Reliable and Interpretable Artificial Intelligence project report

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1 Zonotope representation and transformation

We represent a zonotope Z by its center $a_0 \in \mathbb{R}^d$ and a tensor $A \in \mathbb{R}^{k \times d}$ representing the coefficient of the k error terms.

Zonotope propagation through the neural network is straightforward using the transformations presented during the course. For convolutional layers, it suffices to apply the convolution to A itself (excluding bias). The proof is not reproduced here due to space restrictions.

2 Loss function and learning λ 's

Let $[o_0, o_2, ...o_9]$ be the output layer of the neural network (the logits for the MNIST digit classification). Let $Z_{out} =: Z$ be the zonotope region at the output layer, for a given input region Z_{in} , and for given ReLU-transformation parameters λ .

Then the network is verifiably robust on the input region if:

$$\begin{split} &\forall (o_0,...,o_9) \in Z, \forall i \in \{0,...,9\}, o_i \leq o_t \\ &\iff \forall (x_0,...,x_9) \in Z', \forall i \in \{0,...,9\}, x_i \leq 0 \\ &\iff \max_i \max_{x \in Z_i'} x_i \leq 0 \end{split}$$

where Z'_i are the zonotopes of the "violations" $x_i := o_i - o_t$. Since Z'_i are one-dimensional zonotopes, the innermost max can be computed in O(1) by assigning all the error terms to the sign of the corresponding coefficients.

Recall that Z_{out} (and so Z_i' and Z'') depends on the ReLU-transformation parameters. So the loss function

$$L(\lambda) = \max_{i} \max_{x_i \in Z_i'} x_i \tag{1}$$

can be computed by propagating the input zonotope Z_{in} through the network. The network is verifiably robust if there exists λ such that $L(\lambda) \leq 0$.

Finally, $L(\lambda)$ is differentiable, so we use gradient-based methods to minimize it.

3 Optimizer selection

We used the optimizers from pytorch.optim to optimize the loss function $L(\lambda)$. To select which method and which hyperparameters (e.g. learning rate) to use, we performed a hyperparameter search using Ax. The criterion used was the verifier execution time (capped by a timeout). We were able to do this by using additional test cases, which we generated ourselves.