8253 | 0.8433 |
| 1 | 4 | 0.8933 | 0.9535 |
| 6 | 3 | 0.7600 | 0.7752 |
| 7 | 3 | 0.6735 | 0.7855 |
| 8 | 1 | 0.5461 | 0.9406 |

(b) CIFAR-10

Table 1: Sample probabilities of inter-class distance being more than the intra-class distance for (a) MNIST with \( L = 0.0298 \) and (b) CIFAR-10 with \( L = 0.4516 \). \( p_1 \) and \( p_2 \) are as defined in the text.

Finally, Table 1a and Table 1b show the probability of the inter-class distance being more than the intra-class distance for MNIST and CIFAR-10 respectively, over the test set. For every dataset, we chose 10 pairs of classes and for each pair of classes (denote the two classes in a pair by \( c_1 \) and \( c_2 \)), we considered the transformed representations of 200 random points in each class (denote these by \( \phi(x_1^{(1)}), \phi(x_1^{(2)}), \ldots, \phi(x_1^{(200)}) \) and \( \phi(x_2^{(1)}), \phi(x_2^{(2)}), \ldots, \phi(x_2^{(200)}) \) for \( c_1 \) and \( c_2 \), respectively). Next, for each \( c_i \) such that \( i = \{1, 2\} \) and for each \( j \) such that \( 1 \leq j \leq 100 \), we considered 100 intra-class distance vectors (denote these by \( d_i^{(j,k)} = \phi(x_i^{(j)}) - \phi(x_i^{(j+100)}) \) for \( 1 \leq k \leq 100 \)) and 100 inter-class distance vectors (denote these by \( d_{1,2}^{(j,k)} = \phi(x_1^{(j)}) - \phi(x_2^{(k)}) \) for \( 1 \leq k \leq 100 \)) and 100 inter-class distance vectors (denote these by \( d_{1,2}^{(j,k)} = \phi(x_1^{(j)}) - \phi(x_2^{(k)}) \) for
1 ≤ k′ ≤ 100). Then, p₁ and p₂ (see Table 1a and Table 1b) are mathematically defined as follows:

\[ p_i = \frac{1}{100} \sum_{j=1}^{100} \sum_{k=1}^{100} \sum_{k'=1}^{100} 1 \left( \| d_{1,2}^{(j,k')} \| > \| d_{1,2}^{(j,k)} \| \right) / 100^3 \]

for \( i = \{1, 2\} \)

where 1() is the indicator function and evaluates to 1 if its argument is true else it evaluates to 0.

In other words, p₁ and p₂ are the sample probabilities of the inter-class distance between \( c_1 \) and \( c_2 \) being more than the intra-class distance of \( c_1 \) and \( c_2 \), respectively.

In Table 1a, observe that p₁ and p₂ values are very close to 1 and the corresponding value of \( L \) is 0.0298. The value of \( b_c(0.0298) \) with \( C = 10, \kappa_{c,c'} = C - 1 \) and \( \beta = 4 \) turns out to be 0.7251 approximately. In Table 1b, where \( L = 0.4516 \), the values of p₁ and p₂ are much lower than 1 and mostly in the range of 0.7 – 0.85. The value of \( b_c(0.4516) \) with \( C = 10, \kappa_{c,c'} = C - 1 \) and \( \beta = 4 \) is 0.5750 approximately. Thus, the obtained lower bounds are consistent with the observed values.

Further experiments on SYN-1 and SYN-2 are described in the supplementary material.

5 Conclusions

In this paper, we have attempted to mathematically quantify the separability of classes with the cross-entropy loss function by deriving a lower bound on the probability with which the inter-class distance is more than the intra-class distance (in the feature space learnt by a neural network) as a function of the loss value. The constant \( \beta \) plays an important role in our results. A future line of work could be to analyze the variation of \( \beta \) and its impact on the probability values. One could also possibly look to relax Assumption 1 and extend the work to the case of the entries of \( \mathbf{A}_c \) having a sub-Gaussian distribution by using concentration inequalities for sub-Gaussian random variables, similar to those that have been used to obtain Theorem 4. Finally, we hope that our techniques can be extended or suitably modified to do the same task for other loss functions too.
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6 Supplementary Material

6.1 Proof of Theorem 1

Firstly, we prove Theorem 1. Before proving it, we restate it for the reader’s convenience.

Theorem 1. Consider a general class, say \( c \in [C] \), and two randomly chosen points \( x_1 \) and \( x_2 \) (without loss of generality) belonging to class \( c \). Then their transformed representations in the \( n \)-dimensional \( \phi \) space are \( \phi(x_1) \) and \( \phi(x_2) \), respectively. Let \( \Delta \phi(x) \) denote \( \phi(x) - \phi(x_2) \). Also, let the probabilities of \( x_1 \) and \( x_2 \) belonging to their ground truth class \( c \), predicted by the network be denoted by \( \hat{y}_1 \) and \( \hat{y}_2 \), respectively. Finally, consider the \( (C-1) \times n \) matrix \( A_c \) whose rows are given by \( (a_j - a_c) \) with \( j \in [C] - \{c\} \). Then under the assumption that for each class \( j \neq c \), \( \hat{y}_1^{(j)}/(1 - \hat{y}_1) = \hat{y}_2^{(j)}/(1 - \hat{y}_2) \) (where \( \hat{y}_1^{(j)} \) is the probability of \( x_i \) belonging to class \( j \) predicted by the network for \( i = \{1, 2\} \)), we have:

\[
\|A_c \Delta \phi(x)^{(c)}\|^2 = (C-1) \log^2 \left( \frac{1/\hat{y}_1 - 1}{1/\hat{y}_2 - 1} \right)
\]

Also, the complementary cumulative distribution function (ccdf) of \( \|A_c \Delta \phi(x)^{(c)}\|^2 \) turns out to be:

\[
P(\|A_c \Delta \phi(x)^{(c)}\|^2 > \nu (C-1)) = 1 - \int_0^\infty \left( e^{-h_1(\alpha, -\sqrt{\nu})} - e^{-h_1(\alpha, \sqrt{\nu})} e^{-\alpha} \right) \text{d}\alpha \text{ for } \nu \geq 0,
\]

where \( h_1(w, z) = \frac{\log(1 + e^{(w \mu)^2 - 1})}{\mu} \) (and \( \mu \) is obtained from Lemma 1).

Proof: We have:

\[
1/\hat{y}_i^{(c)} = 1 + \sum_{k \neq c} \exp(\{(a_k - a_c)^T \phi(x_i) + (b_c - b_k)\}) \text{ for } i = \{1, 2\}.
\]

Now, \( 1/\hat{y}_1^{(c)} = 1/\hat{y}_1 \) (as mentioned in the theorem) \( \Rightarrow \) \( \exp(\{(a_j - a_c)^T \phi(x_1) + (b_j - b_c)\}) = \eta_j^{(1)}(1/\hat{y}_1 - 1) \) for some \( \eta_j^{(1)} \) such that \( 0 \leq \eta_j^{(1)} \leq 1 \) and \( \sum_{k \neq c} \eta_k^{(1)} = 1 \). Thus:

\[
(a_j - a_c)^T \phi(x_1) + (b_j - b_c) = \log(\eta_j^{(1)}(1/\hat{y}_1 - 1)). \tag{4}
\]

Similarly, for some \( \eta_j^{(2)} \)’s such that \( 0 \leq \eta_j^{(2)} \leq 1 \) and \( \sum_{k \neq c} \eta_k^{(2)} = 1 \), we have:

\[
(a_j - a_c)^T \phi(x_2) + (b_j - b_c) = \log(\eta_j^{(2)}(1/\hat{y}_2 - 1)). \tag{5}
\]

Subtracting (5) from (4) gives us:

\[
(a_j - a_c)^T \phi(x_1) - \phi(x_2)) = \log\left(\frac{\eta_j^{(1)}(1/\hat{y}_1 - 1)}{\eta_j^{(2)}(1/\hat{y}_2 - 1)}\right). \tag{6}
\]

Therefore, we have:

\[
\|A_c \Delta \phi(x)^{(c)}\|^2 = \sum_{k \neq c} ((a_k - a_c)^T (\phi(x_1) - \phi(x_2)))^2 = \sum_{k \neq c} \log^2 \left(\frac{\eta_k^{(1)}(1/\hat{y}_1 - 1)}{\eta_k^{(2)}(1/\hat{y}_2 - 1)}\right). \tag{7}
\]

Now, since \( x_1 \) and \( x_2 \) belong to the same class \( c \), we assume that \( \eta_j^{(1)} = \eta_j^{(2)} \) for all \( j \neq c \).

From (4), we have:

\[
\eta_j^{(1)} = \frac{\exp(a_j^T \phi(x_1) + b_j)}{\exp(a_c^T \phi(x_1) + b_c)(1/\hat{y}_1 - 1)} = \frac{\hat{y}_1^{(j)}}{\hat{y}_1(1/\hat{y}_1 - 1)} = \frac{\hat{y}_1^{(j)}}{1 - \hat{y}_1}
\]

From the above equation, it can be also seen that \( \eta_j^{(1)} \) is the conditional probability of \( x_1 \) belonging to class \( j \) given that it does not belong to class \( c \), predicted by the network.
Similarly, from (5), we have:

\[ \eta_j^{(2)} = \frac{\hat{y}_2 \cdot j}{1 - \hat{y}_2} \]

Thus, \( \eta_j^{(1)} = \eta_j^{(2)} \) for all \( j \neq c \Rightarrow \frac{\hat{y}_1}{1 - \hat{y}_1} = \frac{\hat{y}_2}{1 - \hat{y}_2} \) for all \( j \neq c \). It also implies that the conditional probability of \( x_1 \) belonging to class \( j \) given that it does not belong to class \( c \), predicted by the network, is the same as that for \( x_2 \), for all \( j \neq c \). We acknowledge that this assumption might not be valid for all points (such as adversarial examples) but we assume that it holds approximately for a large number of points belonging to the same class. Further, without this assumption, our ensuing analysis becomes intractable.

Therefore, under the aforementioned assumption, we get:

\[ \| A_c \Delta \phi(x)^{(c)} \|^2 = (C - 1) \log^2 \left( \frac{1/\hat{y}_1 - 1}{1/\hat{y}_2 - 1} \right) \]  \hspace{1cm} (8)

This proves the first part of Theorem 1.

Next using (8), we have: \( \mathbb{P}(\| A_c \Delta \phi(x)^{(c)} \|^2 < \nu(C - 1)) = \)

\[ \int_1^\infty \mathbb{P} \left( 1 + e^{-\sqrt{\alpha}} \left( \frac{1}{\hat{y}_2} - 1 \right) < \frac{1}{\hat{y}_1} < 1 + e^{\sqrt{\alpha}} \left( \frac{1}{\hat{y}_2} - 1 \right) \right) f \left( \frac{1}{\hat{y}_2} \right) \]  \hspace{1cm} (9)

where \( f(.) \) is the pdf of \( \frac{1}{\hat{y}_2} \).

Now recall that \( \left( \log \left( \frac{1}{\hat{y}^{(c, z)}} \right) \right)^{1/\beta} \) approximately follows an exponential distribution with mean \( \mu \) whose value (as a function of \( L \)) is obtained from Lemma 1 in the main paper. Keeping this in mind, let us introduce a useful reparameterization as follows:

\[ \left( \log \left( \frac{1}{\hat{y}^{(c, z)}} \right) \right)^{1/\beta} = \alpha \mu \text{ where } \alpha \sim \exp(1) \Rightarrow \frac{1}{\hat{y}^{(c, z)}} = e^{(\alpha \mu)^\beta} \text{ where } \alpha \sim \exp(1) \]

Then with the above reparameterization, let \( 1/\hat{y}_1 = e^{(\alpha_1 \mu)^\beta} \) and \( 1/\hat{y}_2 = e^{(\alpha_2 \mu)^\beta} \) where \( \alpha_1, \alpha_2 \) are i.i.d \( \exp(1) \). So we have:

\[ \mathbb{P} \left( 1 + e^{-\sqrt{\alpha}} \left( \frac{1}{\hat{y}_2} - 1 \right) < \frac{1}{\hat{y}_1} < 1 + e^{\sqrt{\alpha}} \left( \frac{1}{\hat{y}_2} - 1 \right) \right) = \mathbb{P}(h_1(\alpha_2, -\sqrt{\mu}) < \alpha_1 < h_1(\alpha_2, \sqrt{\mu})) \]

\[ = (e^{-h_1(\alpha_2, -\sqrt{\mu})} - e^{-h_1(\alpha_2, \sqrt{\mu})}) \text{ where } h_1(w, z) = \left\{ \log \left( 1 + e^{z(e(w\mu)^\beta - 1}) \right) \right\}^{1/\beta} \]

We also have:

\[ f \left( \frac{1}{\hat{y}_2} \right) \]  \hspace{1cm} (11)

Now using (10) and (11) in (9), we finally get:

\[ \mathbb{P}(\| A_c \Delta \phi(x)^{(c)} \|^2 < \nu(C - 1)) = \int_0^\infty (e^{-h_1(\alpha_2, -\sqrt{\mu})} - e^{-h_1(\alpha_2, \sqrt{\mu})}) e^{-\alpha_2} d\alpha_2 \]  \hspace{1cm} (12)

Lastly, replacing \( \alpha_2 \) by \( \alpha \) in (12), we obtain the second part of Theorem 1:

\[ \mathbb{P}(\| A_c \Delta \phi(x)^{(c)} \|^2 > \nu(C - 1)) = 1 - \int_0^\infty (e^{-h_1(\alpha, -\sqrt{\mu})} - e^{-h_1(\alpha, \sqrt{\mu})}) e^{-\alpha} d\alpha \]

with \( h_1(.) \) as defined in (10). \hspace{1cm} (13)

This finishes the proof of Theorem 1. Unfortunately, we could not simplify the integral in (13) further.

### 6.2 Proof of Theorem 2

Next, we restate Theorem 2 and then prove it.
Theorem 2. Consider two distinct classes, say $c$ and $c' \in [C]$. Also, consider two randomly chosen points $x$ and $x'$ (without loss of generality) belonging to classes $c$ and $c'$, respectively. Their transformed representations in the $n$-dimensional $\phi$ space are $\phi(x)$ and $\phi(x')$, respectively. Let $\Delta \phi(x)^{(c,c')}$ be the difference $\phi(x) - \phi(x')$. Also, let the probabilities of $x$ and $x'$ belonging to their respective ground truth classes, $c$ and $c'$, predicted by the network be denoted by $\hat{y}$ and $\hat{y}'$, respectively. Finally, consider the $(C-1) \times n$ matrix $A_c$, whose rows are given by $(a_j - a_{c'})$ with $j \in [C] - \{c\}$. Then under the assumption of Theorem 1, for some constant $\kappa_{c,c'} \geq 1$, we have:

$$
\|A_c \Delta \phi(x)^{(c,c')}\|^2 \geq (C-1) \log^2 \left( \frac{((\kappa_{c,c'} - 1)/\hat{y}') + 1}{((1/\hat{y}') - 1)((1/\hat{y}) - 1)} \right)
$$

Also, the ccdf of $\|A_c \Delta \phi(x)^{(c,c')}\|^2$ turns out to be:

$$
\mathbb{P} \left( \|A_c \Delta \phi(x)^{(c,c')}\|^2 > \nu(C-1) \right) \geq 1 - \int_0^\infty (e^{-h_2(\alpha, -\sqrt{\nu})} - e^{-h_2(\alpha, \sqrt{\nu})}) e^{-\alpha} d\alpha \text{ for } \nu \geq 0,
$$

where $h_2(w, z) = \left\{ \frac{\log \left( 1 + e^{\nu \left( \frac{\kappa_{c,c'} - 1}{1 - \hat{y}} \right)} \right)}{\mu} \right\}^{1/\beta}$ (and $\mu$ is obtained from Lemma 1).

Proof: Similar to the derivation of (4) and (5) in the proof of Theorem 1, we have for some $\eta_j$'s such that $0 \leq \eta_j \leq 1$ and $\sum_{k \neq c} \eta_k = 1$:

$$
(a_j - a_{c'})^T \phi(x) + (b_j - b_{c'}) = \log(\eta_j(1/\hat{y})).
$$

(14)

Now if $x'$ belongs to class $c'$ and the probability of it belonging to $c'$ itself, predicted by the network is assumed to be $\hat{y}'$ (as stated in the theorem), let us say that the probability of $x'$ belonging to class $c$ predicted by the network is $(1 - \hat{y}')/\kappa_{c,c'}$ where $\kappa_{c,c'} \geq 1$. It is easy to see that $1/\kappa_{c,c'}$ is equal to the conditional probability of $x'$ belonging to class $c$ given that it does not belong to class $c'$ (which is its ground truth class). Also, let's recall from the assumption of Theorem 1 that $\kappa_{c,c'}$ is assumed to be a constant for all points belonging to $c'$. Additionally, if all the classes other than $c'$ are equally similar/dissimilar to each other, then obviously $\kappa_{c,c'} = (C-1)$ for all $c \neq c'$ (since $\sum_{j \neq c'} (1/\kappa_{c,j,c'}) = 1$ and if all the classes other than $c'$ are equally similar/dissimilar to each other, then that would imply $\kappa_{j,c'} = (C-1)^{-1}$ for $j \neq c'$). This is exactly the statement of Corollary 1.

So once again, similar to the derivation of (4) and (5) in the proof of Theorem 1, we have for some $\eta_j$'s such that $0 \leq \eta_j \leq 1$ and $\sum_{k \neq c} \eta_k = 1$:

$$
(a_j - a_{c'})^T \phi(x') + (b_j - b_{c'}) = \log(\eta_j \left( \frac{\kappa_{c,c'} - 1}{1 - \hat{y}} \right) - 1) = \log \left( \eta_j \left( \frac{(\kappa_{c,c'} - 1)(1/\hat{y}') + 1}{(1/\hat{y}') - 1} \right) \right).
$$

(15)

Now subtracting (15) from (14), we get:

$$
(a_j - a_{c})^T (\phi(x) - \phi(x')) = \log \left( \frac{\eta_j \left( (1/\hat{y}') - 1 \right)(1/\hat{y}) - 1 \right) \right) \right).
$$

(16)

Therefore, we have:

$$
\|A_c \Delta \phi(x)^{(c,c')}\|^2 = \sum_{k \neq c} \left( (a_k - a_{c})^T (\phi(x) - \phi(x')) \right)^2 = \sum_{k \neq c} \log^2 \left( \frac{\eta_k \left( (1/\hat{y}') - 1 \right)(1/\hat{y}) - 1 \right) \right) \right).
$$

(17)

Note that here we do not assume $\eta_j = \eta_j'$ for $j \neq c$ since $x$ and $x'$ belong to different classes (whereas the assumption of Theorem 1 is for points belonging to the same class). Instead, for this case, we state a lemma which allows us to provide a succinct bound.

Lemma 2. Consider the function $g(u_1, \ldots, u_p, v_1, \ldots, v_p) = \sum_{i=1}^p \log^2 \left( \frac{\eta_k \left( (1/\hat{y}') - 1 \right)(1/\hat{y}) - 1 \right) \right) \right)$. Then under the constraints $0 < u_i, v_i < 1 \forall i \in \{1, \ldots, p\}$ and $\sum_{i=1}^p u_i = \sum_{i=1}^p v_i = 1$, the minimum value of $g$ occurs when $u_i = v_i = (\frac{1}{p}) \forall i$ and the minimum value is equal to $p \log^2(R)$.
We defer the proof of Lemma 2 for now but it can be found immediately after the end of the proof of Theorem 2 in this subsection itself.

Observe that the RHS of (17) has the same form as the function $g$ in Lemma 2 with $p = C - 1$, $R = \frac{((1/\bar{y}) - 1)((1/\bar{y}) - 1)}{((1/\bar{y}) - 1)/\bar{y}+1}$ and $u_i$ and $v_i$ playing the roles of $\eta_k$ and $\eta_k^*$, respectively. Thus using Lemma 2, we have:

$$\|A_\epsilon \Delta \phi(x)^{(C,c',\epsilon)}\|^2 \geq (C - 1) \log^2 \left( \frac{((1/\bar{y}) - 1)((1/\bar{y}) - 1)}{((1/\bar{y}) - 1)/\bar{y}+1} \right)$$

$$= (C - 1) \log^2 \left( \frac{((1/\bar{y}) - 1)/\bar{y}+1}{((1/\bar{y}) - 1)/(1/\bar{y}) - 1)} \right) \quad (18)$$

This completes the proof of the first part of Theorem 2.

Next using (18), we have: $P(\|A_\epsilon \Delta \phi(x)^{(C,c',\epsilon)}\|^2 < \nu(C - 1)) \leq$

$$\int_1^\infty \left\{ P\left(1 + e^{-\sqrt{\nu}} \left( \frac{((1/\bar{y}) - 1)/\bar{y}+1}{(1/\bar{y}) - 1} \right) \right) < \frac{1}{y} < 1 + e^{\sqrt{\nu}} \left( \frac{((1/\bar{y}) - 1)/\bar{y}+1}{(1/\bar{y}) - 1} \right) \right\} f\left(\frac{1}{y}\right) d\left(\frac{1}{y}\right) \quad (19)$$

Using the reparameterization mentioned in the proof of Theorem 1, let us say that $1/\hat{y} = e^{(\alpha \nu)\beta}$ and $1/\bar{y} = e^{(\alpha' \nu)\beta}$ where $\alpha, \alpha'$ are i.i.d. exp(1). Then we have:

$$P\left(1 + e^{-\sqrt{\nu}} \left( \frac{((1/\hat{y}) - 1)/\hat{y}+1}{(1/\hat{y}) - 1} \right) \right) < \frac{1}{y} < 1 + e^{\sqrt{\nu}} \left( \frac{((1/\hat{y}) - 1)/\hat{y}+1}{(1/\hat{y}) - 1} \right)$$

$$= P(h_2(\alpha', -\sqrt{\nu}) < \alpha < h_2(\alpha', \sqrt{\nu})) = (e^{-h_2(\alpha', -\sqrt{\nu})} - e^{-h_2(\alpha', \sqrt{\nu})})$$

$$\text{where } h_2(w, z) = \left\{ \log \left(1 + e^{\nu \left( \frac{((1/\hat{y}) - 1)/\hat{y}+1}{(1/\hat{y}) - 1} \right) \right) \right\}^{1/\beta} \quad (20)$$

We also have:

$$f\left(\frac{1}{y}\right) d\left(\frac{1}{y}\right) = e^{-\alpha' d\alpha'} \quad (21)$$

Now using (20) and (21) in (19), we finally get:

$$P(\|A_\epsilon \Delta \phi(x)^{(C,c',\epsilon)}\|^2 < \nu(C - 1)) \leq \int_0^\infty (e^{-h_2(\alpha', -\sqrt{\nu})} - e^{-h_2(\alpha', \sqrt{\nu})}) e^{-\alpha' d\alpha'} \quad (22)$$

Lastly, replacing $\alpha'$ by $\alpha$ in (22), we obtain the second part of Theorem 2:

$$P(\|A_\epsilon \Delta \phi(x)^{(C,c',\epsilon)}\|^2 > \nu(C - 1)) \geq 1 - \int_0^\infty (e^{-h_2(\alpha, -\sqrt{\nu})} - e^{-h_2(\alpha, \sqrt{\nu})}) e^{-\alpha d\alpha}$$

with $h_2()$ as defined in (20). \quad (23)

This finishes the proof of the second part of Theorem 2. Unfortunately, we could not simplify the integral in (23) further.

Now we prove Lemma 2. We wish to minimize $g(u_1, \ldots, u_p, v_1, \ldots, v_p) = \sum_{i=1}^p \log^2 \left( \frac{u_i}{v_i} R \right)$ under the constraints $0 < u_i, v_i < 1 \forall i \in \{1, \ldots, p\}$ and $\sum_{i=1}^p u_i = \sum_{i=1}^p v_i = 1$. We solve this using the method of Lagrangian multipliers (only imposing the equality constraints). Ideally, we should also impose the inequality constraints (i.e., $0 < u_i, v_i < 1$) and use the KKT conditions. However, it turns out that the solution obtained using the method of Lagrangian multipliers satisfies the inequality constraints due to which we need not worry. Thus, consider:

$$h(u_1, \ldots, u_p, v_1, \ldots, v_p, \lambda_u, \lambda_v) = \sum_{i=1}^p \log^2 \left( \frac{u_i}{v_i} R \right) - \lambda_u (\sum_{i=1}^p u_i - 1) + \lambda_v (\sum_{i=1}^p v_i - 1)$$
We have:

\[
\frac{\partial h}{\partial u} = 2 \log \left( \frac{u_i R}{v_i} \right) - 1 = \frac{1}{u_i} - \lambda_u = 0 \Rightarrow \log \left( \frac{u_i R}{v_i} \right) = \frac{\lambda_u u_i}{2} \tag{24}
\]

\[
\frac{\partial h}{\partial v} = 2 \log \left( \frac{u_i R}{v_i} \right) - 1 = \frac{1}{v_i} + \lambda_v = 0 \Rightarrow \log \left( \frac{u_i R}{v_i} \right) = \frac{\lambda_v v_i}{2} \tag{25}
\]

From (24) and (25), we get:

\[
\frac{u_i}{v_i} = \frac{\lambda_u}{\lambda_v} = \alpha \forall i \tag{26}
\]

Now using (26) along with (24) and (25), we get:

\[
u_i = \frac{2}{\lambda_u} \log(\alpha R), \quad v_i = \frac{2}{\lambda_v} \log(\alpha R) \forall i \tag{27}
\]

Finally using (27) along with the constraint that \(\sum_{i=1}^{p} u_i = 1\) and \(\sum_{i=1}^{p} v_i = 1\), we get -

\[
u_i = v_i = \frac{1}{p} \forall i \tag{28}
\]

Thus, the minimum value is obtained when \(u_i = v_i = 1/p \forall i\). Observe that the obtained solution automatically satisfies the inequality constraints (i.e. \(0 < u_i, v_i < 1\)), as mentioned before. The minimum value obtained for \(u_i = v_i = 1/p \forall i\) is obviously equal to \(p \log^2(R)\). This finishes the proof of Lemma 2.

### 6.3 Proof of Theorem 3

Now, we restate Theorem 3 followed by its proof.

**Theorem 3.** Consider a randomly chosen point \(x_1\) belonging to class \(c \in [C]\). Now consider two points, \(x_2\) also belonging to class \(c\) and \(x_3\) belonging to class \(c' \neq c\). Their transformed representations in the \(n\)-dimensional \(\phi\) space are \(\phi(x_1), \phi(x_2)\) and \(\phi(x_3)\), respectively. Let \(\Delta\phi(x)^{(c)} = \phi(x_1) - \phi(x_2)\) and \(\Delta\phi(x)^{(c,c')} = \phi(x_1) - \phi(x_3)\). Also recall \(A_c\) as defined in Theorem 1 and Theorem 2, the assumption in Theorem 1, \(\kappa_{c,c'}\) in Theorem 2 and \(\mu\) from Lemma 1. Then for any \(\gamma > 1\):

\[
P \left( \|A_c \Delta\phi(x)^{(c,c')}\|^2 > \gamma \|A_c \Delta\phi(x)^{(c)}\|^2 \right) \geq \int_{\alpha_1=0}^{\infty} \int_{\alpha_2=0}^{\infty} \left[ e^{-h_3(\alpha_1,\alpha_2,\gamma)} - e^{-h_3(\alpha_1,\alpha_2,\gamma)} |e^{-\alpha_2} e^{-\alpha_1} da_2 da_1 = b_3(\gamma, L) \right]
\]

where \(b_3(p,q,r) = \frac{1}{\mu} \left\{ \log \left( 1 + \left( e^{(pq)^{\beta}} - 1 \right)^{1+\frac{\beta}{2}} \left( \kappa_{c,c'} - 1 + \frac{\kappa_{c,c'}}{e^{(q\beta)^{\beta}} - 1} \right) \right) \right\}^{1/\beta} \)

**Proof:** From Theorem 1, we have:

\[
\|A_c \Delta\phi(x)^{(c)}\|^2 = (C - 1) \log^2 \left( \frac{1/\hat{y}_1 - 1}{1/\hat{y}_2 - 1} \right) = q_1(\hat{y}_1, \hat{y}_2)
\]

where \(\hat{y}_1\) and \(\hat{y}_2\) are the probabilities predicted by the network of \(x_1\) and \(x_2\) belonging to class \(c\).

Also, from Theorem 2, we have:

\[
\|A_c \Delta\phi(x)^{(c,c')}\|^2 \geq (C - 1) \log^2 \left( \frac{((\kappa_{c,c'} - 1)/\hat{y}_3) + 1}{((1/\hat{y}_3) - 1)((1/\hat{y}_1) - 1)} \right) = q_2(\hat{y}_1, \hat{y}_3)
\]

where \(\hat{y}_3\) is the probability predicted by the network of \(x_3\) belonging to class \(c'\).

Now since \(q_2(\hat{y}_1, \hat{y}_3)\) is a lower bound for \(\|A_c \Delta\phi(x)^{(c,c')}\|^2\):

\[
P \left( \|A_c \Delta\phi(x)^{(c,c')}\|^2 > \gamma \|A_c \Delta\phi(x)^{(c)}\|^2 \right) \geq P \left( q_2(\hat{y}_1, \hat{y}_3) > \gamma q_1(\hat{y}_1, \hat{y}_2) \right) \tag{29}
\]
Let us now use the reparameterization introduced in the proof of Theorem 1. Say, $1/y_1 = e^{(\alpha_2 \mu)^\beta}$ and $1/y_2 = e^{(\alpha_2 \mu)^\beta}$ and $1/y_3 = e^{(\alpha_3 \mu)^\beta}$ where $\alpha_1, \alpha_2, \alpha_3$ are i.i.d $\exp(1)$. We then have:

$$q_1(\hat{y}_1, \hat{y}_2) = \log^2 \left( e^{(\alpha_1 \mu)^\beta} - 1 \right)$$
$$q_2(\hat{y}_1, \hat{y}_3) = \log^2 \left( \frac{\beta}{e^{(\alpha_2 \mu)^\beta} - 1} \right)$$

Using (30) and imposing the condition: $q_2(\hat{y}_1, \hat{y}_3) - \gamma q_1(\hat{y}_1, \hat{y}_2) > 0$, we get:

$$\alpha_1 \in \left( \text{min}(h_3(\alpha_2, \alpha_3, \sqrt{7}), h_3(\alpha_2, \alpha_3, -\sqrt{7})), \text{max}(h_3(\alpha_2, \alpha_3, \sqrt{7}), h_3(\alpha_2, \alpha_3, -\sqrt{7})) \right)$$

where $h_3(p, q, r) = \frac{1}{\mu} \left\{ \log \left( 1 + \left( e^{(\mu)^\beta} - 1 \right) \right) \right\}^{1/\beta}$

Imposing the condition: $q_2(\hat{y}_1, \hat{y}_3) - \gamma q_1(\hat{y}_1, \hat{y}_2) > 0$, gives us a quadratic inequality in $\log \left( e^{(\alpha_2 \mu)^\beta} - 1 \right)$ and the coefficients of the inequality are a function of $\log \left( (\alpha_1 \mu)^\beta - 1 \right)$ as well as $\log \left( \frac{\beta}{e^{(\alpha_2 \mu)^\beta} - 1} \right)$. Solving the quadratic inequality gives us (31).

Next, we have:

$$P(\alpha_1 \in \left( \text{min}(h_3(\alpha_2, \alpha_3, \sqrt{7}), h_3(\alpha_2, \alpha_3, -\sqrt{7})), \text{max}(h_3(\alpha_2, \alpha_3, \sqrt{7}), h_3(\alpha_2, \alpha_3, -\sqrt{7})) \right))$$

$$= |\exp(-h_3(\alpha_2, \alpha_3, -\sqrt{7})) - \exp(-h_3(\alpha_2, \alpha_3, \sqrt{7}))|.$$ (32)

Hence using (32), we get:

$$P(\gamma q_1(\hat{y}_1, \hat{y}_2)) = \int_{\alpha_2=0}^{\infty} \int_{\alpha_3=0}^{\infty} e^{-h_3(\alpha_2, \alpha_3, -\sqrt{7}) - h_3(\alpha_2, \alpha_3, \sqrt{7})} e^{-\alpha_3} e^{-\alpha_2} \alpha_3 \alpha_2$$ (33)

Finally, using (29) along with (33) and replacing the variables $\alpha_3$ and $\alpha_2$ in (33) by $\alpha_2$ and $\alpha_1$ respectively, we get:

$$P(\|A_c \Delta \phi(x)(c,c')\|^2 > \gamma \|A_c \Delta \phi(x)(c')\|^2) \geq \int_{\alpha_1=0}^{\infty} \int_{\alpha_2=0}^{\infty} e^{-h_3(\alpha_2, \alpha_2, -\sqrt{7}) - h_3(\alpha_2, \alpha_2, \sqrt{7})} e^{-\alpha_2} e^{-\alpha_1} \alpha_3 \alpha_2$$ (34)

This concludes the proof of Theorem 3. Unfortunately, we could not simplify the double integral in (34) any further.

6.4 Proof of Theorem 4

We now restate and then prove Theorem 4.

**Theorem 4.** Let $F_c^\gamma(u)$ be the cdf of a chi-squared random variable with $(C - 1)$ degrees of freedom evaluated at $(C - 1)$ units. Then, under Assumption 1, the same settings as in Theorem 3 and with the function $b_A$ as defined in Theorem 3, we have for any $\gamma \geq 1$:

$$P(\|A_c \Delta \phi(x)(c,c')\|^2 > \gamma \|A_c \Delta \phi(x)(c')\|^2) \geq \max_{0 < \epsilon_1, \epsilon_2 < 1} b_A \left( \frac{\gamma + \epsilon_1}{1 - \epsilon_2}, L \right) \left( F_c^\gamma(1 + \epsilon_1) - F_c^\gamma(1 - \epsilon_2) \right) = b(\gamma, L)$$

$$\geq \max_{0 < \epsilon_1, \epsilon_2 < 1} b_A \left( \frac{\gamma + \epsilon_1}{1 - \epsilon_2}, L \right) \left( 1 - \exp \left( -\left( 1 + \epsilon_1 - \sqrt{1 + 2\epsilon_1} \left( \frac{C-1}{2} \right) \right) \right) \right)$$

**Proof:** Firstly, recall our assumption (Assumption 1) that the elements of $A_c$ are zero mean i.i.d Gaussian random variables. Let $\tilde{A_c} \triangleq \frac{A_c}{\sqrt{\sum_{i,j} A_{i,j}^2}}$ where $\sigma_c^2$ is the variance of the elements of $A_c$. Thus, the elements of $\tilde{A_c} \sim N(0, \frac{1}{\sigma_c^2 - 1})$.

Now as shown in [6], both $\|A_c \Delta \phi(x)(c)\|^2 / \|A_c \Delta \phi(x)(c')\|^2$ and $\|A_c \Delta \phi(x)(c,c')\|^2 / \|A_c \Delta \phi(x)(c')\|^2$ are both chi-squared random variables with $(C - 1)$ degrees of freedom each (here $A_c$ is treated
as random variable whereas $\Delta \phi(x)^{(c)}$ and $\Delta \phi(x)^{(c,c')}\) are treated as deterministic/non-random quantities). But unfortunately, the two are not independent (we are talking about independence with respect to $A_c$ of each other. But still, we have the following inequality:

$$
\mathbb{P}\left(\gamma \|\Delta \phi(x)^{(c)}\|^2 < \gamma \frac{\|\hat{A}_c \Delta \phi(x)^{(c)}\|^2}{1 - \epsilon_2}, \|\Delta \phi(x)^{(c,c')}\|^2 > \frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{1 + \epsilon_1}\right) = 
\mathbb{P}\left(\|\Delta \phi(x)^{(c)}\|^2 < \frac{\|\hat{A}_c \Delta \phi(x)^{(c)}\|^2}{1 - \epsilon_2}, \|\Delta \phi(x)^{(c,c')}\|^2 > \frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{1 + \epsilon_1}\right) \geq 
1 - \mathbb{P}\left(\frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{\|\Delta \phi(x)^{(c,c')}\|^2} > 1 + \epsilon_1\right) - \mathbb{P}\left(\frac{\|\hat{A}_c \Delta \phi(x)^{(c)}\|^2}{\|\Delta \phi(x)^{(c)}\|^2} < 1 - \epsilon_2\right) = F_C^\chi(1 + \epsilon_1) - F_C^\chi(1 - \epsilon_2) \text{ where } F_C^\chi(u) = \text{cdf of a } \chi^2_{(C-1)} \text{ random variable at } (C-1)u.
$$

(35)

In order to show how the above inequality is obtained, consider two random variables $X$ and $Y$. Then:

$$
\mathbb{P}(X < x, Y > y) = 1 - \{\mathbb{P}(X > x, Y > y) + \mathbb{P}(X > x, Y < y)\} - \mathbb{P}(X < x, Y < y)
= 1 - \mathbb{P}(X > x) - \mathbb{P}(X < x, Y < y) \geq 1 - \mathbb{P}(X > x) - \mathbb{P}(Y < y)
$$

In the above steps, the first equality follows from the law of total probability, the second equality is obtained by marginalizing out $Y$ and the third inequality follows from the fact that $\mathbb{P}(Y < y) = \mathbb{P}(X < x, Y < y) + \mathbb{P}(X > x, Y < y) \geq \mathbb{P}(X < x, Y < y) \Rightarrow \mathbb{P}(X < x, Y < y) \leq \mathbb{P}(Y < y)$. Also:

$$
\frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{(1 + \epsilon_1)} > \gamma \frac{\|\hat{A}_c \Delta \phi(x)^{(c)}\|^2}{(1 - \epsilon_2)} \Rightarrow \frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{\|\Delta \phi(x)^{(c,c')}\|^2} > \gamma \frac{\|\hat{A}_c \Delta \phi(x)^{(c)}\|^2}{\|\Delta \phi(x)^{(c)}\|^2}
$$

(36)

But from Theorem 3 - $\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2 \geq \gamma \frac{(1 + \epsilon_1)}{(1 - \epsilon_2)} \|\hat{A}_c \Delta \phi(x)^{(c)}\|^2$ w.p. $\geq b_A\left(\gamma \frac{1 + \epsilon_1}{1 - \epsilon_2}, L\right)$. Note that the derivation of (35) is completely oblivious of $\Delta \phi(x)^{(c)}$ and $\Delta \phi(x)^{(c,c')}$, and depends only on the distribution of $A_c$. And the derivation of (36) is completely oblivious of the distribution of $A_c$. Leveraging these two facts, we use (35) and (36) to get:

$$
\|\Delta \phi(x)^{(c,c')}\|^2 > \frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{1 + \epsilon_1} \geq \gamma \frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{1 - \epsilon_2} > \gamma \|\Delta \phi(x)^{(c,c')}\|^2
$$

w.p. $\geq b_A\left(\gamma \frac{1 + \epsilon_1}{1 - \epsilon_2}, L\right)(F_C^\chi(1 + \epsilon_1) - F_C^\chi(1 - \epsilon_2))$. (37)

Notice that (37) holds for all $\epsilon_1, \epsilon_2 \in (0, 1)$. Thus, taking max over all $\epsilon_1, \epsilon_2 \in (0, 1)$, we get:

$$
\mathbb{P}\left(\|\Delta \phi(x)^{(c,c')}\|^2 > \gamma \|\Delta \phi(x)^{(c)}\|^2\right) \geq \max_{0 < \epsilon_1, \epsilon_2 < 1} b_A\left(\gamma \frac{1 + \epsilon_1}{1 - \epsilon_2}, L\right)(F_C^\chi(1 + \epsilon_1) - F_C^\chi(1 - \epsilon_2)).
$$

(38)

This proves the first part of Theorem 4.

The second part of Theorem 4 involves simply upper-bounding $\mathbb{P}\left(\frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{\|\Delta \phi(x)^{(c,c')}\|^2} > 1 + \epsilon_1\right)$ and $\mathbb{P}\left(\frac{\|\hat{A}_c \Delta \phi(x)^{(c,c')}\|^2}{\|\Delta \phi(x)^{(c,c')}\|^2} < 1 - \epsilon_2\right)$. Essentially, we derive some upper bounds on the values of $\mathbb{P}(\chi^2_{(C-1)} > (1 + \epsilon)(C - 1))$ and $\mathbb{P}(\chi^2_{(C-1)} < (1 - \epsilon)(C - 1))$.

We provide tighter bounds than the ones provided in Lemma 1.3 of [6] by using a result provided in Lemma 1, Page 1325 of [8] which is as follows:

$$
\mathbb{P}(\chi^2_k \geq k + 2\sqrt{kx} + 2x) \leq e^{-x} \text{ and } \mathbb{P}(\chi^2_k \leq k - 2\sqrt{kx}) \leq e^{-x}
$$

(39)
Now substituting \((1 + \epsilon)k = k + 2\sqrt{k/2} + 2x\) gives us \(x = \frac{k}{2}(1 + \epsilon - \sqrt{1 + 2\epsilon})\). Similarly, substituting \((1 - \epsilon)k = k - 2\sqrt{k/2}\) gives us \(x = k\epsilon^2/4\). Using this, we get:

\[
\mathbb{P}(\chi_k^2 \geq (1 + \epsilon)k) \leq \exp\left(-\frac{k}{2}(1 + \epsilon - \sqrt{1 + 2\epsilon})\right) \quad \text{and} \quad \mathbb{P}(\chi_k^2 \leq (1 - \epsilon)k) \leq \exp\left(-\frac{k}{4}\epsilon^2\right). \tag{40}
\]

Substituting the bounds obtained above in (40) along with \(k = (C - 1)\) in (35) and then repeating the rest of the process (of the proof) up to (38), we obtain the second part of \textbf{Theorem 4}.

This concludes the proof of \textbf{Theorem 4}.

### 6.5 Proof of \textbf{Theorem 5}

Finally, we restate and then prove the last theorem, i.e. \textbf{Theorem 5}.

**Theorem 5.** Let there be \(N_c\) examples belonging to class \(c \in [C]\). Under the assumption of \textbf{Theorem 1}, define \(\kappa^*_c \triangleq \min_{c' \neq c} \kappa_{c', c}\) (\(\kappa_{c', c}\)'s are the same as in \textbf{Theorem 2}). Then the expected number of examples in class \(c\) correctly classified, say \(N_c^{\text{corr}}\), is:

\[
N_c^{\text{corr}} = N_c\left(1 - \exp\left(-\left(\frac{\Gamma(\beta + 1) \log(1 + \kappa^*_c)}{L}\right)^{\frac{1}{\beta}}\right)\right) \geq N_c\left(1 - \exp\left(-\left(\frac{\Gamma(\beta + 1) \log(2)}{L}\right)^{\frac{1}{\beta}}\right)\right)
\]

The lower bound provided above holds regardless of the validity of the assumption in \textbf{Theorem 1}.

**Proof:** Consider a point \(x\) belonging to class \(c\). Let the probability of it belonging to \(c\), predicted by the network be \(\hat{y}\). As per the notation used in \textbf{Theorem 2}, the probability of \(x\) belonging to \(c' \neq c\), predicted by the network, is \((1 - \hat{y})/\kappa_{c', c}\) and under the assumption of \textbf{Theorem 1}, \(\kappa_{c', c}\) is a constant for all points belonging to \(c\).

Now, for \(x\) to be correctly classified by the network, we must have \(\hat{y} > (1 - \hat{y})/\kappa_{c', c}\) for all \(c' \neq c\). In other words, we must have \(\hat{y} > (1 - \hat{y})/\kappa^*_c\) where \(\kappa^*_c \triangleq \min_{c' \neq c} \kappa_{c', c}\). This is equivalent to \(\hat{y} > 1/(\kappa^*_c + 1)\) or \((-\log(\hat{y}))^{1/\beta} < (\log(\kappa^*_c + 1))^{1/\beta}\). Now using (3) of the main paper and substituting the value of \(\mu\) obtained from \textbf{Lemma 1} in the main paper, we have:

\[
\mathbb{P}\left((-\log(\hat{y}))^{1/\beta} < (\log(\kappa^*_c + 1))^{1/\beta}\right) = 1 - \exp\left(-\left(\frac{\Gamma(\beta + 1) \log(1 + \kappa^*_c)}{L}\right)^{\frac{1}{\beta}}\right) = p_{\text{acc}}(L, \kappa^*_c)
\]

Using (41), the expected number of correctly classified examples actually belonging to \(c\), \(N_c^{\text{corr}}\) will be:

\[
N_c^{\text{corr}} = N_c p_{\text{acc}}(L, \kappa^*_c) \tag{42}
\]

This proves the first part of \textbf{Theorem 5}.

We have \(\kappa^*_c \geq 1\) since \(\kappa_{c', c} \geq 1\) for all \(c' \neq c\). It can be verified that \(p_{\text{acc}}(L, \kappa^*_c)\) is an increasing function of \(\kappa^*_c\). Therefore:

\[
N_c^{\text{corr}} \geq N_c p_{\text{acc}}(L, 1) = N_c\left(1 - \exp\left(-\left(\frac{\Gamma(\beta + 1) \log(2)}{L}\right)^{\frac{1}{\beta}}\right)\right) \tag{43}
\]

Note that (43) can be also derived by just computing the probability with which \(\hat{y} > (1 - \hat{y})\) (notice that this is equivalent to setting \(\kappa^*_c = 1\)) which always ensures that \(x\) is correctly classified. In other words, the probability with which correct classification occurs is at least as large as the probability with which \(\hat{y} > (1 - \hat{y})\). Thus (43) holds irrespective of the validity of the assumption of \textbf{Theorem 1}.

This completes the proof of \textbf{Theorem 5}.

### 6.6 Additional Experiments

We firstly describe the two synthetic datasets (SYN-1 and SYN-2) that we talked about in the main paper. We also provide code to generate SYN-1 and SYN-2.

**First synthetic dataset (SYN-1):** Here, we considered 10 dimensional random Gaussian vectors as input belonging to one out of 20 possible classes. Denote one such random input by \(z = [z_1, z_2, \ldots, z_{10}]^T\). The class of \(z\) is determined by the range in which the value of
$h(z) = \sum_{i=1}^{10} \exp(z_i)/10$ lies in. Specifically, we have interval points $\{r_1, r_2, \ldots, r_{19}\}$. Then, $z$ belongs to class number 0 if $h(z) < r_1$, $z$ belongs to class number $i$ ($0 < i < 19$) if $r_i \leq h(z) < r_{i+1}$ and $z$ belongs to class number 19 if $h(z) \geq r_{19}$. The interval points were chosen such that the number of training points in each interval are all nearly the same. For SYN-1, we fitted a fully connected neural network (the entire architecture can be found in Subsection 6.7) consisting of three hidden layers with ReLU activation. The value of $n$ used was 80. The total number of training set and test set examples were 16000 and 4000 (randomly chosen), respectively. We trained the model for 100 epochs and the obtained loss value over the test set (after 100 epochs) was $L = 0.5632$. We observed that $\beta = 2$ results in the closest resembling exponential distribution for SYN-1.

**Second synthetic dataset (SYN-2):** This is similar to the previous dataset, except that the function for the classification rule was taken to be a simple linear function, $h(z) = (\sum_{i=1}^{10} 2z_i + \sum_{i=6}^{10} z_i)/5$. We used the same architecture as that used for SYN-1 (and so $n = 80$). Here, the total number of training set and test set examples were 24000 and 6000 (again randomly chosen), respectively. The test set loss value after training the model for 20 epochs was $L = 0.1889$. In this case, $\beta = 1.4$ results in the closest resembling exponential distribution.

Figure 4c and Figure 4d in the main paper show the distribution of $\left( -\log \hat{p}_i(c(z_i)) \right)^{1/\beta}$ along with the closest fit exponential distribution for SYN-1 with $\beta = 2$ and SYN-2 with $\beta = 1.4$, respectively, over the test set.

Also, Table 2a and Table 2b show the probability of the inter-class distance being more than the intra-class distance for SYN-1 and SYN-2 respectively, over the test set.

| Class 1 ($c_1$) | Class 2 ($c_2$) | $p_1$    | $p_2$    |
|----------------|----------------|---------|---------|
| 0              | 1              | 0.7575  | 0.8448  |
| 1              | 2              | 0.8317  | 0.7751  |
| 5              | 6              | 0.6196  | 0.6319  |
| 16             | 17             | 0.5677  | 0.5257  |
| 11             | 13             | 0.8278  | 0.7645  |
| 7              | 9              | 0.8216  | 0.7836  |
| 12             | 15             | 0.9675  | 0.8782  |
| 14             | 18             | 0.9951  | 0.9251  |
| 5              | 10             | 0.9985  | 0.9931  |
| 3              | 12             | 1.0000  | 0.9964  |

(a) SYN-1

| Class 1 ($c_1$) | Class 2 ($c_2$) | $p_1$    | $p_2$    |
|----------------|----------------|---------|---------|
| 0              | 1              | 0.8169  | 0.9183  |
| 1              | 2              | 0.8927  | 0.9153  |
| 5              | 6              | 0.9123  | 0.9445  |
| 16             | 17             | 0.9036  | 0.8848  |
| 11             | 13             | 0.9998  | 0.9995  |
| 7              | 9              | 0.9990  | 0.9999  |
| 12             | 15             | 1.0000  | 1.0000  |
| 14             | 18             | 1.0000  | 1.0000  |
| 5              | 10             | 1.0000  | 1.0000  |
| 3              | 12             | 1.0000  | 1.0000  |

(b) SYN-2

Table 2: Sample probabilities of inter-class distance being more than the intra-class distance for (a) SYN-1 with $L = 0.5632$ and (b) SYN-2 with $L = 0.1889$. $p_1$ and $p_2$ are as defined in the text.

Observe that in both Table 2a and Table 2b, the values of $p_1$ and $p_2$ are lower when $|c_1 - c_2|$ is small as compared to when $|c_1 - c_2|$ is large. This is because, based on the description of the two datasets, if $|c_1 - c_2| < |c_1 - c_3|$ then it implies that the interval corresponding to $c_2$ is closer to the interval corresponding to $c_1$ than that corresponding to $c_3$, leading to poorer separability between the points belonging to $c_1$ and $c_2$ as compared to the points belonging to $c_1$ and $c_3$.

In Table 2a with $L = 0.5632$, observe that $p_1$ and $p_2$ values for the first 4 entries of the table where $|c_1 - c_2| = 1$ is in the range of (0.6, 0.85) while their values for the last 2 entries of the table where $|c_1 - c_2| \geq 5$ is nearly 1. In order to illustrate the effect of the choice of $\kappa_{c,c'}$ other than $(C - 1)$, we report the values of $b_c(0.5632)$ with $\beta = 2$, $C = 20$, $\kappa_{c,c'} = 0.2(C - 1)$ and $\kappa_{c,c'} = 5(C - 1)$ (which indicate greater and lesser similarity or poorer and better separation, respectively, between $c$ and $c'$, than if we would have set $\kappa_{c,c'} = C - 1$). These turn out to be approximately 0.5494 and 0.7295, respectively.

In Table 2b with $L = 0.1889$, observe that $p_1$ and $p_2$ values for the first 4 entries of the table where $|c_1 - c_2| = 1$ is in the range of (0.8, 0.95) while their values for the last 4 entries of the table where $|c_1 - c_2| \geq 3$ is exactly 1. Here, the values of $b_c(0.1889)$ with $\beta = 1.4$, $C = 20$, $\kappa_{c,c'} = 0.2(C - 1)$ and $\kappa_{c,c'} = 5(C - 1)$ turn out to be approximately 0.7749 and 0.8986, respectively.

Thus, even here, the obtained values are consistent with the observed values.
6.7 Architectures used and some more training details

Finally, we show the block-diagrams of the network architectures used for the 4 datasets in Figure 5. Observe that the values of \( n \) in Figure 5a, Figure 5b and Figure 5c are 512, 128 and 80, respectively. As usual, the last layer in all 3 cases is a fully connected Softmax layer.

The models described earlier were fitted with Keras (using NVIDIA GeForce 940MX GPU). The batch size used for CIFAR-10, MNIST, SYN-1 and SYN-2 were 64, 128, 200 and 400, respectively. The training set and test set of MNIST and CIFAR-10 were used as provided with sizes of the training set being 60000 and 50000, respectively. As mentioned in the main paper also, size of the test set was 10000 for both the datasets.