Fast Single-Class Classification and the Principle of Logit Separation

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Abstract

We consider neural network training, in applications in which there are many possible classes, but at test time the task is to identify whether the example belongs to one specific class, e.g., when searching for photos of a specific person. We focus on reducing the computational burden at test-time in such applications. We define the Single Logit Classification (SLC) task: training the network so that at test time, it would be possible to accurately identify if the example belongs to a given class, based only on the output logit of the trained model for this class. We propose a natural principle, the Principle of Logit Separation (PoLS), as a guideline for choosing and designing losses suitable for the SLC. We study previously suggested losses and their alignment with the PoLS. We further derive new batch versions of known losses, and show that unlike the standard versions, these new versions satisfy the PoLS. Our experiments show that the losses aligned with the PoLS overwhelmingly outperform the other losses on the SLC task. Tensorflow code for optimizing the new batch losses is publicly available in [https://github.com/cruvadom/Logit_Separation](https://github.com/cruvadom/Logit_Separation).

1 Introduction

With the advent of Big Data, classifiers can learn fine-grained distinctions, and are used for classification in settings with very large numbers of classes. Datasets with up to hundreds of thousands of classes are already in use in the industry [Deng et al., 2009; Partalas et al., 2015], and such classification tasks have been studied in several works (e.g., Weston et al., 2013; Gupta et al., 2014). Classification with a large number of classes appears naturally in vision, in language modeling, and in machine translation [Bahdanau et al., 2015; Józefowicz et al., 2016; Dean et al., 2013].

When using neural network classifiers, one implication of a large number of classes is a high computational burden at test-time. Indeed, the computation needed for finding the pre-normalized outputs of the top network layer (the logits of the classes) is linear in the number of classes [Grave et al., 2016], and can be prohibitively slow for high-load systems, such as search engines and real-time machine translation systems. In this work, we focus on reducing the computation at test-time.

In many applications, the task at test time is not full classification of each example into one of the many possible classes. Instead, the task is to identify whether the example should be classified into one of a small subset of the possible classes, or even a single class. For instance, when searching...
for photos of a specific person, we do not need to identify the person in each photo — we only need to identify whether this is a photo of the person of interest. In this type of application, one would ideally like to have a test-time computation that does not depend on the total number of possible classes. A natural approach is to calculate the network logit of each example only for the class of interest for that example, and use this value alone to infer whether this is the true class of the example. In this paper we consider the goal of training the network in a way that leads to a high accuracy of this approach. We name this problem Single Logit Classification (SLC): training the network so that at test time, it would be possible to accurately predict, based on the logit of a single class, whether this is the true class of the example.

Some training methods might not be suitable for the SLC task, since in these methods, the logits for each class are meaningful only in comparison with the logits of the other classes. For instance, in the standard cross-entropy training paradigm (Hinton, 1989), each logit is normalized by a function of the logits of all classes, which requires computing all the logits.

What properties should a training loss have so as to successfully solve the SLC? In this work we identify a simple principle that such a loss should satisfy. We name this principle the Principle of Logit Separation (PoLS). Informally, it states that to succeed in the SLC task, the training objective should optimize for separating between the set of logits that belong to the true classes of their respective training examples, and all the other logits. We study previously suggested losses and their alignment with the PoLS. We show that the PoLS is satisfied by the approaches proposed in Devlin et al. (2014); Mnih and Teh (2012) for calculating posterior distributions in the context of natural language processing, as well as by the binary cross-entropy loss used in multi-label settings (Wang et al., 2016; Huang et al., 2013), while it is not satisfied by the standard cross-entropy loss and the max-margin loss.

Further, we derive new solutions to the SLC task based on the PoLS. These objectives are novel batch versions of the cross-entropy loss and the max-margin loss. We show that the batch versions, unlike the standard versions of these losses, satisfy the PoLS. These new solutions have several advantages, which we discuss in the sequel.

In total, we study seven different training objectives, showing that two of them do not satisfy the PoLS, while the other five (two of which are new) do. We perform experiments on five benchmark datasets, and compare the accuracy of the seven methods on the SLC task, as well as on multiclass prediction. The experiments show that indeed, on the SLC task, all objectives that satisfy the PoLS overwhelmingly outperform the ones that do not. Moreover, the former obtain a comparable, and sometimes superior, accuracy also in the multiclass classification task. In addition, surprisingly, the performance on the SLC task of the losses that satisfy the PoLS is usually better even than the performance of the normalized logits of the standard cross-entropy loss. Thus, even when one is allowed to compute all the logits so as to normalize the single-class logit, the losses which satisfy the PoLS, which compute only a single logit at test-time, are still preferable for the SLC task.

Our main contributions are therefore

- Defining the SLC, and proposing the Principle of Logit Separation;
- Analyzing the alignment of previously suggested losses with the PoLS;
- Proposing new batch losses for solving the SLC, based on the PoLS; Tensorflow code for optimizing these losses is publicly available in https://github.com/cruvadom/Logit_Separation
- Showing that objectives that satisfy the PoLS overwhelmingly outperform standard objectives on the SLC task, while keeping multiclass classification accuracy the same or higher.
- Showing that the losses that satisfy the PoLS are preferable even to the normalized logits of the standard cross-entropy loss, although the former require only a single logit computation at test-time.

We conclude that the PoLS is a useful principle for selecting losses for the SLC, and that the SLC can be efficiently and practically solved, without hindering the multiclass classification accuracy of the model.

Related Work We review existing methods that are relevant for faster test-time classification. The hierarchical softmax layer (Morin and Bengio, 2005; Mnih and Hinton, 2008) replaces the flat soft-
max layer with a binary tree with classes as leaves, making the computational complexity of calculating the posterior probability of each class logarithmic in the number of classes. A drawback of this method is the additional construction of the binary tree of classes, which requires expert knowledge or data-driven methods. Inspired by the hierarchical softmax approach, Grave et al. (2016) exploit unbalanced word distributions to form clusters that explicitly minimize the average time for computing the posterior probabilities over the classes. The authors report an impressive speed-up factor of between 2 and 10 for posterior probability computation, but their computation time still depends on the total number of classes. Differentiated softmax was introduced in Chen et al. (2016) as a less computationally expensive alternative to the standard softmax mechanism, in the context of neural language models. With differentiated softmax, each class (word) is represented in the last hidden layer using a different dimension, with higher dimensions for more frequent classes. This allows a faster computation for less frequent classes. However, this method is only applicable for highly unbalanced distributions. Several sampling-based approaches were developed in the context of language modeling, with the goal of approximating the softmax function at training-time. Notable examples are importance sampling (Bengio and Senecal, 2003, 2008), negative sampling (Mnih and Teh, 2012), and Noise Contrastive Estimation (NCE) (Gutmann and Hyvärinen, 2010; Mnih and Teh, 2012). These methods do not necessarily improve the test-time computational burden, however we show below that the NCE loss can be used for the SLC task.

2 The Principle of Logit Separation

In the SLC task, the only information about an example is the output logit of the model for the single class of interest. Therefore, a natural approach to classifying whether the class matches the example is to set a threshold: if the logit is above the threshold, classify the example as belonging to this class, otherwise, classify it as not belonging to the class. We refer to logits that belong to the true classes of their respective training examples as true logits and to other logits as false logits. For the threshold approach to work well, values for true and false logits across different examples should be separable from each other. We term this requirement the Principle of Logit Separation, and formalize it below.

Let \([k] := \{1, \ldots, k\}\) be the possible class labels. Assume that the training sample is \(S = ((x_1, y_1), \ldots, (x_n, y_n))\), where \(x_i \in \mathbb{R}^d\) are the training examples, and \(y_i \in [k]\) are the labels of these examples. A standard neural network model calculates for each input example \(x\) a vector of real values \((z_1, \ldots, z_k) \in \mathbb{R}^k\), where \(z_i\) is the logit assigned to example \(x\) for class \(i\). The PoLS can be stated as follows:

**Definition 2.1 (The Principle of Logit Separation (PoLS)).** For any two examples \((x, y), (x', y')\) with logit vectors \(z, z'\) respectively, if \(y \neq y'\) then \(z_y > z'_y\).

This simple principle guarantees, if it holds for all examples, perfect accuracy on the SLC task. Thus, a training objective for SLC should attempt to optimize for this principle.

We now define training losses, and formally define what it means for a loss to satisfy the PoLS. We focus on losses that are a function of the output logits and the labels of the examples. For a neural network model \(\theta\), denote the vector of logits it assigns to example \(x\) by \(z^\theta(x) = (z_1^\theta(x), \ldots, z_k^\theta(x))\). When \(\theta\) and \(x\) are clear from context, we write \(z_j\) instead of \(z_j^\theta(x)\). Denote the logit output of the sample by \(S_\theta = ((z^\theta(x_1), y_1), \ldots, (z^\theta(x_n), y_n))\). A loss function for neural network training is a function \(\ell: \bigcup_{i=1}^\infty (\mathbb{R}^k \times [k])^n \rightarrow \mathbb{R}_+\), which assigns a loss to a training sample based on the output logits of the model and on the labels of the training examples. The goal of training is to find a model \(\theta\) which minimizes \(\ell(S_\theta)\). In almost all the losses we study below, the loss on the training sample is simply the sum over all examples of a loss defined on a single example: \(\ell(S_\theta) \equiv \sum_{i=1}^n \ell(z^\theta(x_i), y_i)\), thus it suffices to define \(\ell(z, y)\). We explicitly define \(\ell(S_\theta)\) below only when it deviates from this paradigm.

We say that a loss \(\ell\) satisfies the PoLS if a small enough value of \(\ell(S_\theta)\) ensures that the requirement in Def. 2.1 is satisfied on the training sample. Formally, we require that for any training sample \(S\):

\[
\exists \epsilon > 0 \text{ such that for any model } \theta \text{ such that } \ell(S_\theta) < \epsilon,
\]

\[
\forall (x, y), (x', y') \in S \text{ such that } y \neq y', \quad z_y^\theta(x) > z_y^\theta(x').
\]

In the following sections we study the alignment with the PoLS of known losses and new losses.
3 Standard objectives in view of the PoLS

In this section we show that the cross-entropy loss (Hinton [1989]), which is the standard loss function for neural network classifiers (e.g., Krizhevsky et al. [2012]) and the multiclass max-margin loss (Crammer and Singer [2001]), do not satisfy the PoLS.

The cross-entropy loss  The cross-entropy loss on a single example is defined as,
\[ \ell(z, y) = -\log(p_y), \quad \text{where} \quad p_y := e^{z_y} / \sum_{j=1}^{k} e^{z_j} = \left( \sum_{j=1}^{k} e^{z_j - z_y} \right)^{-1}. \] (2)

Note that \( p_y \) is the probability assigned by the softmax layer. It is easy to see that the cross-entropy loss does not satisfy the PoLS. Indeed, as the loss depends only on the difference between logits for every example separately, minimizing it does not guarantee that all true logits are larger than all false logits in the training set. Formally, the following counter-example shows that Eq. (1) does not hold. Let \( S = ((x_1, 1), (x_2, 2)) \) be the training sample, and let \( \theta_\alpha \), for \( \alpha > 0 \), be a model such that \( z^{\theta_\alpha}(x_1) = 2\alpha \), \( z^{\theta_\alpha}(x_2) = -2\alpha \). Then \( \ell(S_{\theta_\alpha}) = 2 \log(1 + e^{-\alpha}) \). Therefore for any \( \epsilon > 0 \), there is some \( \alpha > 0 \) such that \( \ell(S_{\theta_\alpha}) \leq \epsilon \), but \( z^{\theta_\alpha}(x_1) > z^{\theta_\alpha}(x_2) \), contradicting Eq. (1).

The max-margin loss  Max-margin training objectives, most widely known for their role in training Support Vector Machines, are used in some cases for training neural networks (Tang [2013]; Socher et al. [2011]; Janocha and Czarnecki [2017]). Here we consider the multiclass max-margin loss suggested by Crammer and Singer [2001],
\[ \ell(z, y) = \max(0, \gamma - z_y + \max_{j \neq y} z_j), \] (3)

where \( \gamma > 0 \) is a hyperparameter, that controls the separation margin between the true logit and the false logits of the example. It is easy to see that this loss too does not satisfy the PoLS. Indeed, consider the same training sample \( S \) as defined in the counter-example for the cross-entropy loss above, and the model \( \theta_\alpha \) defined there. Setting \( \alpha = \gamma \), we have \( \ell(S_{\theta_\alpha}) = 0 \). Thus for any \( \epsilon > 0 \), \( \ell(S_{\theta_\alpha}) < \epsilon \), but \( z^{\theta_\alpha}(x_1) > z^{\theta_\alpha}(x_2) \), contradicting Eq. (1).

4 Objectives that satisfy the PoLS

In this section we consider objectives that have been previously suggested for addressing problems that are somewhat related to the SLC task. We show that these objectives indeed satisfy the PoLS.

4.1 Self-normalization

Self-normalization (Devlin et al. [2014]) was introduced in the context of neural language models, to avoid the costly step of computing the posterior probability distribution over the entire vocabulary when evaluating the trained models. The self-normalization loss is a sum of the cross-entropy loss with an additional term. Let \( \alpha > 0 \) be a hyperparameter, and \( p_y \) as defined in Eq. (2). The self-normalization loss is defined by
\[ \ell(z, y) = -\log(p_y) + \alpha \cdot \log(\sum_{j=1}^{k} e^{z_j}). \]

The motivation for this loss is self-normalization: The second term is minimal when the softmax normalization term \( \sum_{j=1}^{k} e^{z_j} \) is equal to 1. When it is equal to 1, the exponentiated logit \( e^{z_j} \) can be interpreted as the probability that the true class for the example is \( j \). Devlin et al. [2014] report a speed-up by a factor of 15 in evaluating models trained when using this loss, since the self-normalization enables computing the posterior probabilities for only a subset of the vocabulary. Intuitively, this loss should also be useful for the SLC task: If the softmax normalization term is always close to 1, there should be no need to compute it, thus only the logit of the class in question should be required.
We show that indeed the self-normalization loss satisfies the PoLS. Assume a training sample \( S \) and a neural network model \( \theta \), and consider an example \((x, y) \in S\). We consider the two terms of the loss in order. First, consider \(- \log(p_y)\). From the definition of \( p_y \) (Eq. 2) we have that

\[
- \log(p_y) = \log(\sum_{j=1}^{k} e^{z_j - z_y}) = \log(1 + \sum_{j \neq y} e^{z_j - z_y}).
\]

Set \( \epsilon_0 := \log(1 + e^{-2}) \). Then, if \(- \log(p_y) < \epsilon_0\), we have \( \sum_{j \neq y} e^{z_j - z_y} \leq e^{-2} \), which implies that (a) \( \forall j \neq y, z_j \leq z_y - 2 \) and (b) \( e^{z_j} \geq \sum_{j \neq y} e^{z_j} / (1 + e^{-2}) \geq \frac{1}{2} \sum_{j \neq y} e^{z_j} \). Second, consider the second term. There is an \( \epsilon_1 > 0 \) such that if \( \log^2(\sum_{j \neq y} e^{z_j}) < \epsilon_1 \) then (c) \( 2e^{-1} < \sum_{j \neq y} e^{z_j} < e \), which implies \( e^{z_y} < e \) and hence (d) \( z_y < 1 \).

Now, consider \( \theta \) such that \( \ell(S_\theta) \leq \epsilon := \min(\epsilon_0, \epsilon_1) \). Then for every \((x, y) \in S\), \( \ell(z^g(x), y) \leq \epsilon \). From (b) and (c), \( e^{-1} < \frac{1}{2} \sum_{j \neq y} e^{z_j} < e^{z_y} \), hence \( z_y > -1 \). Combining with (d), it follows that \(-1 < z_y < 1 \). Combined with (a), it follows that for \( j \neq y \), \( z_j < -1 \). To summarize, we have shown that for every \((x, y), (x', y') \in S\), if \( y \neq y' \) then \( z^g_\theta(x) > -1 > z^g_\theta(x') \), implying Eq. (1).

### 4.2 Noise Contrastive Estimation

Noise Contrastive Estimation (NCE) ([Gutmann and Hyvärinen, 2010; Mnih and Teh, 2012]) was considered, like self-normalization, in the context of natural language learning. This approach was developed to speed up neural-language model training over large vocabularies. In NCE, the multiclass classification problem is treated as a set of binary classification problems, one for each class. Each binary problem classifies, given a context and a word, whether this word is from the data distribution or from a noise distribution. Using only \( t \) words from the noise distribution instead of the entire vocabulary leads to a significant speedup at training-time. Similarly to the self-normalization objective, NCE, in the version appearing in [Mnih and Teh, 2012], is known to produce a self-normalized logit vector ([Andreas and Klein, 2015]). This property makes NCE a good candidate for the SLC task.

The loss function used in NCE for a single training example, as given by [Mnih and Teh, 2012], is defined based on a distribution over the possible classes, denoted by \( \mathbf{q} = (q(1), \ldots, q(k)) \), where \( \sum_{i=1}^{k} q(i) = 1 \). The NCE loss, in our notation, is

\[
\ell(z, y) = - \log g_j - t \cdot \mathbb{E}_{j \sim q}[\log(1 - g_j)], \quad \text{where } g_j := (1 + t \cdot q(j) \cdot e^{-z_j})^{-1} \tag{4}
\]

and \( t \) is an integer hyperparameter. During training, the second term in the loss is usually approximated by Monte-Carlo approximation, using \( t \) random samples of \( j \sim q \), to speed up training time ([Mnih and Teh, 2012]).

We show that the NCE loss satisfies the PoLS. The proof relies on the observation that \( g_j \) is monotonic increasing in \( z_j \). Therefore, if the loss is small, \( g_y \) must be large and \( g_j \), for \( j \neq y \), must be small. Formally, fix \( t \), and assume a training sample \( S \). There exists an \( \epsilon_0 > 0 \) such that if \(- \log g_j \leq \epsilon_0 \), then \( z_j > 0 \). In addition, there exists an \( \epsilon_1 > 0 \) (which depends on \( q \)) such that if \(- \mathbb{E}_{j \sim q}[\log(1 - g_j)] \leq \epsilon_1 \) then for all \( j \neq y \), \( \log(1 - g_j) \) must be small enough so that \( z_j < 0 \). Now, consider \( \theta \) such that \( \ell(S_\theta) \leq \epsilon := \min(\epsilon_0, \epsilon_1) \). Then for every \((x, y) \in S\), \( \ell(z^g_\theta(x), y) \leq \epsilon \). This implies that for every \((x, y), (x', y') \in S\) such that \( y' \neq y \), \( z^g_\theta(x) > 0 > z^g_\theta(x') \), thus Eq. (1) holds.

### 4.3 Binary cross-entropy

The last known loss that we consider is often used in multilabel classification settings. In multilabel settings, each example can belong to several classes, and the goal is to identify the set of classes relevant to each example. A common approach ([Wang et al., 2016; Huang et al., 2013]) is to try to solve \( k \) binary classification problems of the form “Does \( x \) belong to class \( j \)?” using a single neural network model, by minimizing the sum of the cross-entropy losses that correspond to these binary problems.

In this setting, the label of each example is a binary vector \((r_1, \ldots, r_k)\), where \( r_j = 1 \) if \( x \) belongs to class \( j \) and 0 otherwise. The loss for a single training example with logits \( z \) and label-vector \( r \) is

\[
\ell(z, (r_1, \ldots, r_k)) = - \sum_{j=1}^{k} r_j \log(\sigma(z_j)) + (1 - r_j) \log(1 - \sigma(z_j)),
\]
When training using Stochastic Gradient Descent, the gradient computation and parameter updates are usually calculated for a single batch at a time. We train our batch losses using the same procedure, so that the gradient of \( L \) for a single batch \( B \) is calculated and applied in each iteration.

Below we define two batch-losses which satisfy the PoLS, generalizing the cross-entropy loss and the max-margin loss. For each case, we define \( L \) and show that it satisfies the PoLS.

**Batch cross-entropy.** Our first batch-loss generalizes the cross-entropy loss, which was defined in Eq. (2). The cross-entropy loss can be given as the Kullback–Leibler (KL) divergence between two distributions, as follows. The KL divergence between two discrete probability distributions \( P \) and \( Q \) over \([k]\) is defined as

\[
\text{KL}(P||Q) := \sum_{j=1}^{k} P(j) \log(P(j)/Q(j)).
\]

For an example \((x, y)\), let \( P_{(x,y)} \) be the distribution over \([k]\) which deterministically outputs \( y \), and let \( Q^y_j \) be the distribution defined by the softmax normalized logits, 

\[
Q^y_j = \frac{e^{\theta_j}}{\sum_{i=1}^{k} e^{\theta_i}}.
\]

Then it is easy to see that for \( p_y \) as defined in Eq. (2), \( \text{KL}(P_{(x,y)}||Q^y_j) = -\log p_y \), exactly the cross-entropy loss in Eq. (2). We define a batch version of this loss, using the KL-divergence between distributions over batches. Recall that the \( i \)’th example in a batch \( B \) is denoted \((x'_i, y'_i)\). Let \( P_B \) be the distribution over \([m] \times [k]\) defined by

\[
P_B(i,j) := \begin{cases} \frac{1}{m} & j = y'_i, \\ 0 & \text{otherwise}. \end{cases}
\]

5 New training objectives for the SLC task

In this section we propose new training objectives for the SLC task, designed to satisfy the PoLS. These objectives adapt the training objectives from Section 3, that do not satisfy the PoLS, by generalizing them to optimize over *batches* of training samples. We show that the revised losses satisfy the PoLS. This approach requires no new hyper-parameters, since the batch size is already a hyper-parameter in standard Stochastic Gradient Descent [Robbins and Monro, 1951]. Further, this allows an easy adaptation of available neural network implementations to the SLC task.

Our general approach is to define a loss over batches of examples, and then minimize its expectation over uniformly random batches. Let \( m > 1 \) be an integer representing the batch size, and let \( B \subseteq S \) be a batch of examples of size \( m \). Denote \( B = ((x'_1, y'_1), \ldots, (x'_m, y'_m)) \). And let \( B_\theta = ((z^0(x'_1), y'_1), \ldots, (z^0(x'_m), y'_m)) \). We define a loss function for batches, denoted \( L(B_\theta) \), and set

\[
\ell(S_\theta) = \mathbb{E}_B[L(B_\theta)],
\]

where \( B \) is a uniformly random batch of size \( m \) from \( S \). The loss \( L \) is designed so as to enforce the PoLS within the batch. When true logits are greater than false logits in every batch separately, the PoLS is satisfied on the whole sample, since every pair of examples appears together in some batch. The following lemma formalizes this claim:

**Lemma 5.1.** If \( \ell \) is defined as in Eq. (5), and \( L \) satisfies the PoLS, then \( \ell \) also satisfies the PoLS.

**Proof.** Assume a training sample \( S \) and a neural network model \( \theta \). Since \( L \) satisfies Eq. (1), there is some \( \epsilon' > 0 \) such that if \( L(B_\theta) < \epsilon' \), then for each \((x, y), (x', y') \in B\), if \( y \neq y' \), then \( z^0_{y}(x) > z^0_{y'}(x') \). Let \( \epsilon = \epsilon' / \binom{m}{2} \), and assume \( \ell(S_\theta) < \epsilon \). Since there are \( \binom{m}{2} \) batches of size \( m \) in \( S \), this implies that for every batch \( B \) of size \( m \), \( L(B_\theta) \leq \epsilon' \). For any \((x, y), (x', y') \in S\), there is a batch \( B \) which includes both examples. Therefore, if \( y \neq y' \), \( z^0_{y}(x) > z^0_{y'}(x') \). Since this holds for any pair of examples in \( S \), Eq. (1) holds for \( \ell \), thus proving that it satisfies the PoLS. \( \square \)

When training using Stochastic Gradient Descent, the gradient computation and parameter updates are usually calculated for a single batch at a time. We train our batch losses using the same procedure, so that the gradient of \( L(B_\theta) \) for a single batch \( B \) is calculated and applied in each iteration.

Below we define two batch-losses which satisfy the PoLS, generalizing the cross-entropy loss and the max-margin loss. For each case, we define \( L \) and show that it satisfies the PoLS.
Let $Q^\theta_B$ be the distribution defined by the soft-max normalized logits over the entire batch $B$. Formally, denote $Z(B) := \sum_{i=1}^m \sum_{j=1}^k e^{\theta^i_j(x^i_j)}$. Then $Q^\theta_B(i, j) := e^{\theta^i_j(x^i_j)}/Z(B)$.

Definition 5.2 (The batch cross-entropy loss). Let $m > 1$ be an integer, and let $B$ be a uniformly random batch of size $m$ from $S$. The batch cross-entropy loss of a training sample $S$ with model $\theta$ is

\[
\ell(S_B) := E_B[L(B_\theta)], \quad \text{where} \quad L(B_\theta) := KL(P_B || Q^\theta_B)].
\]

To show that the batch cross-entropy satisfies the PoLS, we show that $L$ does, which by Lemma 5.1 implies this for $\ell$. By the continuity of $KL$, and since for discrete distributions, $KL(P || Q) = 0 \iff P \equiv Q$, there is an $\epsilon > 0$ such that if $L(B_\theta) = KL(P_B || Q^\theta_B]) < \epsilon$, then for all $i, j$, $|P_B(i, j) - Q^\theta_B(i, j)| \leq \frac{1}{\epsilon_m}$. Therefore, for each example $(x, y) \in B$,

\[
e^{\theta^i_j(x^i_j)}/Z(B) > \frac{1}{2m}, \quad \text{and} \quad \forall j \neq y, \quad e^{\theta^i_j(x^i_j)}/Z(B) < \frac{1}{2m}.
\]

It follows that for any two examples $(x, y), (x', y') \in B$, if $y \neq y'$, then $z^\theta_+(x) > z^\theta_+(x')$. Therefore $L$ satisfies the PoLS, which completes the proof.

**Batch max-margin.** Our second objective is a batch version of the max-margin loss, which was defined in Eq. (3). For a batch $B$ and a model $\theta$, denote the minimal true logit in $B_\theta$, and the maximal false logit in $B_\theta$, as follows:

\[
z^B_+ := \min_{(x, y) \in B} z^\theta_+(x), \quad \text{and} \quad z^B_- := \max_{(x, y) \in B \neq y} z^\theta_+(x).
\]

Definition 5.3 (The batch max-margin loss). Let $m > 1$ be an integer, and let $B$ be a uniformly random batch of size $m$ from $S$. Let $\ell$ be the single-example max-margin loss defined in Eq. (3), let $\gamma > 0$ be the max-margin hyper-parameter. The batch max-margin is defined by

\[
\ell(S_B) := E_B[L(B_\theta)], \quad \text{where} \quad L(B_\theta) := \frac{1}{m} \max(0, \gamma - z^B_+ + z^B_-) + \frac{1}{m} \sum_{(x, y) \in B} \ell(z^\theta_+(x), y).
\]

To show that the batch max-margin loss satisfies the PoLS, we show this for $L$ and invoke Lemma 5.1. Set $\epsilon = \gamma/m$. If $L(B_\theta) < \epsilon$, then $\gamma - z^B_+ + z^B_- < \epsilon$, implying $z^B_+ > z^B_-$. Hence, any $(x, y), (x', y') \in B$ such that $y \neq y'$ satisfy $z^\theta_+(x) \geq z^B_+ > z^B_- \geq z^\theta_+(x')$. Thus Eq. (1) holds for $L$, implying the PoLS for $\ell$. Note: The second term in $L(B_\theta)$ is not required for the PoLS; we add it to make training effective, since the gradients of the first term are zero for most batch examples.

6 Experiments

We compared the performance of neural networks trained with each of the objectives studied above, on the SLC task and on multiclass classification. To evaluate a learned model on the SLC task, for each class $j$ and a threshold $T$, we measured the precision and recall in identifying examples from class $j$ using the test $z_j > T$, and calculated the Area Under the Precision-Recall curve (AUPRC) defined by the entire range of possible thresholds. We also measured the precision at fixed recall values 0.9 (Precision@0.9) and 0.99 (Precision@0.99). We report the averages of these values over all the classes in the dataset. We further report the multiclass accuracy (Acc.) of each model.

We evaluated the methods on five computer-vision classification benchmark datasets: MNIST (LeCun et al. 1998), SVHN (Netzer et al. 2011), CIFAR-10 and CIFAR-100 (Krizhevsky and Hinton 2009). The last dataset is ImageNet (Russakovsky et al. 2015), which has 1000 classes, demonstrating the scalability of the PoLS approach to many classes. Due to its size, training on ImageNet is highly computationally intensive, therefore we evaluated its performance using two representative methods, which do not require tuning additional hyperparameters. We report the results obtained for this dataset after $2 \cdot 10^6$ iterations. For every dataset, a single network architecture was used for all training objectives.

For the MNIST dataset, we used an MLP comprised of two fully-connected layers with 500 units each, and the output layer (its values are the logits) with 10 units. For other datasets, we used a
<table>
<thead>
<tr>
<th>Dataset</th>
<th>Method</th>
<th>1-AUPRC</th>
<th>1-Precision@0.9</th>
<th>1-Precision@0.99</th>
<th>1-Acc.</th>
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<td>0.978</td>
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<tr>
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<td>0.739</td>
<td>0.932</td>
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<td><strong>0.865</strong></td>
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<td>0.566</td>
<td>0.872</td>
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</table>

Table 1: Results of experiments, see details in Section 6.

convolutional neural network ([LeCun et al., 1989]) with six convolutional layers and one dense layer with 1024 units. The first, third and fifth convolutional layers utilized a 5 × 5 kernel, where other convolutional layers utilized a 1 × 1 kernel. The first two convolutional layers were comprised of 128 feature maps, where convolutional layers three and four had 256 feature maps, and convolutional layers five and six had 512 feature maps. Max-pooling layers with 3 × 3 kernel size and a 2 × 2 stride were applied after the second, fourth and sixth convolutional layers. In all networks, batch normalization ([Ioffe and Szegedy, 2015]) was applied to the output of every fully-connected or convolutional layer, followed by a rectified-linear non-linearity. For every combination of a training objective and a dataset (with its fixed network architecture), we optimized for the best learning rate among 1, 0.1, 0.01, 0.001 using the classification accuracy on a validation set. Except for Imagenet, each model was trained for 10⁶ steps, which was always enough to reach a convergence state. For the Imagenet experiments, we use an inception-v3 architecture ([Szegedy et al., 2016]) as appears in the tensorflow ([Abadi et al., 2015]) repository. We used all the default hyperparameters from this
implementation, changing only the loss function used. For every tested loss function, we trained the model for $2 \cdot 10^6$ iterations.

Experiment results are reported in Table 1. Since many of the measures in our experiments are close to the maximal value of 1, we report the value of one minus each measure, so that a smaller number indicates a better accuracy. For each dataset, the losses above the dashed line do not satisfy the PoLS (Section 3), while the losses below the line do (Sections 4 and 5). Finally, the bottom row in each dataset stands for the normalized Cross-Entropy: here we used the output logits of the cross-entropy loss after normalization, a method which requires computing all the logits, unlike the other methods we consider. We compare to this method, since it is probably the default approach one would take if the standard cross-entropy loss is used. We mark in boldface the best result for each dataset and measure, out of all the losses excluding the normalized CE.

The results lead to several observations:

1. All training objectives that satisfy the PoLS obtain a considerably superior performance on the SLC task, compared to the training objectives that do not satisfy the PoLS.
2. Despite its advantageous computational resources, the default approach of normalized cross-entropy is at best comparable with the other methods that satisfy the PoLS, although they require only a single logit computation per test example.
3. The objectives that satisfy the PoLS usually also have a better classification accuracy.

We conclude from these experiments that indeed, the PoLS presents itself as a good measurement stick for the suitability of objectives to the SLC task. Further, it can be seen that the SLC task can be achieved, while keeping the accuracy on the multiclass classification task the same or higher.

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References


