Neural Network Classifier as Mutual Information Evaluator

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Abstract
Cross-entropy loss with softmax output is a standard choice to train neural network classifiers. We give a new view of neural network classifiers with softmax and cross-entropy as mutual information evaluators. We show that when the dataset is balanced, training a neural network with cross-entropy maximises the mutual information between inputs and labels through a variational form of mutual information. Thereby, we develop a new form of softmax that also converts a classifier to a mutual information evaluator when the dataset is imbalanced. Experimental results show that the new form leads to better classification accuracy, in particular for imbalanced datasets.

1. Introduction
Neural network classifiers play an important role in contemporary machine learning and computer vision (LeCun et al., 2015). Although many architectural choices and optimisation methods have been explored, relatively fewer considerations have been shown on the final layer of the classifier: the cross-entropy loss with the softmax output.

The combination of softmax with cross-entropy is a standard choice to train neural network classifiers. It measures the cross-entropy between the ground truth label $y$ and the output of the neural network $\hat{y}$. The network’s parameters are then adjusted to reduce the cross-entropy via backpropagation. While it seems sensible to reduce the cross-entropy between the labels and predicted probabilities, it still remains a question as to what relation the network aims to model between input $x$ and label $y$ via this loss function, i.e., softmax with cross-entropy.

In this work, for neural network classifiers, we explore the connection between cross-entropy with softmax and mutual information between inputs and labels. From a variational form of mutual information, we prove that optimising model parameters using the softmax with cross-entropy is equal to maximising the mutual information between input data and labels when the distribution over labels is uniform. This connection provides an alternative view on neural network classifiers: they are mutual information estimators. We further propose a probability-corrected version of softmax that relaxes the uniform distribution condition. We empirically demonstrate that our mutual information estimators can accurately evaluate mutual information. We also show mutual information estimators can perform classification more accurately than traditional neural network classifiers. When the dataset is imbalanced, the estimators outperform the state-of-the-art classifier for our example.

2. Preliminaries
In this section, we first define the notations used throughout this paper. We then introduce the definition of mutual information and variational forms of mutual information.

2.1. Notation
We let training data consist of $M$ classes and $N$ labelled instances as $\{(x_i, y_i)\}_{i=1}^N$, where $y_i \in Y = \{1, ..., M\}$ is a class label of input $x_i$. We let $n_\phi(x) : \mathcal{X} \to \mathbb{R}_+^M$ be a neural network parameterised by $\phi$, where $\mathcal{X}$ is a space of input $x$. We assume $\mathcal{X}$ to be a compact subset of $D$-dimensional Euclidean space. We denote by $P_{XY}$ some joint distribution over $\mathcal{X} \times \mathcal{Y}$, with $(X, Y) \sim P_{XY}$ being a pair of random variables. $P_X$ and $P_Y$ are the marginal distributions of $X$ and $Y$, respectively. We remove a subscript from the distribution if it is clear from context.

2.2. Variational Bounds of Mutual Information
Mutual information evaluates the mutual dependence between two random variables. The mutual information between $X$ and $Y$ can be expressed as:

$$I(X, Y) = \int_{x \in \mathcal{X}} \left[ \sum_{y \in \mathcal{Y}} P(x, y) \log \left( \frac{P(x, y)}{P(x)P(y)} \right) \right] dx.$$  (1)

Equivalently, following (Poole et al., 2019), we may ex-
press the definition of mutual information in Equation 2.2 as:
\[
\mathbb{I}(X, Y) = \mathbb{E}_{(X,Y)} \left[ \log \frac{P(y|x)}{P(y)} \right],
\]
where \(\mathbb{E}_{(X,Y)}\) is the abbreviations of \(\mathbb{E}_{(X,Y) \sim P_{X,Y}}\). Computing mutual information directly from the definition is, in general, intractable due to integration.

**Variational form:** Barber and Agakov introduce a commonly used lower bound of mutual information via a variational distribution \(Q\) (Barber & Agakov, 2003), derived as the following form:
\[
\mathbb{I}(X, Y) = \mathbb{E}_{(X,Y)} \left[ \log \frac{P(y|x)}{P(y)} \right] = \mathbb{E}_{(X,Y)} \left[ \log \frac{Q(y|x)}{P(y)} + \log \frac{P(y|x)}{Q(y|x)} \right] + \mathbb{E}_{(X,Y)} \left[ \log \frac{P(x,y)}{Q(x,y)} \right] - \mathbb{E}_{(X)} \left[ \log \frac{P(x)}{Q(x)} \right] \geq \mathbb{E}_{(X,Y)} \left[ \log \frac{Q(y|x)}{P(y)} \right]. \tag{3}
\]

The inequality in Equation 3 holds since KL divergence maintains non-negativity. This lower bound is tight when variational distribution \(Q(x, y)\) converges to joint distribution \(P(x, y)\), i.e., \(Q(x, y) = P(x, y)\).

The form in Equation 3 is, however, still hard to compute since it is not easy to make a tractable and flexible variational distribution \(Q(x, y)\). Variational distribution \(Q(x, y)\) can be considered as a constrained function which has to satisfy the probability axioms. Especially, the constraint is challenging to model with a function estimator such as a neural network. To relax the function constraint, McAllester et al. (McAllester & Statos, 2018) further apply reparameterisation and define \(Q(x, y)\) in terms of an unconstrained function \(f_\phi\) parameterised by \(\phi\) as:
\[
Q(x, y) = \frac{P(x)P(y)}{E_{y' \sim P_{Y}}[\exp(f_\phi(x, y'))]} \exp(f_\phi(x, y)). \tag{4}
\]

As a consequence, the variational lower bound of mutual information \(\mathbb{I}(X, Y)\) can be rewritten with function \(f_\phi\) as:
\[
\mathbb{I}(X, Y) \geq \mathbb{E}_{(X,Y)} \left[ \log \frac{\exp(f_\phi(x, y))}{E_{y' \sim P_{Y}}[\exp(f_\phi(x, y'))]} \right]. \tag{5}
\]

Thus, one can estimate mutual information without any constraint on \(f\). Through the reparameterisation, the MI estimation can be recast as an optimisation problem.

### 3. NN Classifiers as MI Estimators

In this section, we prove that a neural network classifier with cross entropy loss and softmax output estimates the mutual information between inputs and labels. To view neural network classifiers as mutual information estimators, we need to discuss two separate cases related to the dataset: whether it is balanced or imbalanced.

#### 3.1. Softmax with Balanced Dataset

Softmax is widely used to map outputs of neural networks into a categorical probabilistic distribution for classification. Given neural network \(n(x) : \mathcal{X} \rightarrow \mathbb{R}^M\), softmax \(\sigma : \mathbb{R}^M \rightarrow \mathbb{R}^M\) is defined as:
\[
\sigma(n(x))_y = \frac{\exp(n(x)_y)}{\sum_{y'=1}^M \exp(n(x)_{y'})}, \tag{6}
\]

Expected cross-entropy is often employed to train a neural network with softmax output. The expected cross-entropy loss is
\[
L = -\mathbb{E}_{(X,Y)}[n(x)_y \log(\sum_{y'=1}^M \exp(n(x)_{y'}))], \tag{7}
\]

where the expectation is taken over the joint distribution of \(X\) and \(Y\). Given a training set, one can train the model with an empirical distribution of the joint distribution. We present an interesting connection between cross-entropy with softmax and mutual information in the following theorem. In a bid for conciseness, we only provide proof sketches for **Theorem 1** and **Theorem 2** here. Please refer to the appendix for rigorous proofs.

**Theorem 1.** Let \(f_\phi(x, y) = n(x)_y\). Infimum of the expected cross-entropy loss with softmax outputs is equivalent to the mutual information between input and output variables up to constant \(\log M\) under uniform label distribution.

*Proof. See Appendix.*

Note that the constant does not change the gradient of the objective. Consequently, the solutions of both the mutual information maximisation and the softmax cross-entropy minimisation optimisation problems are the same.

#### 3.2. Softmax with Imbalanced Dataset

The uniform label distribution assumption in **Theorem 1** is restrictive since we cannot access the true label distribution, often assumed to be non-uniform. To relax the restriction, we propose a probability-corrected softmax (PC-softmax):
\[
\sigma_p(n(x))_y = \frac{\exp(n(x)_y)}{\sum_{y'=1}^M \exp(n(x)_{y'})}, \tag{8}
\]

The form in Equation 3 is, however, still hard to compute since it is not easy to make a tractable and flexible variational distribution \(Q(x, y)\). Variational distribution \(Q(x, y)\) can be considered as a constrained function which has to satisfy the probability axioms. Especially, the constraint is challenging to model with a function estimator such as a neural network. To relax the function constraint, McAllester et al. (McAllester & Statos, 2018) further apply reparameterisation and define \(Q(x, y)\) in terms of an unconstrained function \(f_\phi\) parameterised by \(\phi\) as:
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\[
\mathbb{I}(X, Y) \geq \mathbb{E}_{(X,Y)} \left[ \log \frac{\exp(f_\phi(x, y))}{E_{y' \sim P_{Y}}[\exp(f_\phi(x, y'))]} \right]. \tag{5}
\]

Thus, one can estimate mutual information without any constraint on \(f\). Through the reparameterisation, the MI estimation can be recast as an optimisation problem.
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| \( y \) | \( \mu \) | # samples | \( p(y) \) |
|---|---|---|---|
| 0 | 0 | 6,000 | 0.07 |
| 1 | +2 | 12,000 | 0.13 |
| 2 | −2 | 18,000 | 0.20 |
| 3 | +4 | 24,000 | 0.27 |
| 4 | −4 | 30,000 | 0.33 |

Table 1. Synthetic dataset description. \( \mu \) is a mean vector for each Gaussian distribution. # samples denotes the number (resp. prior distribution) of samples with the non-uniform prior assumption. For the test with the uniform prior assumption, we use 12,000 samples from each distribution.

4. Impact of PC-softmax on Classification

In this section, we measure the empirical performance of PC-softmax as mutual information (MI) and the influence of PC-softmax on the classification task. Since it is impossible to obtain correct MI from real-world datasets, we first construct synthetic data with known properties to measure the MI estimation performance, and then we use two real-world datasets to measure the impact of PC-softmax on classification tasks.

4.1. Mutual information estimation task

To construct a synthetic dataset with a pair of continuous and discrete variables, we employ a Gaussian mixture model:

\[
P(x) = \sum_{y=1}^{M} P(y)N(x|\mu_y, \Sigma_y)
\]

\[
P(x|y) = N(x|\mu_y, \Sigma_y),
\]

where \( P(y) \) is a prior distribution over the labels. To form classification, we use \( x \) as an input variable, and \( y \) as a label.

For the experiments, we use five mixtures of isotropic Gaussian, each of which has a unit diagonal covariance matrix with different means. We set the parameters of the mixtures to make them overlap in significant proportions.

We generate two sets of datasets: one with uniform prior and the other with non-uniform prior distribution over labels, \( p(y) \). For the uniform prior, we sample 12,000 data points from each Gaussian, and for the non-uniform prior, we sample unequal number of data points from each Gaussian. In addition, we vary the dimension of Gaussian distribution from 1 to 10. The detailed statistics for the Gaussian parameters and the number of samples are available in Table 1. To train classification models, we divide the dataset into training, validation and test sets. We use the validation set to find the best parameter configuration of the classifier.

We aim to compare the difference of true and softmax-based estimated mutual information \( I(X, Y) \). The mutual information is, however, intractable. We thus approximate it via Monte Carlo (MC) methods using the true probability density function, expressed as:

\[
I(X, Y) \approx \frac{1}{N} \sum_{i=1}^{N} \log \left( \frac{P(x_i|y_i)}{P(x_i)} \right),
\]

where \( (x_i, y_i) \) forms a paired sample. Equation 9 attains equality as \( N \) approaches infinity.

We use four layers of a feed-forward neural network with the ReLU as an activation for internal layers and soft-
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max as an output layer. We train the model with softmax on balanced dataset and with PC-softmax on unbalanced dataset. We compare the experimental results against mutual information neural estimator (MINE) proposed in (Belghazi et al., 2018). Note that MINE requires having a pair of input and label variables as an input of an estimator network, the classification-based MI-estimator seems more straightforward for measuring mutual information between inputs and labels of classification tasks.

Table 2a summarises the experimental results with the balanced dataset. With the balanced dataset, there is no difference between softmax and PC-softmax. Note that the MC estimator has access to explicit model parameters for estimating mutual information, whereas the softmax estimator measures mutual information based on the model outputs without accessing the true distribution. We could not find a significant difference between MC and the softmax estimator. Additionally, we report the accuracy of the trained model on the classification task.

Table 2b summarises the experimental results with the unbalanced dataset. The results show that the PC-softmax slightly under-estimates mutual information when compared with the other two approaches. It is worth noting that the classification accuracy of PC-softmax consistently outperforms the original softmax. The results show that the MINE slightly under-estimates the MI as the input dimension increases.

4.2. Classification task

We test the classification performance of softmax and PC-softmax with two real-world datasets: MNIST (LeCun et al., 2010) and CUB-200-2011 (Wah et al., 2011).

We construct balanced and unbalanced versions of the MNIST dataset. For the balanced-MNIST, we use a subset of the original dataset. For the unbalanced-MNIST, we randomly subsample one tenth of instances for digits 0, 2, 4, 6 and 8 from the balanced-MNIST. With CUB-200-2011, we follow the same training and validation splits as in (Cui et al., 2018). As a result of such splitting, the training set is approximately balanced, where out of the total 200 classes, 196 of them contain 30 instances and the remaining 6 classes include 29 instances. To construct an unbalanced dataset, similar to MNIST, we randomly drop one half of the instances from one half of the bird classes.

We adopt a simple convolutional neural network as a classifier for MNIST. The model contains two convolutional layers with max pooling layer and the ReLU activation, followed by two fully connected layers with the final softmax. For CUB-200-2011, we apply the same architecture as Inception-V3 (Cui et al., 2018). We measure both the micro accuracy and the average per-class accuracy of the two softmax versions on both datasets. The average per-class accuracy alleviates the dominance of the majority classes in unbalanced datasets. The classification results are shown in Table 3. PC-softmax is significantly more accurate on unbalanced datasets for the average per-class accuracy.

5. Conclusion

We have shown the connection between mutual information estimators and neural network classifiers through the variational form of mutual information. The connection explains the rationale behind the use of sigmoid, softmax and cross-entropy from an information-theoretic perspective. There is previous work that called the negative log-likelihood (NLL) loss as maximum mutual information estimation (Bahl et al., 1986). Despite this naming similarity, that work does not show the relationship between softmax and mutual information that we have shown here. The connection between neural network classifiers and mutual information evaluators provides more than an alternative view on neural network classifiers. Thereby, we improve the classification accuracy, in particular when the datasets are unbalanced. The new mutual information estimators even outperform the prior state-of-the-art neural network classifiers.

| Dataset | MNIST | CUB-200-2011 |
|---------|-------|-------------|
|         | Balanced | Unbalanced | Balanced | Unbalanced |
| softmax | 97.95 | 96.81 | 89.23 | 89.21 |
| PC-softmax | 97.91 | 96.86 | 89.18 | 89.73* |

(a) Classification accuracy (%).

| Dataset | MNIST | CUB-200-2011 |
|---------|-------|-------------|
|         | Balanced | Unbalanced | Balanced | Unbalanced |
| softmax | 97.95 | 95.05 | 89.21 | 84.63 |
| PC-softmax | 97.91 | 96.30 | 89.16 | 87.69 |

(b) Average per-class accuracy (%).

Table 3. Classification accuracy of using softmax and PC-softmax. Numbers of instances for different labels are the same for a balanced dataset and are significantly distinct for an unbalanced dataset. Bold values denote p-values less than 0.05 with the Mann-Whitney U statistical test.²
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A. Proofs

In this section, we provide rigorous proofs of Theorem 1 and Theorem 2. The structure of proof is similar to the proof used in (Belghazi et al., 2018). We assume the input space $\Omega = X \times Y$ being a compact domain of $\mathbb{R}^d$, where all measures are Lebesgue and are absolutely continuous. We restrict neural networks to produce a single continuous output, denoted as $n(x)$. We restate the two theorems for quick reference.

**Theorem 1.** Let $f(x, y) = n(x)$. Minimising the cross-entropy loss of softmax-normalised neural network outputs is equivalent to maximising Equation 5, i.e., the lower bound of mutual information, under the uniform label distribution. That is, if the dataset is balanced, then training a neural network via minimising cross-entropy with softmax equals enhancing a estimator toward more accurately evaluating the mutual information between data and label.

**Theorem 2.** The mutual information between two random variable $X$ and $Y$ can be obtained via the infimum of cross-entropy with PC-softmax in Equation 8. Such an evaluation is strongly consistent.

The proof technique that we have used to prove Theorem 2 is similar to the one used in (Belghazi et al., 2018).

**Lemma 1.** Let $\eta > 0$. There exists a family of neural network functions $n_\phi$ with parameter $\phi$ in some compact domain such that

$$|\mathbb{I}(X; Y) - \mathbb{I}_\phi(X; Y)| \leq \eta,$$

where

$$\mathbb{I}_\phi(X; Y) = \sup_{\phi} \mathbb{E}_{(X, Y)}[n_\phi] - \mathbb{E}_X \log \mathbb{E}_Y[\exp(n_\phi)_y].$$

**Proof.** Let $n_\phi^*(X, Y) = \text{PMI}(X, Y) = \log \frac{P(X, Y)}{P(X)P(Y)}$. We then have:

$$\mathbb{E}_{(X, Y)}[n_\phi^*(X, Y)] = \mathbb{I}(X; Y) \quad \text{and} \quad \mathbb{E}_X \mathbb{E}_Y[\exp(n_\phi^*(X))_y] = 1.$$  

Then, for neural network $n_\phi$, the gap $\mathbb{I}(X; Y) - \mathbb{I}_\phi(X; Y)$:

$$\mathbb{I}(X; Y) - \mathbb{I}_\phi(X; Y) = \mathbb{E}_{(X, Y)}[n_\phi^*(X, Y) - n_\phi(X, Y)] + \mathbb{E}_X \log \mathbb{E}_Y[\exp(n_\phi)_y]$$

$$\leq \mathbb{E}_{(X, Y)}[n_\phi^*(X, Y) - n_\phi(X, Y)] + \mathbb{E}_X \mathbb{E}_Y[\exp(n_\phi)_y]$$

$$\leq \mathbb{E}_{(X, Y)}[n_\phi^*(X, Y) - n_\phi(X, Y)]$$

$$+ \mathbb{E}_X \mathbb{E}_Y[\exp(n_\phi)_y - \exp(n_\phi)_y].$$

**Equation 13** is positive since the mutual neural information estimator evaluates a lower bound. The equation uses Jensen’s inequality and the inequality $\log x \leq x - 1$.

We assume $\eta > 0$ and consider $n_\phi^*(x)_y$ is bounded by a positive constant $M$. Via the universal approximation theorem (Hornik et al., 1989), there exists $\eta_0(x)_y \leq M$ such that

$$\mathbb{E}_{(X, Y)}|n_\phi^*(X, Y) - n_\phi(X, Y)| \leq \frac{\eta}{2} \quad \text{and} \quad \mathbb{E}_X \mathbb{E}_Y|n_\phi(x)_y - n_\phi^*(x)_y| \leq \frac{\eta}{2} \exp(-M).$$

By utilising that $\exp$ is Lipschitz continuous with constant $\exp(M)$ over $(-\infty, M]$, we have

$$\mathbb{E}_X \mathbb{E}_Y|\exp(n_\phi(x)_y) - \exp(n_\phi^*(x)_y)| \leq \exp(M) \cdot \mathbb{E}_X \mathbb{E}_Y|n_\phi(x)_y - n_\phi^*(x)_y| \leq \frac{\eta}{2}.$$  

**Equation 15**

Combining **Equation 13**, **Equation 14** and **Equation 15**, we then obtain

$$|\mathbb{I}(X; Y) - \mathbb{I}_\phi(X; Y)| \leq \mathbb{E}_{(X, Y)}|n_\phi^*(X, Y) - n_\phi(X, Y)|$$

$$+ \mathbb{E}_X \mathbb{E}_Y|\exp(n_\phi(x)_y) - \exp(n_\phi^*(x)_y)|$$

$$= \frac{\eta}{2} + \frac{\eta}{2} = \eta.$$  

$\square$
Lemma 2. Let $\eta > 0$. Given a family of neural networks $n_\phi$ with parameter $\phi$ in some compact domain, there exists $N \in \mathbb{N}$ such that

$$\forall n \geq N, \Pr(\hat{I}_n(X;Y) - n_\phi(X;Y) \leq \eta) = 1.$$  \hspace{1cm} (17)

Proof. We start by employing the triangular inequality:

$$\hat{I}_n(X;Y) - I_\phi(X;Y) \leq \sup \phi |E_{(X,Y)}[n_\phi^*(X,Y)] - E_{(X,Y)}[n_\phi^*(X,Y)]|$$

$$+ \sup \phi |E_X \log E_Y[\exp(n_\phi(y))] - E_X \log E_Y[\exp(n_\phi(y))]|$$  \hspace{1cm} (18)

We have stated previously that neural network $n_\phi$ is bounded by $M$, i.e., $n_\phi(x) \leq M$. Using the fact that $\log$ is Lipschitz continuous with constant $\exp(M)$ over the interval $[\exp(-M), \exp(M)]$, we have

$$|\log E_Y[\exp(n_\phi(y))] - \log E_{Y_n}[\exp(n_\phi(y))]| \leq \exp(M) \cdot |E_Y[\exp(n_\phi(y))] - E_{Y_n}[\exp(n_\phi(y))]|$$  \hspace{1cm} (19)

Using the uniform law of large numbers (Geer & van de Geer, 2000), we can choose $N \in \mathbb{N}$ such that for $\forall n \geq N$ and with probability one

$$\sup \phi |E_Y[\exp(n_\phi(y))] - E_{Y_n}[\exp(n_\phi(y))]| \leq \frac{\eta}{4}\exp(-M).$$  \hspace{1cm} (20)

That is,

$$|\log E_Y[\exp(n_\phi(y))] - \log E_{Y_n}[\exp(n_\phi(y))]| \leq \frac{\eta}{4}$$  \hspace{1cm} (21)

Therefore, using the triangle inequality we can rewrite Equation 18 as:

$$\hat{I}_n(X;Y) - I_\phi(X;Y) \leq \sup \phi |E_{(X,Y)}[n_\phi^*(X,Y)] - E_{(X,Y)}[n_\phi^*(X,Y)]|$$

$$+ \sup \phi |E_X \log E_Y[\exp(n_\phi(y))] - E_X \log E_Y[\exp(n_\phi(y))]| + \frac{\eta}{4}.$$  \hspace{1cm} (22)

Using the uniform law of large numbers again, we can choose $N \in \mathbb{N}$ such that for $\forall n \geq N$ and with probability one

$$\sup \phi |E_X \log E_Y[\exp(n_\phi(y))] - E_{X_n} \log E_Y[\exp(n_\phi(y))]| \leq \frac{\eta}{4}$$  \hspace{1cm} (23)

and:

$$\sup \phi |E_{(X,Y)}[n_\phi^*(X,Y)] - E_{(X,Y)}[n_\phi^*(X,Y)]| \leq \frac{\eta}{2}.$$  \hspace{1cm} (24)

Combining Equation 22, Equation 23 and Equation 24 leads to

$$\hat{I}_n(X;Y) - \sup \phi I_\phi(X;Y) \leq \frac{\eta}{2} + \frac{\eta}{4} + \frac{\eta}{4} = \eta.$$  \hspace{1cm} (25)

Now, combining the above two lemmas, we prove that our mutual information evaluator is strongly consistent.

Proof. Using the triangular inequality, we have

$$|I(X;Y) - \hat{I}_n(X;Y)| \leq |I(X;Y) - I_\phi(X;Y)| + |\hat{I}_n(X;Y) - n_\phi(X;Y)| \leq \epsilon.$$  \hspace{1cm} (26)