ReLU activated Multi-Layer Neural Networks trained with Mixed Integer Linear Programs

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Abstract

This paper is a case study to demonstrate that, in principle, multi-layer feedforward Neural Networks activated by ReLU functions can be iteratively trained with Mixed Integer Linear Programs. To this end, two simple networks were trained with a backpropagation-like algorithm on the MNIST dataset that contains handwritten digits.

Keywords: Neural Networks, Mixed Integer Linear Programs

1 Introduction

Neural Networks typically learn by adjusting weights via non-linear optimization in a training phase. Often, variants of gradient descent are used. These techniques require some differentiability. Therefore, non-smooth but piecewise linear activation functions like ReLU or the Heaviside function raise the question if techniques of linear and mixed integer linear programming are also suited for network training.

Theoretical results are proved for certain network architectures in [2] showing that learning to near optimality can be performed with Linear Programs (LP) of exponential size. Mixed Integer Linear Programs (MILPs) are proposed in [5] to find inputs of ReLU networks that maximize activation of units. This might help to understand features computed within the network. To this end, weights are not variable. The output of a neuron is modeled by the same constraints as in [7] where MILPs are used to count maximum numbers of linear regions in outputs of ReLU networks. A trained binary Neural Network is attacked by a MILP in [6]. In this MILP as well as in [1], the weights are considered as constants, too. Another approach to evaluate robustness of networks is described in [8]. A network layout consisting of nodes and edges is optimized via a MILP in [4].

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In the given paper, we investigate suitability of training with MILPs, i.e. weights are variables. Oracle Inc. holds US patent US10068170B2 that protects the idea to use MILPs for (deep) Neural Network training at least in a scenario with piecewise constant activation functions for hidden neurons as well as piecewise linear activation functions on the output layer. In contrast to gradient descent methods, a MILP determines best possible weights in the sense of a global optimum. The restriction to piecewise constant activation functions is necessary to avoid multiplication of weights (that are variables in the optimization problem) which would lead to a non-linear problem. Thus, deep Neural Networks with ReLU activation (on subsequent layers) cannot be trained with a corresponding single MILP by means of the patent.

By applying ReLU function $\sigma$ to each component of vector $W \vec{x} + \vec{c}$, output $\vec{\phi}$ is obtained ($\vec{x} \in \mathbb{R}^d$, $\vec{a} \in \mathbb{R}^n$, $\vec{c} \in \mathbb{R}^n$, $W \in \mathbb{R}^{n \times d}$).

$$\vec{\phi} = \sigma(W \vec{x} + \vec{c}).$$

Fig. 1: Building block of ReLU-activated feedforward network: Blocks can be concatenated to realize a deep network. The output $\vec{\phi}$ of one layer then is seen as the input $\vec{x}$ of the next layer, i.e., dimensions of subsequent building blocks have to fit. Building blocks do not share weights.

**Algorithm 1 Iterative backpropagation-like learning with MILPs**

```plaintext
procedure LEARN_WEIGHTS(training_input_data, training_ground_truth_data)
    Randomly initialize all weights
    accuracy := 0, last_accuracy := -1, target_values := training_ground_truth_data
    while accuracy > last_accuracy do
        last_accuracy := accuracy
        Compute all neuron outputs $\vec{\phi}$ for training_input_data
        for i := number of output layer back to number 1 of first hidden layer do
            Update weights of (output or hidden) layer i with LP/MILP, see Section 2.1:
            Minimize $l^1$ norm of differences between output values of layer i and target_values. Input values of layer i are fixed, weights are variables.
            if i > 1 then
                Compute optimal input values $\vec{x}$ of this layer (which are output values $\vec{\phi}$ of the preceding layer) using a second LP/MILP, see Section 2.2:
                Minimize $l^1$ norm of differences between output values of layer i and target_values. Weights of the layer are now fixed. Input values are variables.
                target_values := computed optimal input values
                For updated weights and training_input_data, update inputs and outputs of all neurons
                Re-compute accuracy
            if accuracy < 1 then
                Update weights with those belonging to best accuracy that occurred in while-loop
                Finally optimize weights of the last layer, see LP in Section 2.3.
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We investigate a backpropagation-like algorithm (see Algorithm 1) to iteratively train a ReLU network with LPs and MILPs. Prerequisite is a Neural Network with ReLU activation that is a concatenation of building blocks as shown in Figure 1. All hidden layers and the output layer consist of such a building block. In a convolutional layer, most weights are fixed to zero. The input layer just passes values to the building block of the first hidden layer.

To evaluate the algorithm, we use the MNIST dataset\(^1\), see [3], that consists of 60,000 images (28 × 28 pixels) of hand-written digits for training and 10,000 digits for testing, in connection with two small example networks. One network consists of 784-8-8-8-10 neurons on five layers (three hidden fully connected layers), cf. [5, DNN1]. Values of ten output neurons encode the recognized number. Another example is a 49-25-10 network with a convolutional and a subsequent fully connected layer. To apply the network, images are downsampled to a size of 7 × 7 gray values by taking mean values of 4 × 4 areas. The size of the convolution kernel is 3 × 3, all offsets \(c_j\) are set to zero. For both networks, the index of an output neuron with output closest to one represents the detected number. The accuracy is the relative number of true detections.

On subsets of training data (which unfortunately have to be small due to running times), we determine weights using Algorithm 1 that utilizes three MILPs. The next section specifies these MILPs. Then results are discussed.

### 2 Mixed Integer Linear and Linear Programs

#### 2.1 Computation of weights

We determine weights \(W \in \mathbb{R}^{n \times d}\), \(W = [w_{l,j}]_{l \in [n], j \in [d]} = \{1, \ldots, d\}\) and \(\vec{c} \in \mathbb{R}^n\) (with components \(c_j\)) of one building block (see Figure 1) with \(d\) inputs and \(n\) outputs. In order to formulate rules (4)–(6) below, we need to bound the weights. Thus, we choose \(-1 \leq w_{l,j}, c_j \leq 1\). Given are \(m\) input vectors \(\vec{x}_1, \ldots, \vec{x}_m\) with \(d\) non-negative components each. We denote component \(j\) of \(\vec{x}_k\) with \(x_{k,j} \geq 0\). The weights have to be chosen such that the \(m\) output vectors \(\vec{o}_1, \ldots, \vec{o}_m\) are closest to given target vectors \(\vec{t}_1, \ldots, \vec{t}_m\) in the \(l^1\) norm \(\sum_{k=1}^{m} \sum_{j=1}^{n} |o_{k,j} - t_{k,j}|\). To this end, we express difference \(o_{k,j} - t_{k,j}\) via two non-negative variables \(\delta_{k,j}^+, \delta_{k,j}^- \geq 0\):

\[
o_{k,j} - t_{k,j} = \delta_{k,j}^+ - \delta_{k,j}^-. \tag{1}\]

This leads to the problem

\[
\text{minimize} \sum_{k=1}^{m} \sum_{j=1}^{n} \delta_{k,j}^+ + \delta_{k,j}^- \tag{2}\]

under following restrictions (3), (4), (5), and (6) that deal with computing \(o_{k,j}\). For each \(k \in [m]\) and \(j \in [n]\) we compute \(o_{k,j} = \sigma(a_{k,j}) \geq 0\),

\[
a_{k,j} := c_j + \sum_{i=1}^{d} w_{j,i} x_{k,i}. \tag{3}\]

\(^1\)http://yann.lecun.com/exdb/mnist/
where $\sigma(x) := \max\{0, x\}$ is the ReLU function. Let $\tilde{M} := \max\{x_{k,j} : k \in [m], j \in [d]\}$. Both $a_{k,j}$ and $|a_{k,j}|$ are bounded by $d\tilde{M} + 1$. In Section 2.2 we determine new inputs that are not necessarily bounded by $M$ but by $1.1 \cdot M + 0.1$. Thus, values of $a_{k,j}$ and $|a_{k,j}|$ are generally bounded by $M := d \cdot (1.1 \cdot \tilde{M} + 0.1) + 1$.

To realize the piecewise definition of ReLU, we introduce binary variables $b_{k,j}$ that model for input $\tilde{x}_k$ whether a neuron $j$ does (value 1) or does not fire (value 0), i.e., if the input of ReLU exceeds zero (cf. [5], [6], [7]):

$$-(1 - b_{k,j})M \leq a_{k,j} \leq b_{k,j}M. \quad (4)$$

If $b_{k,j} = 1$, output $a_{k,j}$, $0 \leq a_{k,j} \leq M$, of neuron $j$ equals $a_{k,j}$ for input $\tilde{x}_k$. Otherwise for $b_{k,j} = 0$, the output $a_{k,j}$ has to be set to zero:

$$-M(1 - b_{k,j}) \leq a_{k,j} - a_{k,j} \leq M(1 - b_{k,j}), \quad (5)$$
$$0 \leq a_{k,j} \leq Mb_{k,j}. \quad (6)$$

The MILP can be divided into $n$ independent MILPs that calculate $d + 1$ weights for each of the $n$ neurons of the layer separately.

To test the network, we use ground truth data that consist of one-hot vectors. If the digit to be detected is $j$, $0 \leq j \leq 9$, then the $j$th component is one, all other components are zero. Due to the way we determine the predictions by an output closest to one, the last layer MILP can be replaced by a potentially much faster LP. To this end, we replace ReLU in the last layer with the identity function, i.e. $a_{k,j} := a_{k,j}$ without restrictions (4)–(6) allowing $a_{k,j}$ to become negative. Instead of objective function (2) we deal with

$$\min \sum_{k=1}^{m} \sum_{j=1}^{n} \delta_{k,j}, \quad \delta_{k,j} := \left\{ \begin{array}{ll}
\delta^+_{k,j} & : \text{ground truth } t_{k,j} = 0 \\
\delta^+_{k,j} + \delta^-_{k,j} & : \text{ground truth } t_{k,j} = 1 
\end{array} \right., \quad (7)$$

ignoring negative distances to ground truth zero (that would be cut away by ReLU).

### 2.2 Proposing layer inputs

After optimizing the weights of a layer, we slightly adjust the input data of the layer such that the output error of this layer becomes even smaller. However, only small adjustments promise not to lead to larger changes of weights in subsequent steps. This is important since we do not want to forget already learned information.

To adjust the input of a layer, basically the same MILP/LP as before can be used. Now weights $W \in \mathbb{R}^{n \times d}$ and $\tilde{c} \in \mathbb{R}^n$ of one building block (see Figure 1) with $d$ inputs and $n$ outputs are given and are not variable. We have to find $m$ input vectors $\tilde{x}_1, \ldots, \tilde{x}_m$ with $d$ components each (these are now variables $x_{k,j} \geq 0$, $k \in [m], j \in [d]$) such that for the given weights problem (3) is solved under restrictions (3), (4), (5), and (6) for all but the last layer. For the last layer, problem (7) is solved under restriction (3). Let $\tilde{x}_{k,j}$ be the input of the layer previous to this optimization step. Then we add bounds

$$\max\{0, 0.9 \cdot \tilde{x}_{k,j} - 0.1\} \leq x_{k,j} \leq 1.1 \cdot \tilde{x}_{k,j} + 0.1. \quad (8)$$

Inputs can be calculated for each of the $m$ training input vectors independently. Instead of adjusting inputs to optimally match desired outputs of one single layer, one could also consider all subsequent layers with the goal to minimize distance to ground truth. With weights fixed, this is a linear problem similar to the tasks in [3], [6], etc.
2.3 Post-processing of weights of last layer

So far, we have minimized an $l^1$ error that is especially required for weight computation of hidden layers. But now we adjust the weights of the last layer with a LP by minimizing $\sum_{k=1}^{m} \sum_{j=1}^{n} \delta_{k,j} - s_{k,j}$ where variables $\delta_{k,j}$ are defined in (7), and slack variables $0 \leq s_{k,j} \leq 0.49$ are additionally restricted by $s_{k,j} \leq \delta_{k,j}$. Thus, we allow deviations up to 0.49 such that zeroes and ones of ground truth vectors are still separated.

3 Results and batch learning

Fig. 2: For training with 100 MNIST images and randomly initialized weights, bars show the contribution of while-iterations (bottom to top) in Algorithm 1 to the final learning accuracy 1.0 of the 784-8-8-8-10 network on these 100 images. Post-processing step was not required. Running times were measured with CPLEX 12.8.0, i5 (two cores) Macbook Pro, 16 MB RAM.

Limitation of training with MILPs is the running time. Therefore, we did not apply all steps of Algorithm 1 to all 60,000 training images but only to small subsets (batches) containing hundred images. However, the LP of the post-processing step is capable of dealing with the complete training set. The outcome of Algorithm 1 heavily depends on the initialization of weights. A good random initialization of weights $w_{j,i}, c_j \in [-1, 1]$ lead to results shown in Figure 2 for the 784-8-8-8-10 network. Whereas one can experimentally determine a suitable initialization, a bigger issue is that the accuracy on all 60,000 training images after training on 100 images is low. Therefore, we experimented with iterative batch learning. Algorithm 1 was applied to an initial batch of images 1-100, and weights were updated accordingly. Then the algorithm was used with images 101-200 on these updated weights, etc. An immediate idea to better remember previously learned images is not only to initialize weight variables for a warm start with values of the preceding batch training but to also limit weight changes of consecutive batch learning steps. Beginning with training of the second batch, each weight $w := w_{j,i}$ or $w := c_j$ is additionally bounded depending on the corresponding computed weight $\tilde{w}$ of the same layer for the preceding batch (factor 0.6 was determined experimentally):

$$\tilde{w} - 0.6 \cdot |\tilde{w}| - 0.01 \leq w \leq \tilde{w} + 0.6 \cdot |\tilde{w}| + 0.01.$$  

(9)

This approach yielded a best case accuracy of 0.69 on the 10,000 test images, see Figure 3. Bound (9) also reduced processing times. We also trained with multiple epochs on shuffled data. To avoid overfitting, we added noise to ground truth vectors and tested a dropout strategy. However, all these methods did not improve accuracy significantly.
Fig. 3: Iterative training of the 784-8-8-8-10 network with 20 batches of 100 consecutive images. Weights are bounded due to (9). The top curve shows training accuracy with respect to each single batch. The middle curve represents the accuracy with respect to all training data so far seen. This consists of the current and all preceding batches. The lower curve visualizes the accuracy on the MNIST test dataset with 10,000 images. Running time was 1,448 s.

Fig. 4: Reduction of resolution contributes to wrong detections. Ground truth is stated in brackets.

- in contrast to running the LP of the post-processing step on all 60,000 training images. To this end, we did not apply it for each batch but performed it after finishing ten batches (i.e., training on 1000 images). It then achieved test accuracies of up to 75.84% within about thousand seconds processor time. A majority vote using three networks trained with different sets of 1,000 images increased accuracy to 79.19%.

For the convolutional network (randomly initialized with weights in [0, 1]), we similarly trained weights iteratively on ten batches of 100 images (first 1000 images of training set) with rule (9) and then ran the post-processing step (Algorithm 1, Section 2.3) on all 60,000 training images in 3,933 seconds processor time to achieve an accuracy of 87.11%. Downsampling of image resolution was necessary to run MILPS in reasonable time. This influences detection results, see Figure 4. Thus, accuracy can be increased only slightly by taking a majority vote of multiple networks.

4 Conclusion

In principle, it is possible to iteratively train networks based on MILPs. Running times did limit this approach to small training sets. However, iterative training of very simple networks brought accuracies up to 87%.
References

[1] Anderson, R., Huchette, J., Ma, W., et al.: Strong mixed-integer programming formulations for trained neural networks. Math. Program. (2020). URL https://doi.org/10.1007/s10107-020-01474-5

[2] Bienstock, D., Muñoz, G., Pokutta, S.: Principled deep neural network training through linear programming. arXiv 1810.03218, 1–26 (2018)

[3] Cun, Y.L.L., Bottou, L., Bengio, Y., Haffner, P.: Gradient-based learning applied to document recognition. Proceedings of IEEE 85(11), 2278–2324 (1998)

[4] Dua, V.: A mixed-integer programming approach for optimal configuration of artificial neural networks. Chemical Engineering Research and Design 88(1), 55–60 (2010)

[5] Fischetti, M., Jo, J.: Deep neural networks and mixed integer linear optimization. Constraints 23, 296–309 (2018)

[6] Khalil, E.B., Gupta, A., Dilkina, B.: Combinatorial attacks on binarized neural networks. In: ICLR (2019)

[7] Serra, T., Tjandraatmadja, C., Ramalingam, S.: Bounding and counting linear regions of deep neural networks. CoRR p. abs/1711.02114 (2017)

[8] Tjeng, V., Xiao, K., Tedrake, R.: Evaluating robustness of neural networks with mixed integer programming. arXiv 1711.07356, 1–21 (2017)