Effectiveness of MPC-friendly Softmax Replacement

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Abstract

Softmax is widely used in deep learning to map some representation to a probability distribution. As it is based on exp/log functions that is relatively expensive in multi-party computation, Mohassel and Zhang (2017) proposed a simpler replacement based on ReLU to be used in secure computation. However, we could not reproduce the accuracy they reported for training on MNIST with three fully connected layers. Later works (e.g., Wagh et al., 2019 and 2021) used the softmax replacement not for computing the output probability distribution but for approximating the gradient in back-propagation. In this work, we analyze the two uses of the replacement and compare them to softmax, both in terms of accuracy and cost in multi-party computation. We found that the replacement only provides a significant speed-up for a one-layer network while it always reduces accuracy, sometimes significantly. Thus we conclude that its usefulness is limited and one should use the original softmax function instead.

Changelog: We fixed a bug in our software affecting the accuracy. The new figures support our conclusion more strongly.

1 Introduction

We use multi-class classification as a typical example where softmax is applied in deep learning. Consider recognizing hand-written digits, where the input is an image and the output is a class label from 0 to 9, signifying the digit it represents. Given the input, a deep neural network can learn a vector representation \( x = (x_0, \ldots, x_9) \in \mathbb{R}^{10} \), where a larger \( x_i \) means a higher likelihood of the input being the digit \( i \). In order to turn \( x \) into a probability distribution (and to define a learning process), the softmax function

\[
p_i := \frac{e^{x_i}}{\sum_j e^{x_j}}
\]

is commonly used. It is easy to check that \( p = (p_0, p_1, \ldots) \) defines a probability distribution. Indeed, by eq. (1), all entries of \( p \) are non-negative and sum up to one.

Usually, a loss function is minimized to implement learning. For a training sample, its loss, indicating the incorrectness of the model, is defined in terms of the output distribution \( p \) as well as the ground truth one-hot vector \( y = (y_0, y_1, \ldots) \) with \( y_i = 1 \) for the true class label \( i \) and \( y_i = 0 \) otherwise. The global loss is a sum of the per-sample losses. A commonly used loss function is the cross-entropy:

\[
\ell := -\sum_i y_i \cdot \log p_i = -\sum_i y_i \cdot \log \frac{e^{x_i}}{\sum_j e^{x_j}} = -\sum_i y_i \cdot x_i + \log \sum_j e^{x_j},
\]

which attains its minimum when \( p = y \). It is easy to see that a loss of zero indicates a perfect prediction. On the other hand, assigning a small probability to the ground truth can yield a large loss.
Finally, for the optimization process we take the partial derivative of the loss function in every coordinate, and then perform gradient descent. This indicates the “correction” on the output values needed for a better model. In our example, this is
\[
\nabla_i := \frac{\partial \ell}{\partial x_i} = \frac{\partial}{\partial x_i} \left( - \sum_k y_k \cdot x_k + \log \sum_j e^{x_j} \right) = -y_i + \frac{e^{x_i}}{\sum_j e^{x_j}} = - (y_i - p_i).
\]

For a good model, the loss reaches a local minimum and the partial derivatives are close to zero. Due to the derivatives of \( \exp \) and \( \log \), softmax appears again in the expression of the gradient of \( \ell \). This is not generally true for any map from real vectors to probability distributions as we will see below.

**Multi-Party Computation (MPC)** is a technology for collaborative computation without individual parties learning the input or intermediate data. As such, it has been proposed as a key tool for federated learning. However, the underlying mathematics only offer modular addition and multiplication as core operations. While it is possible to build non-linear computation using these, the relative cost compared to the core operations is much higher than with microprocessors. In particular for exponential computation, there is only recent literature \[AS19\] on how to do this compared to comparison and division \[CS10\], which are the only ingredients on the softmax replacement defined below.

### 2 A Softmax Replacement

Mohassel and Zhang \[MZ17\] suggested to replace softmax with
\[
\hat{p}_i := \begin{cases} 
\frac{\text{ReLU}(x_i)}{\sum_i \text{ReLU}(x_i)}, & \text{if } \sum_i \text{ReLU}(x_i) > 0 \\
1/L, & \text{otherwise}
\end{cases}
\]

where \( L = \dim(x) \) is the number of possible classes and \( \text{ReLU} \) \[GBB11\] is defined as follows:
\[
\text{ReLU}(x) := \begin{cases} 
x, & \text{if } x > 0 \\
0, & \text{otherwise}
\end{cases}
\]

It is easy to recognize the appeal of this function. The vector \( \hat{p} = (\hat{p}_0, \hat{p}_1, \cdots) \) in eq. (2) is clearly a probability distribution. Similar to eq. (1), it assigns the highest probability to the largest value of \( x \). Furthermore, piece-wise linear approximations are proven successful in other contexts such as logistic regression. Mohassel and Zhang have proposed to replace the sigmoid function by three-piece linear approximation, which has shown to closely match the accuracy without the replacement on several datasets \[MZ17\] \[HHL\+20\].

The back-propagation implied by using the softmax replacement as an output probability distribution has not been spelled out in previous work. Using the softmax replacement with cross-entropy loss results in the following (ignoring the special case when \( \text{ReLU}(x_i) = 0 \)):
\[
\hat{\ell} := - \sum_i y_i \cdot \log \hat{p}_i = - \sum_i y_i \cdot \log \frac{\text{ReLU}(x_i)}{\sum_j \text{ReLU}(x_j)}
\]
\[
= - \sum_i y_i \cdot \log \text{ReLU}(x_i) + \log \left( \sum_j \text{ReLU}(x_j) \right),
\]

where \( y_i \) denotes the ground truth as a one-hot vector. For back-propagation, we take the partial derivate:
\[
\frac{\partial \hat{\ell}}{\partial x_i} = -y_i \cdot \frac{[x_i > 0]}{x_i} + \frac{[x_i > 0]}{\sum_j \text{ReLU}(x_j)}
\]
\[
= - [x_i > 0] \cdot \left( y_i \frac{1}{x_i} - \frac{1}{\sum_j \text{ReLU}(x_j)} \right)
\]
\[
= - [x_i > 0] \cdot \left( y_i - \frac{\text{ReLU}(x_i)}{\sum_j \text{ReLU}(x_j)} \right),
\]
We found that it is not really necessary to treat small values of \( \hat{x} \). We implemented training for the MNIST dataset [LBBH98] in MP-SPDZ [Kel20] with one to three dense layers. All but the last layer consist of 128 ReLU units [GBB11]. We use fixed-point representation of fractional numbers, that is \( x \in \mathbb{R} \) is represented as \( \text{round}(x \cdot 2^{16}) \). For rounding

where \([\cdot]\) denotes the Iverson bracket (1 if the condition is true otherwise 0). The obvious issue is division by zero and numerical instability caused by the first term in the parentheses. We found that this can be fixed by defining the gradient flow

\[
\nabla_i := \begin{cases} 
0 & y_i = 0, \ x_i < \varepsilon \\
-1 & y_i = 1, \ x_i < \varepsilon \\
-\left(\frac{y_i - \sum_j \text{ReLU}(x_j)}{x_i}\right) & \text{otherwise}
\end{cases}
\]

for some \( \varepsilon \in (0, 1) \). The reason to use a non-zero \( \varepsilon \) is to limit the scale of the partial derivative. Using softmax, \( \nabla_i \) is guaranteed to be in \((-1, 1)\), and thus we aim to constrain \( \nabla_i \) in a similar range. If \( x_i \geq \varepsilon \),

\[
\left|\frac{y_i}{x_i} - \frac{1}{\sum_j \text{ReLU}(x_j)}\right| = \frac{1}{x_i} |y_i - \tilde{p}_i| \leq \frac{1}{x_i} \leq \frac{1}{\varepsilon},
\]

(3)

Therefore \( \nabla_i \in [-\frac{1}{\varepsilon}, \frac{1}{\varepsilon}] \). In our experiments, we simply fix \( \varepsilon = 0.1 \) and show that this suffices for convergence albeit with lower accuracy than softmax. Neither \( \ell \) nor \( \nabla_i \) is a continuous function with respect to \( x \). Therefore the learning process may suffer from instability.

Kaina et al. [KFYA18] have suggested to mitigate the instability using the following probability distribution:

\[
\tilde{p}_i := \frac{\text{ReLU}(x_i) + \varepsilon}{\sum_j (\text{ReLU}(x_j) + \varepsilon)}
\]

for \( \varepsilon = 10^{-8} \). Computing the gradient as above, we get

\[
\frac{\partial \ell}{\partial x_i} = -\left[ x_i > 0 \right] \cdot \left( y_i - \frac{\text{ReLU}(x_i) + \varepsilon}{\sum_j (\text{ReLU}(x_j) + \varepsilon)} \right),
\]

whose absolute value is bounded by \( 1/(x_i + \varepsilon) \). This is similar to our implementation \( \nabla_i \). Both have bounded gradient.

**Replacing softmax directly in the back-propagation.** Following Mohassel and Zhang’s proposal, a number of works [WTB+20, WGB+19, CRS20, PSS+20] used the softmax replacement directly in back-propagation. This is to say, they implement gradient descent by manually modifying the gradient of \( \ell \) with respect to \( x_i \) as

\[
-y_i + \frac{\text{ReLU}(x_i)}{\sum_j \text{ReLU}(x_j)}.
\]

Taking into account the special case when \( \sum_j \text{ReLU}(x_j) = 0 \), we implement this approach as follows:

\[
\nabla_i := \begin{cases} 
-y_i, & \text{if } \sum_j \text{ReLU}(x_j) = 0 \\
-y_i + \frac{\text{ReLU}(x_i)}{\sum_j \text{ReLU}(x_j)} & \text{otherwise}
\end{cases}
\]

We found that it is not really necessary to treat small values of \( \sum_j \text{ReLU}(x_j) \) because it is unlikely to arise for a random model.

While this is less likely to require treatment of special cases, and it comes closer to the softmax back-propagation, the above works do not provide a formal justification in the form of a loss function. Nevertheless, a loss function or probability distribution is not necessary to measure the accuracy because that can simply be done by taking the maximum of the output values. We did so in our implementation. However, while we managed to stabilize accuracy, it remained considerably below either using softmax or the softmax replacement as output probability distribution.

### 3 Experiments

We implemented training for the MNIST dataset [LBBH98] in MP-SPDZ [Kel20] with one to three dense layers. All but the last layer consist of 128 ReLU units [GBB11]. We use fixed-point representation of fractional numbers, that is \( x \in \mathbb{R} \) is represented as \( \text{round}(x \cdot 2^{16}) \). For rounding
Table 1: Time and accuracy for various models and parameters. “⊥” stands for divergence even with the smallest possible learning rate. “Rounding” denotes the rounding after multiplication in fixed-point representation (probabilistic or nearest), and “ReLU probability” and “ReLU gradient” denote using the softmax replacement for output probability and the gradient, respectively.

| No. layers | Rounding | Back-propagation | s/epoch | Accuracy after n epochs |
|------------|----------|------------------|---------|------------------------|
|            |          |                  |         | n = 5 | n = 10 | n = 15 | n = 20 |
| 1          | Prob.    | Softmax          | 12.0    | 91.6 | 92.2 | 92.2 | 92.4 |
|            |          | ReLU probability | 7.0     | 87.8 | 89.0 | 90.8 | 91.6 |
|            |          | ReLU gradient    | 5.6     | 86.7 | 86.7 | 86.7 | 86.7 |
|            | Nearest  | Softmax          | 24.3    | 91.7 | 92.1 | 92.3 | 92.5 |
|            |          | ReLU probability | 16.0    | 90.4 | 90.5 | 90.3 | 88.5 |
|            |          | ReLU gradient    | 13.9    | 86.5 | 86.6 | 86.7 | 86.5 |
| 2          | Prob.    | Softmax          | 28.2    | 95.8 | 96.9 | 97.2 | 97.6 |
|            |          | ReLU probability | 23.2    | 92.2 | 92.4 | 93.3 | 93.4 |
|            |          | ReLU gradient    | ⊥       | ⊥    | ⊥    | ⊥    | ⊥    |
|            | Nearest  | Softmax          | 55.3    | 96.2 | 97.2 | 97.4 | 97.5 |
|            |          | ReLU probability | 46.8    | 92.9 | 92.1 | 91.4 | 87.2 |
|            |          | ReLU gradient    | ⊥       | ⊥    | ⊥    | ⊥    | ⊥    |
| 3          | Prob.    | Softmax          | 33.8    | 96.7 | 97.4 | 97.7 | 97.9 |
|            |          | ReLU probability | 28.8    | 92.3 | 93.1 | 93.5 | 94.2 |
|            |          | ReLU gradient    | ⊥       | ⊥    | ⊥    | ⊥    | ⊥    |
|            | Nearest  | Softmax          | 70.1    | 96.8 | 97.4 | 97.5 | 97.5 |
|            |          | ReLU probability | 61.4    | 94.2 | 95.3 | 95.0 | 95.6 |
|            |          | ReLU gradient    | ⊥       | ⊥    | ⊥    | ⊥    | ⊥    |

after multiplication, we consider two variants: nearest and probabilistic rounding. The latter is particularly efficient in secure computation and rounds according to proximity. For example, 0.25 is rounded down to 0 with 0.75 probability.

To implement the exponential function we use the approach by Aly and Smart [AS19]. They proposed to compute exponentials via computing exponentiation with base 2 because $e^x = 2^{x \log_2 e}$. Powers of two can be computed by splitting the input into the integer and fractional components $a = x + y$, where $x$ is an integer and $y \in [0, 1)$. The former can be computed exactly using bit decomposition. If $x = \sum x_i \cdot 2^i$, where $x_i = 0$ or 1, then $2^x = \prod (1 - x_i + x_i \cdot 2^i)$. On the other hand, $2^y$ for $y \in [0, 1]$ can be computed using Taylor approximation. Finally, $e^a = 2^x \cdot 2^y$.

Table 1 lists our timings and accuracy results for one run of each variant with honest-majority semi-honest three-party computation on AWS c5.9xlarge. Our code is available as a Docker container for reproduction.

Our results show that the ReLU-based softmax replacement only improves the running time per epoch by less than 25 percent for two layers or more while it considerably deteriorates the accuracy for any number of layers. If measuring the time it takes until a certain accuracy is reached, softmax always produces the best results. Furthermore, using the ReLU-based replacement directly in the back-propagation does not produce convergence at all with more than one layer.

Further notable is the fact that three layers do not improve the accuracy for the reported number of epochs. We found that 98 percent are achieved after 50 epochs with both two or three layers. The same occurs in plaintext training, where we found that a three-layer model would not improve over two layers. This was done using the TensorFlow MNIST tutorial [Bra] by running it as is (two dense layers) and duplicating the first dense layer.

The three-layer model was used by Mohassel and Zhang [MZ17] and later dubbed Network A by Wagh et al. [WGC19]. Neither makes an argument for using three instead of two layers, however. Mohassel and Zhang claim to reach 93.4% accuracy after 15 epochs. They provide neither code nor

1https://github.com/mkskeller/mnist-mpc
Table 2: Comparison of softmax with the two replacement variants.

| Variant          | Gradient | Established | Differentiable | Known loss | Computation |
|------------------|----------|-------------|----------------|------------|-------------|
| Softmax          | ▽_i     | ✓           | ✓              | ✓          | ✓ ✓ ✓ ✓ ✓ ✓ |
| ReLU probability | ▽_i     | ✗           | ✗              | ✓          | ✓ ✓ ✓ ✗ ✓ ✓ |
| ReLU gradient    | ▽_i     | ✗           | ✗              | ✗          | ✓ ✓ ✓ ✓ ✗ ✓ |

a detailed description of their protocol. We therefore lack the information to further evaluate the considerable difference to our accuracy results.

The recent work of Wagh et al. [WTB+20] reports a timing of 0.17 hours for 15 epochs of training, which corresponds to 41 seconds per epoch. They improve on previous works [MR18, WGC19] in the same security model, which shows that our implementation is competitive even when using softmax.

We have also run two-party training for one dense layer with probabilistic rounding. We found that one epoch takes 1173, 993, and 892 seconds with softmax, ReLU probability, and ReLU gradient, respectively. However, MP-SPDZ does not support matrix multiplication via triples generated using homomorphic encryption. This would only benefit the dense layer computation and thus increase the relative cost of the activation layer.

4 Conclusion

We conclude that the softmax replacement by Mohassel and Zhang [MZ17] is of limited use. For inference, finding the index with the maximum value in a vector (argmax) is often enough. For training on the other hand, the replacement proves to deteriorate the accuracy and slow the convergence to the extent that it is more efficient to use softmax in order to reach a certain accuracy. Table 2 shows a comparison of the three variants considered in this work.

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