Scalable and Modular Robustness Analysis of Deep Neural Networks

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Abstract. As neural networks are trained to be deeper and larger, the scalability of neural network analyzer is urgently required. The main technical insight of our method is modularly analyzing neural networks by segmenting a network into blocks and conduct the analysis for each block. In particular, we propose the network block summarization technique to capture the behaviors within a network block using a block summary and leverage the summary to speed up the analysis process. We instantiate our method in the context of a CPU-version of the stateof-the-art analyzer DeepPoly and name our system as Bounded-Block *Poly* (*BBPoly*). We evaluate BBPoly extensively on various experiment settings. The experimental result indicates that our method yields comparable precision as DeepPoly but runs faster and requires less computational resources. Especially, BBPoly can analyze *really* large neural networks like SkipNet or ResNet that contain up to one million neurons in less than around 1 hour per input image, while DeepPoly needs to spend even 40 hours to analyze one image.

Keywords: Abstract Interpretation · Formal Verification · Neural Nets.

1 Introduction

Deep neural networks are one of the most well-established techniques and have been applied in a wide range of research and engineering domains such as image classification, autonomous driving etc. However, researchers have found out that neural nets can sometimes be brittle and show unsafe behaviors. For instance, a well-trained network may have high accuracy in classifying the testing image dataset. But, if the testing image is perturbed subtly without changing the context of the image, it could fool the network into classifying the perturbed image as something else; this perturbation is known as adversarial attack [1, 2]. To tackle the issue, robustness verification is used to guarantee that unsafe states will not be reached within a certain perturbation size. Several verification techniques have been proposed to verify the robustness of neural networks.

In general, these techniques can be categorized into incomplete methods (e.g. abstract interpretation [3–5]) and complete methods (e.g. constraint solving [6, 7]). Complete methods reason over exact result, but also require long execution time and heavy computational power. On the contrary, incomplete methods run much faster but will lose precision along the way.

One of the most state-of-the-art neural network verification methods proposed in recent years is DeepPoly [5]. It is an incomplete but efficient method that uses abstract interpretation technique to over-approximate operations in neural network. In particular, DeepPoly designs the abstract domain to contain symbolic lower and upper constraints, together with concrete lower and upper bounds of a neuron's value. The symbolic constraints of a neuron are defined over neurons in the previous layer; during analysis, they will be revised repeatedly into constraints defined over neurons of even earlier layers. This computation is named as *back-substitution* and is aimed to obtain more precise analysis results [5].

Considering a network with n affine layers and each layer has at most N neurons, the time complexity of this back-substitution operation is $O(n^2 \cdot N^3)$ [8]. When the neural network has many layers (n is large), this computation is heavy and it also demands extensive memory space. This is the main bottleneck of the abstract-interpretation-based analysis used by DeepPoly.

Motivation. As deep neural networks are trained to be larger and deeper to achieve higher accuracy or handle more complicated tasks, the verification tools will inevitably need to scale up so as to analyze more advanced neural networks.

To mitigate the requirement for high computational power of DeepPoly, we propose a *network block summarization* technique to enhance the scalability of the verification tool. Our key insight is to define a method that enables tradeoff between precision requirement, time-efficiency requirement and computingresource limitation. Our method, specially tailored to handle very deep networks, leads to faster analysis and requires less computational resources with reasonable sacrifice of analysis precision. We instantiate our method in the context of a CPU-version of DeepPoly, but it can also be implemented for the GPU version of DeepPoly (named as GPUPoly [8]) which can lead to even more gain in speed.

Contribution. We summarize our contributions below:

- We propose block summarization technique supplemented with bounded backsubstitution heuristic to scale up the verification process to handle large networks like ResNet34 [9] with around one million neurons.
- We design two types of block summaries that allow us to take "shortcuts" in the back-substitution process for the purpose of reducing the time complexity and memory requirement during the analysis process.
- We implement our proposal into a prototype analyzer called BBPoly, which is built on top of the CPU-version of DeepPoly, and conduct extensive experiments on fully-connected, convolutional and residual networks. The experimental results show that BBPoly is faster and requires less memory allocation compared to the original DeepPoly, while achieves comparable precision.

2 Overview

We present an overview of the whole analysis process with an illustrative example. Our analyzer is built on top of DeepPoly system, leveraging their design of abstract domains and abstract transformers. But we will analyze the network *in blocks* and generate block summarization to speed up the analysis process. Formal details of our proposed method will be provided in Section 3.

The illustrative example is a fully-connected network with ReLU activation function as shown in Figure 1. The network has 4 layers with 2 neurons in each layer and the two input neurons i_1, i_2 can independently take any real number between [-1, 1]. The weights of the connections between any two neurons from two adjacent layers are displayed at their corresponding edges, the bias of each neuron is indicated either above or below the neuron. Computation for a neuron in a hidden layer undergoes two steps: (i) an *affine transformation* based on the inputs, weights and biases related to this neuron, which generates a value v, followed by (ii) a *ReLU activation* which outputs v if v > 0, or 0 if $v \leq 0$. For the output layer, only affine transformation is applied to generate the final output of the entire network.

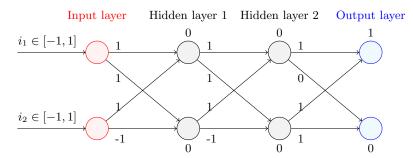


Fig. 1: Example fully-connected network with ReLU activation (cf. [5])

To analyze a neural network, we follow the approach taken by DeepPoly where each hidden layer is perceived as a combination of an affine layer and a ReLU layer. Therefore, network in Figure 1 will be represented by the network depicted in Figure 2 for analysis purpose, where a neuron in a hidden layer is expanded into two nodes: (i) one affine node for the related affine transformation (such as x_3, x_4, x_7, x_8), and (ii) one ReLU node which is the output of ReLU function (such as $x_5.x_6, x_9, x_{10}$).

2.1 Preliminary Description on Abstract Domain

We use the abstract domain designed from DeepPoly system [5] to verify neural networks. For each neuron x_i , its abstract value is comprised of four elements: a symbolic upper constraint u_i^s , a symbolic lower constraint l_i^s , a concrete lower bound l_i and a concrete upper bound u_i . And we have $l_i^s \leq x_i \leq u_i^s$, $x_i \in [l_i, u_i]$. All the symbolic constraints associated with x_i can be formulated as $b_i + \sum_j w_j \cdot x_j$, where $w_j \in \mathbb{R}, b_i \in \mathbb{R}, j < i$. Here, the constraint j < i asserts that the constraints for x_i only refer to variables "before" x_i , since the value of

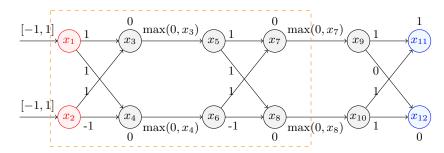


Fig. 2: The transformed network from Figure 1 to perform analysis (cf. [5])

one neuron (at a layer) only depends on the values of the neurons at preceding layers. For the concrete bounds of x_i , we have $l_i \in \mathbb{R}, u_i \in \mathbb{R}, l_i \leq u_i$ and the interval $[l_i, u_i]$ over-approximates all the values that x_i can possibly take.

2.2 Abstract Interpretation on the Example Network

We now illustrate how to apply abstract interpretation on the example network in order to get the output range of the network, given an abstract input [-1, 1]for both the input neurons.

The analysis starts at the input layer and processes layer by layer until output layer. The abstract values of the inputs x_1, x_2 are respectively $\langle l_1^s = -1, u_1^s =$ $1, l_1 = -1, u_1 = 1 \rangle$ and $\langle l_2^s = -1, u_2^s = 1, l_2 = -1, u_2 = 1 \rangle$. Next, the affine abstract transformer (designed by DeepPoly [5]) for x_3 and x_4 generates the following symbolic constraints, where the coefficients (and the constant terms, if any) in constraints are the weights (and bias) in the fully connected layer:

$$x_1 + x_2 \le x_3 \le x_1 + x_2; \quad x_1 - x_2 \le x_4 \le x_1 - x_2 \tag{1}$$

The concrete bounds are computed using concrete intervals of x_1, x_2 and symbolic constraints in Equation (1), thus $l_3 = l_4 = -2$ and $u_3 = u_4 = 2$ (the process of computing concrete bound is formally described in Appendix A).

The activation transformer (designed by DeepPoly [5]) is then applied to get the abstract elements for x_5, x_6 from x_3, x_4 respectively. In general, given that $x_i = \text{ReLU}(x_j)$, if $u_j \leq 0, x_i$ is always 0, therefore we have $0 \leq x_i \leq 0, l_i =$ $0, u_i = 0$. If $l_j \geq 0$, then $x_i = x_j$ and we get $x_j \leq x_i \leq x_j, l_i = l_j, u_i = u_j$. For the case where $l_j < 0$ and $u_j > 0$, an over-approximation error will be introduced and we set the abstract element as followed for x_i :

$$x_i \ge c_i \cdot x_j, \quad x_i \le \frac{u_j(x_j - l_j)}{u_j - l_j}, \quad l_i = 0, \quad u_i = u_j,$$
 (2)

where $c_i = 0$ if $|l_j| > |u_j|$ and $c_i = 1$ otherwise. For example, $x_5 = \text{ReLU}(x_3)$ and since $l_3 < 0, u_3 > 0$, it belongs to the last case described in Equation (2). $|l_3| = |u_3| = 2$ therefore $c_5 = 1$. Finally, we get the abstract value for x_5 : $l_5 = 0, u_5 = 2, l_5^s = x_3, u_5^s = 0.5 \cdot x_3 + 1$. Similar computation can be done for x_6 to yield $l_6 = 0, u_6 = 2, l_6^s = x_4, u_6^s = 0.5 \cdot x_4 + 1$. Next, we work on the symbolic bounds for x_7, x_8 , beginning with:

$$x_5 + x_6 \le x_7 \le x_5 + x_6; \quad x_5 - x_6 \le x_8 \le x_5 - x_6 \tag{3}$$

From the symbolic constraints in Equation (3), we recursively substitute the symbolic constraints *backward* layer by layer until the constraints are expressed in terms of the input variables. Upon reaching back to an earlier layer, constraints defined over neurons in that layer are constructed and concrete bound values are evaluated and recorded (refer to Appendix A). Finally the most precise bound among all these layers will be selected as the actual concrete bound for x_7 and x_8 respectively. This process is called *back-substitution* and is the key technique proposed in DeepPoly to achieve tighter bounds. We follow the back-substitution procedure in DeepPoly and construct constraints for x_7, x_8 defined over x_3, x_4 :

$$x_3 + x_4 \le x_7 \le 0.5 \cdot x_3 + 0.5 \cdot x_4 + 2$$

$$x_3 - (0.5 \cdot x_4 + 1) \le x_8 \le 0.5 \cdot x_3 + 1 - x_4,$$
(4)

And we further back-substitute to have them defined over x_1, x_2 :

$$2x_1 \le x_7 \le x_1 + 2$$

$$0.5 \cdot x_1 + 1.5 \cdot x_2 - 1 \le x_8 \le -0.5 \cdot x_1 + 1.5 \cdot x_2 + 1$$
(5)

Finally, we determine the best bound for x_7 to be $l_7 = 0, u_7 = 3$ and that for x_8 to be $l_8 = -2, u_8 = 2$. Note that we have additionally drawn a dashed orange box in Figure 2 to represent a network *block*. Here, we propose a *block summarization* method which captures the relations between the input (leftmost) layer and output (rightmost) layer of the block. Thus Equation (5) can function as the block summarization for the dashed block in Figure 2; we leverage on this block summarization to make "jumps" during back-substitution process so as to save both running time and memory (details in Section 3).

To continue with our analysis process, we obtain next:

$$l_{9} = 0, \quad u_{9} = 3, \quad l_{9}^{s} = x_{7}, \quad u_{9}^{s} = x_{7}$$

$$l_{10} = 0, \quad u_{10} = 2, \quad l_{10}^{s} = x_{8}, \quad u_{10}^{s} = 0.5 \cdot x_{8} + 1$$

$$l_{11} = 1, \quad u_{11} = 6, \quad l_{11}^{s} = x_{9} + x_{10} + 1, \quad u_{11}^{s} = x_{9} + x_{10} + 1$$

$$l_{12} = 0, \quad u_{12} = 2, \quad l_{12}^{s} = x_{10}, \quad u_{12}^{s} = x_{10},$$
(6)

Here, we can quickly construct the constraints of x_{11} defined over x_1, x_2 by using the block summarization derived in Equation (5); yielding $2.5 \cdot x_1 + 1.5 \cdot x_2 \le x_{11} \le 0.75 \cdot x_1 + 0.75 \cdot x_2 + 4.5$. By doing so, our analysis will return $x_{11} \in [1, 6]$ and $x_{12} \in [0, 2]$. Note that we lose some precision when making "jumps" through block summarization; the interval for x_{11} would be [1, 5.5] if we were to stick to layer-by-layer back-substitution as originally designed in DeepPoly.

2.3 Scaling up with block summarization

As illustrated in Equation (4) and Equation (5), we conduct back-substitution to construct symbolic constraints defined over neurons at earlier layer in order to

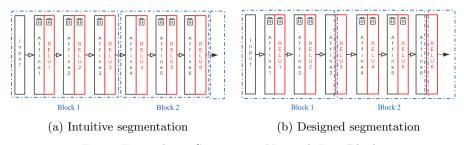


Fig. 3: Example on Segmenting Network Into Blocks

obtain a tighter concrete bound. In DeepPoly, every affine layer initiates layer-bylayer back-substitution until the input layer. Specifically, we assume a network with n affine layers, maximum N neurons per layer and consider the k^{th} affine layer (where the input layer is indexed as 0). Every step of back-substitution for layer k through a preceding affine layer requires $O(N^3)$ time complexity and every back-substitution through a preceding ReLU layer requires $O(N^2)$, it takes $O(k \cdot N^3)$ for the k^{th} affine layer to complete the back-substitution process. Overall, DeepPoly analysis requires $O(n^2 \cdot N^3)$ time complexity. This can take a toll on DeepPoly when handling large networks. For example, in our evaluation platform, DeepPoly takes around 40 hours to analyze one image on ResNet18 [9] with 18 layers. Therefore, we propose to divide the neural networks into blocks, and compute the summarization for each block. This summarization enables us to charge up the back-substitution operation by speeding across blocks, as demonstrated in Equation (5) where constraints of neuron x_7 are directly defined over input neurons.

3 Network Block Summarization

3.1 Network analysis with modularization

For better scalability, we propose a modularization methodology to decrease the computational cost as well as the memory usage, where we segment the network into blocks and analyze each block in sequence. Specifically, we propose the following two techniques to reduce computation steps:

- 1. Generate summarization between the input and output neurons for each block, and leverage block summarization to make "jumps" during backsubstitution instead of doing it layer by layer.
- 2. Leverage block summarization by bounding back-substitution operation to terminate early.

As illustrated by the simplified network representation in Figure 3, we segment a network into two blocks. We then show (1) how to generate summarization given the network fragment and (2) how to leverage the summarization to perform back-substitution. The details are as follows.

Network segmentation. We parameterize network segmentation with a parameter σ , which is the number of affine layers required to form a block.

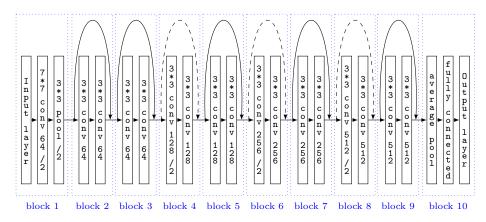


Fig. 4: ResNet18 [9] and the corresponding block segmentation

For example, σ is set to 3 in Figure 3. Since each layer in the neural network ends with the ReLU function, an intuitive segmentation solution is to divide the network so that each block always *ends at a ReLU layer*, as depicted in Figure 3a. However, doing so requires more computation during the back-substitution but does not gain more accuracy as compared to the segmentation method in which *each block ends by an affine layer*.³ Therefore, we choose the later segmentation option, as shown in Figure 3b.

Moreover, special care is required to segment a residual network. As illustrated in Figure 4, the most important feature of residual network is the *skip* connection that enables a layer to take "shortcut connections" with a much earlier layer [9] (displayed by the curved line). Thus, a set of layers residing in between a layer and its skip-connected layer forms an "intrinsic" residual block, to be used to segment the network (eg., blocks #2 to #9 in Figure 4). A more dynamic choice of block size or block number could potentially lead to better trade-off between speed and precision; we leave it as future work.

Back-substitution with block summarization. We present the analysis procedure which implements our block summarization method (Section 3.2) and bounded back-substitution heuristic in Algorithm 1. Given an input neural network, it will be first segmented (line 1) using the method described in previous subsection. For a block consisting of layers $\gamma_a, \ldots, \gamma_k$, the start layer and the end layer of the block will be remembered by the markers **GetStartLayer** and **IsEndLayer** respectively. The analysis of ReLU layers (line 3) only depends on the preceding affine layer it connects to (line 4). The computation of ReLU layer (line 5) follows the process described in Section 2.2 and Equation (2).

To handle affine layer with back-substitution, we firstly assign γ_{pre} to be the preceding layer of γ_k (line 7). Then, we initialize the constraint set of γ_k to be the symbolic lower and upper constraints for neurons in γ_k (line 8). Constraints Υ_k

 $^{^3}$ An explanation of our choice to end blocks at an affine layer instead of a ReLU layer can be found in Appendix B

are defined over neurons in layer γ_{pre} and directly record the affine transformation between layer γ_k and γ_{pre} . Thus, we could use Υ_k and the concrete bounds of neurons in γ_{pre} to compute the initial concrete bounds for neurons in layer γ_k (line 9), using the constraint evaluation mechanism described in Appendix A. As such, we conduct back-substitution to compute the concrete bounds for neurons in affine layer γ_k (lines 11-27).

Algorithm 1: Overall analysis procedure in BBPoly						
Input: M is the network (eg. Figure 2); τ is the back-substitution threshold	1:					
σ is the network segmentation parameter						
Annotatation: input layer of M as γ_{in} ; constraint set of affine layer γ_k as γ_{in}	Υ_k :					
the set of concrete bounds for neurons in layer $\gamma_k \in M$ as C_k ; the segment network model as \mathcal{M}						
Assumption: the analysis is conducted in ascending order of the layer inde	v					
Output: tightest concrete bounds C_k computed for all layer $\gamma_k \in M$						
1: $\mathcal{M} \leftarrow \text{SegmentNetwork}(\mathcal{M}, \sigma)$						
2: for all layer $\gamma_k \in \mathcal{M}$ do						
3: if IsReluLayer(γ_k) then						
4: $\gamma_{pre} \leftarrow PredecessorLayer(\gamma_k)$						
5: $C_k \leftarrow ComputeReluLayer(\gamma_{pre})$						
6: else						
7: $\gamma_{pre} \leftarrow PredecessorLayer(\gamma_k)$						
8: $\Upsilon_k \leftarrow GetSymbolicConstraints(\gamma_k)$						
9: $C_k \leftarrow EvaluateConcreteBounds(\Upsilon_k, \gamma_{pre})$						
10: $counter_k = 0$						
11: while $\gamma_{pre} \neq \gamma_{in} \mathbf{do}$						
12: if $lsEndLayer(\gamma_{pre})$ then						
13: $sum \leftarrow ReadSummary(\gamma_{pre})$						
14: $\Upsilon_k \leftarrow BacksubWithBlockSummary(\Upsilon_k, sum)$						
15: $counter_k \leftarrow counter_k + 1$						
16: $\gamma_{pre} \leftarrow GetStartLayer(\gamma_{pre})$						
17: else						
18: $sym_cons \leftarrow GetSymbolicConstraints(\gamma_{pre})$						
19: $\Upsilon_k \leftarrow BacksubWithSymbolicConstraints(\Upsilon_k, sym_cons)$						
20: $counter_k \leftarrow counter_k + 1$						
21: $\gamma_{pre} \leftarrow PredecessorLayer(\gamma_{pre})$						
22: if $lsEndLayer(\gamma_k)$ and $\gamma_{pre} = GetStartLayer(\gamma_k)$ then						
23: StoreSummary (γ_k, Υ_k)						
24: $temp_ck \leftarrow EvaluateConcreteBounds(\Upsilon_k, \gamma_{pre})$						
25: $C_k \leftarrow UpdateBounds(C_k, temp_ck)$	_					
26: if $counter_k \ge \tau$ and $\neg (IsEndLayer(\gamma_k) \text{ and } LackSummary(\gamma_k))$ the set of the se	hen					
27: break						
28: return all C_k for all layer $\gamma_k \in \mathcal{M}$						

We have two types of back-substitution and executing either one of the two will be considered as one step of back-substitution which leads to an increment of the counter for layer γ_k (lines 15, 20):

- If γ_{pre} is the end layer of a block, we first read the block summary of γ_{pre} (lines 12-13), and then call BacksubWithBlockSummary(Υ_k , sum) to perform back-substitution over a block (line 14). After execution, Υ_k will be updated to be defined over the start layer of the block. Lastly, in preparation for next iteration of execution, γ_{pre} is set to the start layer of the block (line 16).
- Otherwise, we conduct *layer-by-layer* back-substitution (lines 18-21) similarly to DeepPoly. We obtain sym_cons , the symbolic constraints built for γ_{pre} , and call BacksubWithSymbolicConstraints(Υ_k, sym_cons) (line 19). Then, Υ_k will be updated to be defined over the predecessor layer of γ_{pre} . Pertaining to block summarization construction, if γ_{pre} and γ_k are the start and the end layer of the same block, Υ_k will be recorded as the block summary (lines 22-23).

After generating a new set of constraints (lines 14, 19), we can compute a set of potential concrete bounds $temp_ck$ using the new constraints Υ_k defined over the new γ_{pre} (line 24). Then we update C_k by the most precise bounds between $temp_ck$ and the previous C_k (line 25) as proposed in DeepPoly, where the most precise means the smallest upper bound and biggest lower bound.

Bounded Back-substitution. Normally, we continue new constraint construction, constraint evaluation and concrete bound update for γ_k until the input layer (line 11). The goal here is to explore the opportunity for cancellation of variables in the constraints defined over a particular layer. Such opportunity may lead to attaining tighter bounds for abstract values of neurons at layer k. Nevertheless, it is possible to terminate such back-substitution operation earlier to save computational cost, at the risk of yielding less precise results.⁴ This idea is similar in spirit to our introduction of block summarization. We term such earlier termination as *bounded back-substitution*. It may appear similar to the "limiting back-substitution" suggested in DeepPoly [5] or GPUPoly [8]. However, we note that one step in back-substitution in our approach can either be a back-substitution over one layer or over a block summary. Please note the difference between our bounded back-substitution and the limiting back-substitution in DeepPoly [5] or GPUPoly [8]. We count either a layer back-substitution or a back-substitution over block summary as one step of back-substitution. Therefore, even though we bound the same number of steps of back-substitution, our method allows us to obtain constraints defined over more preceding layers compared to limiting back-substitution in DeepPoly or GPUPoly.

Bounded back-substitution is incorporated in Algorithm 1, by accepting an input τ , which is a threshold for the maximum number of steps to be taken during back-substitution. More specifically, we initialize a counter when processing layer γ_k (line 10), and increment the counter accordingly during the analysis (lines 15, 20). Finally, we end the back-substitution iteration for layer γ_k once the threshold is reached (line 26).

⁴ As a matter of fact, our empirical evaluation (detailed in Appendix C) shows that the degree of improvement in accuracy degrades as we explore further back into earlier layers during back-substitution.

During the construction of block summarization, we suspend this threshold checking when γ_k is the end layer of a block (second test in line 26). This ensures that the algorithm can generate its block summarization without being forced to terminate early. In summary, suppose each block has at most ℓ layers, under bounded back-substitution, the layer γ_k will back-substitute either ℓ layers (if γ_k is the end layer of a block) or τ steps (if γ_k is not the end layer of a block).

Summarization within block 3.2

Block Summarization. The summarization captures the relationship between the output neurons and input neurons within a block. Given a block with kaffine layers inside, we formally define it as $\Gamma = \{\gamma_{in}, \gamma_1, \gamma'_1, \dots, \gamma_k\}$ (e.g. block1 in Figure 3b) or $\Gamma = \{\gamma'_0, \gamma_1, \gamma'_1, \dots, \gamma_k\}$ (like block2 in Figure 3b), where γ_i refers to an affine layer, γ_{in} refers to the input layer and γ'_i refers to the ReLU layer with ReLU function applied on γ_i , for $i \in \{0, 1, 2, \dots, k\}$.

Suppose the last layer $\gamma_k = \{x_{k1}, \dots, x_{kN}\}$ contains N neurons in total. The block summarization $\Phi_{\Gamma} = \{\langle \phi_{x_{k1}}^L, \phi_{x_{k1}}^U \rangle, \dots, \langle \phi_{x_{kN}}^L, \phi_{x_{kN}}^U \rangle\}$ is defined as a set of constraint-pairs. For $j \in \{1, 2, \dots, N\}$, each pair $\langle \phi_{x_{kj}}^L, \phi_{x_{kj}}^U \rangle$ corresponds to the lower and upper constraints of neuron x_{kj} defined over the neurons in the first layer of the block (be it an affine layer $\gamma_{\rm in}$ or a ReLU layer γ'_0). As these lower and upper constraints encode the relationship between output neurons and input neurons with respect to the block Γ , they function as the block summarization.

Back-substitution with Block Summarization. To explain our idea, we present the overall back-substitution process as the matrix multiplication (cf. [8]) depicted in Figure 5. Matrix M^k encodes the current constraints for neurons in layer l defined over neurons in previous layer k, where $1 \leq k < l$. The cell indexed by the pair (x_{hm}^l, x_{ic}^k) in the matrix records the coefficient between neuron x_{hm}^l in layer l and neuron x_{ic}^k in layer k. The same notation also applies for matrix F^k and M^{k-1} , where F^k denotes next-step back-substitution and M^{k-1} represents a newly generated constraint for neurons in layer l defined over neurons in the preceding layer k-1. As we always over-approximate ReLU function to a linear function, without loss of generality, we therefore discuss further by considering a network as a composition of affine layers.

	x_{i1}^k	x_{i2}^k		x_{is}^k	5	x_{j1}^{k-1}	x_{j2}^{k-}	¹ ;	r_{jr}^{k-1}		3	c_{j1}^{k-1}	x_{j2}^{k-2}	۱ :	x_{jr}^{k-1}
x_{h1}^l	*	*		*	x_{i1}^k	*	*		*		l h1	*	*	•••	*
x_{h2}^l	*	*		*	x_{i2}^k	*	*		*	$\begin{bmatrix} x \\ - \end{bmatrix}$	l h2	*	*		*
					•••										
x_{ht}^l	*	*		*	x_{is}^k	*	*		*		l_{ht}	*	*	•••	*
		1	M^k				1	$\overline{\gamma}^k$					M	k - 1	

Fig. 5: Back-substitution process can be represented as matrix multiplication with constant terms (e.g. biases) being omitted, cf. [8]

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Next, we describe how to perform back-substitution with the generated block summarization. After completing the layer-by-layer back-substitution process within a given block (take block 2 in Figure 3b as example), we obtain constraints of neurons in the affine layer 6 (γ_6) defined over neurons in the ReLU layer 3 (γ'_3), which corresponds to M^k . This matrix is then multiplied with matrix F^{k1} which captures the affine relationship between neurons in layer γ'_3 and γ_3 (this affine relationship is actually an over-approximation since $\gamma'_3 = \text{ReLU}(\gamma_3)$), followed by another multiplication with matrix F^{k2} constructed from block summarization for block 1 (in Figure 3b), denoted here by Φ_{Γ_1} . Φ_{Γ_1} is a set of constraints for neurons in the affine layer 3 (γ_3) defined over neurons in the input layer (γ_{in}) and is computed already during the analysis of block 1. Hence, the resulting matrix $M^k \circ F^{k1} \circ F^{k2}$ encodes the coefficients of neurons in layer γ_6 defined over neurons in layer γ_6 to the input layer.

Memory Usage and Time Complexity. In the original method, the memory usage of DeepPoly is high since it associates all neurons with symbolic constraints and maintains all symbolic constraints throughout the analysis process for the sake of layer-by-layer back-substitution. In work of [10] and [11], they all faced with out-of-memory problem when running DeepPoly on their evaluation platform. In our block summarization approach, a block captures only the relationship between its end and start layers. Consequently, all the symbolic constraints for intermediate layers within the block can be released early once we complete the block summarization computation (illustrated by a delete icon in the layer in Figure 3). Thus our method requires less memory consumption when analyzing the same network, and the memory usage can also be controlled using the network segmentation parameter σ .

For time complexity, consider a network with n affine layers and each layer has at most N neurons, DeepPoly's complexity is $O(n^2 \cdot N^3)$. In our method, with bounded back-substitution (detail in Section 3.1), we can bound the number of steps for back-substitution to a constant for each layer. Thus the time complexity can be reduced to $O(n \cdot N^3)$. Without bounded back-substitution, we have constant-factor reduction in time complexity, yielding the same $O(n^2 \cdot N^3)$.

3.3 Summarization defined over input layer

Previously, Section 3.2 describes a back-substitution mechanism on "block-byblock" basis. To further simplify the back-substitution process and save even more on the execution time and memory, we also design a variation of block summarization that is *defined over the input layer*. As the overall procedure of back-substitution with summarization defined over input layer is similar to the block summarization described in Algorithm 1, we provide the algorithm for this new summary in Appendix G.

Summary over Input. Just as in Section 3.2, the summary-over-input is still formulated as Φ_{Γ} . However, $\langle \phi_{x_{jk}}^L, \phi_{x_{jk}}^U \rangle$ corresponds to constraints of neuron x_{jk} which are now *defined over the input neurons*. To generate summary for block Γ_i , we firstly do layer-by-layer analysis within the block, then we back-substitute

further with the summary for block Γ_{i-1} which is defined over input neurons, thus we get Φ_{Γ_i} defined over the input neurons.

Back-substitution with Summary over Input. The back-substitution process also follows the formulation described in Section 3.2. The resulting matrix $M^k \circ F^{k1} \circ F^{k2}$ will directly be defined over input neurons since F^{k2} is the summary of preceding block directly defined over input neurons.

Memory Requirement and Time Complexity. Once the summary generation for block Γ_i has completed, all symbolic constraints and summaries from previous i-1 blocks could be released, only the input layer needs to be kept. For time complexity, each layer back-substitutes at most l + 1 steps (if each block has maximum l layers), the time complexity will be $O(n \cdot N^3)$.

4 Experiment

We have implemented our proposed method in a prototype analyzer called BBPoly, which is built on top of the state-of-the-art verifier DeepPoly. Then, we conducted extensive experiments to evaluate the performance of both our tool and DeepPoly, in terms of precision, memory usage and runtime. In the following subsections, we will describe the details of our experiment.

4.1 Experiment Setup

We propose two types of block summary in our BBPoly system:

- Block summarization as described in Section 3.2. It can be supplemented with bounded back-substitution heuristic in Section 3.1 to facilitate the analysis even more for extremely large network;
- Block summary defined over input layer that is introduced in Section 3.3

We compare our methods with the state-of-the-art system DeepPoly [5], on top of which our prototype tool is built. DeepPoly is publicly available at the GitHub repository of the ERAN system [12]. On the other hand, we do not compare with existing approach using MILP solving [13] since the latter can only handle small networks, such as MNIST/CIFAR10 networks with 2 or 3 hidden layers while our BBPoly can analyze large networks of up to 34 hidden layers.

Evaluation datasets. We choose the popular MNIST [14] and CIFAR10 [15] image datasets that are commonly used for robustness verification. MNIST contains gray-scale images with 28×28 pixels and CIFAR10 consists of RGB 3-channel images of size 32×32 . Our test images are provided from DeepPoly paper where they select out the first 100 images of the test set of each dataset. The test images are also publicly available at [12].

Evaluation platform and networks. The evaluation machine is equipped with a 2600 MHz 24 core GenuineIntel CPU with 64 GB of RAM. We conducted experiments on networks of various sizes as itemized in Table 1; these include fully-connected, convolutional and (large sized) residual networks where the number of hidden neurons is up to 967K. All networks use ReLU activation, and we list the layer number and number of hidden neurons in the table.

Specifically, the networks whose names suffixed by "DiffAI" were trained with adversarial training DiffAI [16]. These benchmarks are also collected from [12].

Verified robustness property. We verify robustness property against the L_{∞} norm attack [17] which is paramterized by a constant ϵ of perturbation. Originally, each pixel in an input image has a value p_i indicating its color intensity. After applying the L_{∞} norm attack with a certain value of ϵ , each pixel now corresponds to an intensity interval $[p_i - \epsilon, p_i + \epsilon]$. Therefore we constructed an adversarial region defined as $\sum_{i=1}^{n} [p_i - \epsilon, p_i + \epsilon]$. Our job is to verify that whether a given neural network can classify all perturbed images within the given adversarial region as the same label as of the original input image. If so, we conclude that robustness is verified for this input image, the given perturbation ϵ and the tested network. For images that fail the verification, due to the over-approximation error, we fail to know if the robustness actually holds or not, thus we report that the results are inconclusive. We set a 3-hour timeout for the analysis of each image, if the verifier fails to return the result within 3 hours, we also state that the result is inconclusive.

Neural Network	Dataset	#Layer	#Neurons	Type	Candidates
MNIST_9_200	MNIST	9	1,610	fully connected	97
$ffcnRELU_Point_{6}_{500}$	MNIST	6	3,000	fully connected	100
convBigRELU	MNIST	6	48,064	convolutional	95
convSuperRELU	MNIST	6	88,544	convolutional	99
$ffcnRELU_Point_6_500$	CIFAR10	6	3,000	fully connected	56
convBigRELU	CIFAR10	6	62,464	convolutional	60
SkipNet18_DiffAI	CIFAR10	18	558K	residual	41
ResNet18_DiffAI	CIFAR10	18	558K	residual	46
ResNet34_DiffAI	CIFAR10	34	967K	residual	39

Table 1: Experimental Networks

4.2 Experiments on fully-connected and convolutional networks

We firstly present the experiment results on fully-connected and convolutional networks for both the MNIST and CIFAR10 datasets. We set the block segmentation parameter to be 3;⁵ this means there will be 3 affine layers contained in a block. We conduct experiments on both block-summarization and summary-over-input methods. And the bounded back-substitution heuristic is disabled for this part of experiments. We set six different values of perturbation ϵ for different networks according to the settings in DeepPoly (details in Appendix D).

The verified precision is computed as follows:

⁵ We have conducted preliminary experiments with the effectiveness of having different block sizes; the results are available in Appendix F. A more thorough investigation on the effectiveness is left as future work.

where candidate images are those which have been correctly classified by a network. The numbers of candidate images for each network are presented in Table 1. Figure 6 shows the precision comparison among different methods on MNIST networks, and Figure 7 shows the precision on CIFAR10 networks. Due to page constraint, full details of the precision and average execution time per image for the experiments are recorded in Table 5 of Appendix E. As expected, DeepPoly \geq BBPoly (using block summary) \geq BBPoly (using input summary) with respect to precision and execution time. Apart from MNIST_9_200 network, our methods actually achieve comparable precision with DeepPoly.

With regard to the execution time, for larger networks such as the three convolutional networks experimented, our block-summarization method can save around half of the execution time in comparison with that by DeepPoly. Interested reader may wish to refer to Table 5 in Appendix E for detail. The execution time can be significantly reduced for even larger network, such as the deep residual networks, as demonstrated in Section 4.3.

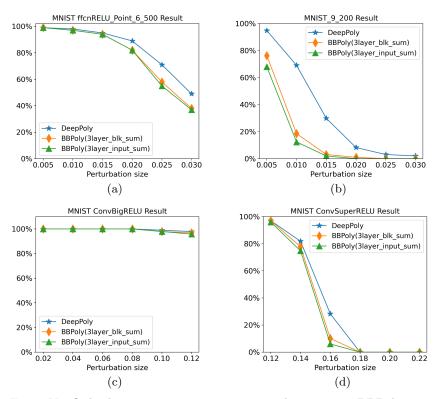


Fig. 6: Verified robustness precision comparison between our BBPoly system and DeepPoly for MNIST fully-connected and convolutional networks

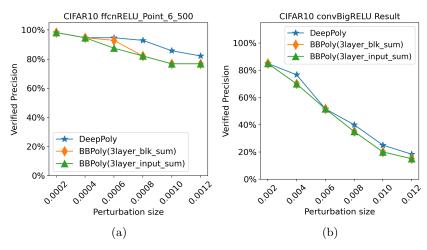


Fig. 7: Verified robustness precision comparison between our BBPoly system and DeepPoly for CIFAR10 fully-connected and convolutional networks.

4.3 Experiments on residual networks

Network description. We select three residual networks that have 18 or 34 layers and contain up to almost one million neurons as displayed in Table 1. The SkipNet18, ResNet18 and ResNet34 are all trained with DiffAI defence.

Perturbation size. DeepPoly is not originally designed to handle such large networks and is inconclusive within our timeout. However, an efficient GPU implementation of DeepPoly (called GPUPoly) [8] is proposed for much larger networks. GPUPoly achieves the same precision as DeepPoly and it selects $\epsilon = 8/255$ for our experimental residual networks. Thus we follow the same setting as in GPUPoly. Unfortunately, GPUPoly does not run in one-CPU environment, and thus not comparable with our experimental setting.

Precision comparison with DeepPoly. We only conduct robustness verification on candidate images as in Section 4.2. We set our baselines to be block-summarization method with bounded back-substitution in four steps, and summary-over-input method. The number of candidate images, verified images and the average execution time per image for our experiment are listed in Table 2, where column "BlkSum_4bound" refers to block-summarization method together with bounded back-substitution in four steps and "Input_Sum" refers to our summary-over-input method. As illustrated in Table 2, the summary-overinput method verifies more or at least the same number of images compare to the block-summarization method with bounded back-substitution but requires less execution time, which demonstrates the competitive advantage of our summaryover-input method.

Verified precision is computed using formula 7 with data from Table 2; the results are displayed in Table 3 for residual networks. DeepPoly fails to verify any image within the timeout of 3 hours in our evaluation platform (indicated by '-')

Neural Net	ϵ	ε	Cand- idates	(BlkSun	Poly n_4bound)	BBI (Input	Poly Sum)	Deep	Poly
			Verified	$\operatorname{Time}(s)$	Verified	$\operatorname{Time}(s)$	Verified	$\operatorname{Time}(s)$	
SkipNet18_DiffAI	8/255	41	35	4027.08	36	1742.93	-	-	
ResNet18_DiffAI	8/255	46	29	3212.26	29	984.43	-	-	
ResNet34_DiffAI	8/255	39	21	2504.89	22	1296.78	-	-	

Table 2: The number of verified images and average execution time per image for CIFAR10 residual networks

Neural Net	ϵ	BBPoly (BlkSum_4bound)	BBPoly (Input_Sum)	DeepPoly
$SkipNet18_DiffAI$	8/255	85.3%	87.8%	-
ResNet18_DiffAI	8/255	63.0%	63.0%	-
ResNet34_DiffAI	8/255	53.8%	56.4%	-

Table 3: Verified precision comparison computed from Table 2

whereas our method yields reasonable verified precision within this time limit, supporting our hypothesis that BBPoly can scale up to analyze large networks with fair execution time and competitive precision.

Time comparison with DeepPoly. To the best of our knowledge, there is no public experimental result of using DeepPoly to analyze ResNets. We initially used DeepPoly to analyze input images in our dataset with a smaller $\epsilon = 0.002$ for ResNet18_DiffAI. Since DeepPoly took around 29 hours to complete the verification of an image, we could not afford to run DeepPoly for all 100 test images. In contrast, our summary-over-input method takes only 1319.66 seconds (≈ 22 minutes) for the same image. We also try to analyze ResNet18_DiffAI with $\epsilon = 8/255$ according to the original perturbation setting, and DeepPoly takes around 41 hours to complete the verification of one image. On the other hand, our block-summarization with bounded back-substitution in 4 steps uses average 3212.26 seconds (≈ 54 minutes) for one image.

Memory comparison with DeepPoly. We mention earlier that our methods utilize less memory. To empirically testify this, we compare the peak memory usage between DeepPoly and summary-over-input method with respect to ResNet18_DiffAI, on the first input image in our dataset and $\epsilon = 8/255$. We use the following command to check the peak memory usage of our analysis process: \$ grep VmPeak /proc/\$PID/status

According to the result, DeepPoly takes up to 20.6 GB of memory while our summary-over-input method needs much less memory. It takes only 11.4 GB of

memory, which is 55% of the memory usage of DeepPoly.

5 Discussion

We now discuss the limitation of our work. There are two limitations as follows. Firstly, although the experimental results in Section 4.2 demonstrate that our tool yields comparable precision with DeepPoly for majority of the tested networks, it still significantly less precise than DeepPoly in certain benchmarks, such as the MNIST_9_200 network. We have explained earlier that this loss of precision is due to our current block summarization technique which cannot capture a precise enough relationship between neurons in the start and the end layer of a block. In the future, we aim to generate a more tightened summarization to reduce the over-approximation error and increase the precision of our analyzer. Secondly, our current construction of a block is simple and straightforward. We currently fix the block size to be a constant (eg. 3), and have not considered the intricate information related to the connectivity between layers when choosing the block size. For future work, we will investigate how to utilize such information to assign the block size dynamically. This could potentially help the analysis to find a better trade-off between speed and precision.

Our proposed method on block summarization could potentially be applied to other neural network verification techniques to enhance their scalability. For instance, in constraint-based verification, the network is formulated by the conjunction of the encoding of all neurons and all connections between neurons [18]. This heavy encoding is exact but lays a huge burden on the constraint solver. Following our block summary method, we could generate over-approximate encoding of the network block to summarize the relationship between the start layer and end layer of the block. This could potentially lead to a significant decrease in the number of constraints and make such analyzer more amenable to handle larger networks.

6 Related Work

Existing works on analyzing and verifying the robustness of neural networks can be broadly categorized as *complete* or *incomplete* methods: given sufficient time and computational resource, a complete verifier can always provide a definite answer (*yes* or *no*) indicating whether a neural network model is robust or not, while an incomplete verifier might return an *unknown* answer.

Typical complete methods include the works in [6,7,19,20], which encode the verification problems into arithmetic constraints, and utilize the corresponding sound and complete solvers to solve them. In particular, the techniques in [6,19] are based on MILP (mixed integer liner program) solvers, while the verifiers in [7,20] use SMT (satisfiability modulo theory) solvers in the theory of linear real arithmetic with ReLU constraints. Although these solvers can give precise answers, they are also costly when handling a large set of constraints with many variables. Hence, it is difficult for complete verifiers to scale up.

In a different approach, the works [3–5] introduce incomplete methods which over-approximate the behavior of neural networks using techniques like abstraction interpretation, reachability analysis etc. Even though they might lose precision in certain situations, they are more scalable than those complete methods. The abstract domain devised for abstract interpretation is the essential part of the analysis. There has been progress in the design of abstract domains, from interval domains in [3] to zonotope domains in [4] and finally to polyhedral domains

in [5]. These domains allow the verifiers to prove more expressive specifications, such as the robustness of neural networks, and handle more complex networks, like the deep convolutional networks. Especially, the polyhedral domain in [5] can scale up the performance of the verifier DeepPoly to handle large networks. Recently, there have been also efforts on combining both incomplete method (such as abstraction) and complete method (MILP encoding and solving), such as the works [19] and [21].

All above-mentioned verification methods are actually doing qualitative verification by considering only two cases: whether the network satisfies the property, or not. In most recent years, researchers have been looking into quantitative verification to check how often a property is satisfied by a given network under a given input distribution. For instance, the work [10] examines if majority portion of the input space still satisfies the property with a high probability.

7 Conclusion

We have proposed the block summarization and bounded back-substitution to reduce the computational steps during back-substitution process, making it more amenable for analyzer to handle larger network with limited computational resources, such as having only CPU setup. We instantiated our idea on top of Deep-Poly and implement a system called BBPoly. Experiment shows that BBPoly can achieve the verified precision comparable to DeepPoly but save both running time and memory allocation. Furthermore, our system is capable of analyzing large networks with up to one million neurons while DeepPoly cannot conclude within a decent timeout. We believe that our proposal can assist with efficient analysis and be applied to other methods for better scalability.

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A Concrete Bound Computation from Symbolic Constraints

As can be seen from the illustrative example in Section 2.2, the symbolic constraints are used to compute the concrete bounds of affine neurons and this is the stratagem proposed in DeepPoly to achieve tighter intervals. To do so, it requires us to evaluate the minimum or maximum value for the symbolic constraints.

For symbolic lower constraint of neuron m, suppose we have $m \ge w_1 \cdot x_1 + \cdots + w_n \cdot x_n$. Note that x_1, \ldots, x_n represent the neurons from some preceding layer. Since the analysis of the preceding neurons has completed, we know the concrete bounds for each $x_i \in \{x_1, \ldots, x_n\}$ and have $x_i \in [l_i, u_i]$.

To evaluate the expression $w_1 \cdot x_1 + \cdots + w_n \cdot x_n$ for lower bound computation, we will calculate the minimum value β of $w_1 \cdot x_1 + \cdots + w_n \cdot x_n$. The minimum value is computed by the following rules:

- For positive coefficient w_i , replace x_i with the concrete lower bound l_i .
- For *negative* coefficient w_i , replace x_i with the concrete *upper* bound u_i .

Therefore, we have $m \ge w_1 \cdot x_1 + \cdots + w_n \cdot x_n \ge \beta$, and β functions as the concrete lower bound of neuron m. Similarly for the upper bound computation of m, we have symbolic constraint $m \le w_1 \cdot x_1 + \cdots + w_n \cdot x_n$ and calculate the maximum value δ of $w_1 \cdot x_1 + \cdots + w_n \cdot x_n$ by:

- For positive coefficient w_i , replace x_i with the concrete upper bound u_i
- For negative coefficient w_i , replace x_i with the concrete lower bound l_i

So we have $m \le w_1 \cdot x_1 + \cdots + w_n \cdot x_n \le \delta$ and δ is the concrete upper bound of neuron m.

B Explanation why a block is ended by an affine layer

Without loss of generality, suppose the symbolic lower constraint for a neuron m at a layer is expressed as a linear combination of neurons \vec{x}_i at a preceding layer: $m \ge w_1 \cdot x_1 + \cdots + w_n \cdot x_n$. In a back-substitute step, \vec{x}_i will be replaced by its own symbolic lower constraint expressed in terms of its preceding layer: $x_i \ge u_{i1} \cdot y_1 + \cdots + u_{in} \cdot y_n$. Expressing the symbolic lower constraint of m in terms of \vec{y}_j would require n^2 computation for combining coefficients \vec{w}_i and \vec{u}_{ij} . On the other hand, some of these combining computations can be eliminated if the ReLU neurons connecting neuron m and layer \vec{x}_i can be set to 0. As it is not infrequent for ReLU neuron values to be set to 0 (for its symbolic lower constraint), by letting a block to end at an affine layer and begin at an ReLU layer, we increase the opportunity to leverage on the symbolic lower constraint of the ReLU neurons being 0, which will lead to elimination of n^2 coefficient computation when back propagating from one block to another. Thus, to preserve the back-substitution approach in DeepPoly and speed up our back-substitution over block summary, we elect to end summary block with an affine layer.

C Empirical proof of bounded back-substitution heuristic

To empirically test the idea of bounded back-substitution, we experiment on the networks enumerated in Table 4, where the classified dataset, the layer number and the number of hidden neurons are listed as well. Please be noted that one actual layer in the network corresponds to one affine layer and one ReLU layer in the analysis. Therefore networks with 9 layers totally have 18 layers in DeepPoly's representation, so setting *max_backsub_steps* as 18 meaning that we will NOT bound the back-substitution process and it will be equal to DeepPoly method.

	v		1	
Network	Type	Dataset	#Layer	#hidden neurons
mnist_9_200	fully connected	MNIST	9	1,610
mnist_9_100	fully connected	MNIST	9	810
mnist_ffcnRELU_Point_6_500	fully connected	MNIST	6	3,000
mnist_6_100	fully connected	MNIST	6	510
$convSuperRELU_mnist$	convolutional	MNIST	6	88,544
convBigRELU_mnist	convolutional	MNIST	6	48,064
cifar_6_100	fully connected	CIFAR10	6	610
convBigRELU_cifar	convolutional	CIFAR10	6	62,464

Table 4: Networks for early termination experiment

Figure 8 demonstrates the tendency of interval length of output neuron with respect to different setting of *max_backsub_steps*. The interval length is averaged over different input images, different perturbations applied and different output neurons. From the outline, we can see that as we allow deeper back-substitution, the benefit will become less and less significant.

D Perturbation size for fully-connected and convolutional networks

We set six different values for perturbation size ϵ according to the following settings made in DeepPoly paper:

- $ϵ ∈ {0.005, 0.01, 0.015, 0.02, 0.025, 0.03}$ for MNIST fully-connected networks;
- $-\epsilon \in \{0.02, 0.04, 0.06, 0.08, 0.1, 0.12\}$ for MNIST convolutional networks;
- $\epsilon \in \{0.0002, 0.0004, 0.0006, 0.0008, 0.001, 0.0012\}$ for CIFAR10 fully-connected networks;
- $ε ∈ {0.002, 0.004, 0.006, 0.008, 0.01, 0.012}$ for CIFAR10 convolutional networks.

Note that, since the specified ϵ set couldn't really differentiate between various ϵ and methods for MNIST convolutional big network as demonstrated in Figure 6c, so we choose a larger set $\epsilon \in \{0.12, 0.14, 0.16, 0.18, 0.2, 0.22\}$ for MNIST convolutional super network.

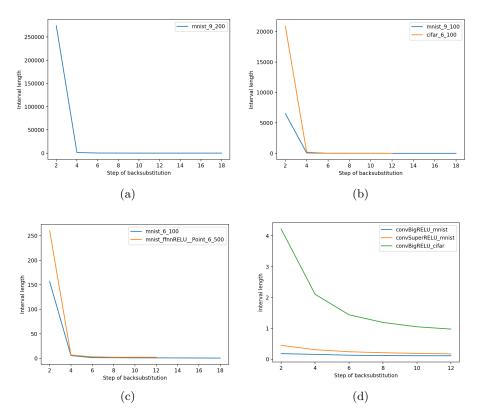


Fig. 8: Empirical result of bounded back-substitution

E Precision and time comparison in table

We also demonstrate the precision and average execution time per image in tables. The experimental result of fully-connected and convolutional networks for MNIST/CIFAR10 is given in Table 5. In the table, we record the number of verified images out of 100 test images together with the average execution time per image (which is recorded within the square brackets) for different experiment settings and three different methods. The three methods include

- DeepPoly;
- Our method with block summarization, which is denoted as "Block_sum";
- Our summary-over-input method, denoted as "Input_sum".

F Additional experimental result on the neural network MNIST 9x200 with different block sizes of 3, 4, 5

In Table 6, the record "83[2.658]" indicates that BBPoly verifies robustness for 83 images, with average execution time 2.658 seconds for each image.

Neural	ral Perturbation #Verified Images out of 100 Images and Time(s)						
Network	Size	DeepPoly	BBPoly	BBPoly			
			(Block_sum)	(Input_sum)			
	0.005	92[3.299]	74[2.773]	66[2.644]			
	0.01	67[3.598]	18[3.170]	12[3.068]			
MNIST	0.015	29[4.011]	3[3.544]	2[3.368]			
_9_200	0.02	8[4.466]	1[3.838]	0[3.566]			
	0.025	3[4.720]	0[4.026]	0[3.751]			
	0.03	2[4.897]	0[4.135]	0[3.851]			
	0.005	99[7.244]	99[5.494]	99[5.336]			
	0.01	98[7.357]	97[5.452]	97[5.467]			
MNIST_ffcn	0.015	95[7.673]	94[5.634]	94[5.622]			
_Point_6_500	0.02	89[8.039]	82[6.065]	82[5.966]			
	0.025	71[8.754]	58[6.668]	55[6.717]			
	0.03	49[9.545]	38[7.489]	37[7.390]			
	0.02	95[33.96]	95[18.87]	95[12.40]			
MNICT	0.04	95[33.12]	95[18.74]	95[17.76]			
MNIST	0.06	95[33.68]	95[18.85]	95[18.31]			
_convBig _RELU	0.08	95[34.21]	95[18.92]	95[17.37]			
LU	0.1	94[33.55]	93[18.59]	93[17.96]			
	0.12	93[34.06]	92[19.38]	91[18.21]			
	0.12	96[133.5]	96[75.22]	95[73.94]			
MNIST	0.14	81[138.7]	77[78.12]	74[78.12]			
	0.16	28[148.7]	10[84.84]	6[82.90]			
₋convSuper _RELU	0.18	0[159.5]	0[93.19]	0[90.12]			
LU	0.2	0[179.8]	0[102.6]	0[98.21]			
	0.22	0[197.9]	0[114.4]	0[109.8]			
	0.0002	55[22.32]	55[14.43]	55[15.18]			
CIFAR10	0.0004	53[22.63]	53[14.53]	53[15.18]			
_ffcn_Point	0.0006	53[22.75]	52[14.76]	49[15.08]			
_6_500	0.0008	52[22.71]	46[14.74]]	46[15.16]			
_0_300	0.001	48[22.76]	43[14.88]	43[15.36]			
	0.0012	46[22.70]	43[15.07]	43[15.35]			
	0.002	51[89.07]	51[42.45]	51[37.46]			
CIFAR10	0.004	46[89.69]	42[41.38]	42[37.49]			
	0.006	31[91.04]	31[41.88]	31[37.78]			
_convBig _RELU	0.008	24[91.26]	21[41.87]	21[37.94]			
LU	0.01	15[91.58]	12[41.87]	12[38.32]			
	0.012	11[92.56]	9[41.79]	9[38.87]			

Table 5: Precision for convolutional and fully-connected networks

G Algorithm of analysis with summary-over-input method

We present the overall procedure of analysis with summary-over-input in Algorithm 2. The algorithm is very similar to Algorithm 1, the differences between the two algorithms are:

NT	D	#Verified Images out of 100 Images and Time(
Neural Network	Perturbation Size	DeepPoly	BBPoly (Block_sum)	BBPoly (Input_sum)			
	0.005	92[3.299]	74[2.773]	66[2.644]			
MNIST	0.01	67[3.598]	18[3.170]	12[3.068]			
_9_200	0.015	29[4.011]	3[3.544]	2[3.368]			
blk_size=3	0.02	8[4.466]	1[3.838]	0[3.566]			
DIK_SIZE=0	0.025	3[4.720]	0[4.026]	0[3.751]			
	0.03	2[4.897]	0[4.135]	0[3.851]			
	0.005	92[3.299]	83[2.658]	82[2.683]			
MNIST	0.01	67[3.598]	29[3.174]	29[3.118]			
_9_200	0.015	29[4.011]	6[3.561]	6[3.530]			
blk size=4	0.02	8[4.466]	2[3.725]	2[3.767]			
DIK_SIZE=4	0.025	3[4.720]	0[3.910]	0[3.900]			
	0.03	2[4.897]	0[3.960]	0[3.968]			
	0.005	92[3.299]	88[2.617]	88[2.643]			
MNIST	0.01	67[3.598]	37[3.041]	37[3.047]			
_9_200	0.015	29[4.011]	9[3.504]	9[3.473]			
blk_size=5	0.02	8[4.466]	2[3.712]	2[3.729]			
DIK_SIZE=0	0.025	3[4.720]	0[3.831]	0[3.854]			
	0.03	2[4.897]	0[3.930]	0[3.940]			

Table 6: Precision and execution time for different block sizes

 The bounded back-substitution heuristic is not involved in summary-overinput method;

 In the summary-over-input method, the summary is directly defined over the actual input layer of the network in stead of the start layer of the given block. Therefore, after back-substitution with summary, the new constraint will directly be defined over input layer (line 13-14);

- If γ_k is the end layer of a block and the current preceding layer γ_{pre} is the input layer of the network, we then store the current Υ_k as the block summary of layer γ_k (line 19-20).

Algorithm 2: Overall analysis procedure with summary-over-input							
Input: M is the network (eg. Figure 2);							
σ is the network segmentation parameter							
Annotatation: input layer of M as γ_{in} ;							
constraint set of affine layer γ_k as Υ_k ;							
the set of concrete bounds for neurons in layer $\gamma_k \in M$ as C_k ;							
the segmented network model as \mathcal{M}							
Assumption: the analysis is conducted in ascending order of the layer index							
Output: tightest concrete bounds C_k computed for all layer $\gamma_k \in M$							
1: $\mathcal{M} \leftarrow SegmentNetwork(M, \sigma)$							
2: for all layer $\gamma_k \in \mathcal{M}$ do							
3: if IsReluLayer (γ_k) then							
4: $\gamma_{pre} \leftarrow PredecessorLayer(\gamma_k)$							
5: $C_k \leftarrow ComputeReluLayer(\gamma_{pre})$							
6: else							
7: $\gamma_{pre} \leftarrow PredecessorLayer(\gamma_k)$							
8: $\Upsilon_k \leftarrow GetSymbolicConstraints(\gamma_k)$							
9: $C_k \leftarrow EvaluateConcreteBounds(\Upsilon_k, \gamma_{pre})$							
10: while $\gamma_{pre} \neq \gamma_{in} \mathbf{do}$							
11: if $lsEndLayer(\gamma_{pre})$ { γ_{pre} is the end layer of a block} then							
12: $sum \leftarrow ReadSummary(\gamma_{pre})$							
13: $\Upsilon_k \leftarrow BacksubWithBlockSummary(\Upsilon_k, sum)$							
14: $\gamma_{pre} \leftarrow \gamma_{in}$							
15: else							
16: $sym_cons \leftarrow GetSymbolicConstraints(\gamma_{pre})$							
17: $\Upsilon_k \leftarrow BacksubWithSymbolicConstraints(\Upsilon_k, sym_cons)$							
18: $\gamma_{pre} \leftarrow PredecessorLayer(\gamma_{pre})$							
19: if $lsEndLayer(\gamma_k)$ and $\gamma_{pre} = \gamma_{in}$ then							
20: StoreSummary (γ_k, Υ_k)							
21: $temp_ck \leftarrow EvaluateConcreteBounds(\Upsilon_k, \gamma_{pre})$							
22: $C_k \leftarrow UpdateBounds(C_k, temp_ck)$							
23: return all C_k for all layer $\gamma_k \in \mathcal{M}$							