Efficient Exact Verification of Binarized Neural Networks (Supplementary Material)

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1 Details of BNN encoding

We present details for encoding the inference computation of a single linear-BatchNorm-binarize module in a BNN. Recall that such a module is defined for an input $x \in \{0,1\}^n$, an output $y \in \{0,1\}^m$, and a weight $W \in \mathbb{R}^{m \times n}$:

$$y = \operatorname{bin}_{act}(\operatorname{BatchNorm}(\operatorname{bin}_{w}(W)x)) \tag{1}$$

where:

$$bin_w(W) = sign(W) \in \{-1, 1\}^{m \times n}$$

BatchNorm(x) = $\gamma \odot \frac{x - E[x]}{\sqrt{Var[x] + \epsilon}} + \beta$

is the Batch Normalization [1] with parameters $\gamma \in \mathbb{R}^m$ and $\beta \in \mathbb{R}^m$

$$bin_{act}(x) = (x \ge 0) = (sign(x) + 1)/2 \in \{0, 1\}^m$$

Batch Normalization becomes a linear transformation in inference:

$$x^{\rm BN} = k^{\rm BN} \odot x + b^{\rm BN} \tag{2}$$

where:

$$\begin{split} k^{\rm BN} &= \frac{\gamma}{\sqrt{\sigma^2 + \epsilon}} \\ b^{\rm BN} &= \beta - k^{\rm BN} \mu \\ \mu \quad \text{is the mean of } x \text{ on training set} \\ \sigma^2 \quad \text{is the variance of } x \text{ on training set} \end{split}$$

With $W^{\text{bin}} = \text{bin}_w(W)$ being a fixed parameter, we can rewrite the computation of a single element of y in (1) as the following:

$$y_i = \left(k_i^{\text{BN}} \sum_{j=1}^n W_{ij}^{\text{bin}} x_j + b_i^{\text{BN}} \ge 0\right)$$
(3)

To encode (3) as a reified cardinality constraint, we consider 1 and TRUE interchangeably and 0 and FALSE interchangeably. If $W_{ij}^{\rm bin}=1$, we have $W_{ij}^{\rm bin}x_j=x_j$, and if $W_{ij}^{\rm bin}=-1$, we rewrite

34th Conference on Neural Information Processing Systems (NeurIPS 2020), Vancouver, Canada.

 $W_{ij}^{\text{bin}}x_j = -x_j = (1-x_j) - 1 = \neg x_j - 1$. With such substitutions of $W_{ij}^{\text{bin}}x_j$ we obtain a reified cardinality constraint:

$$y_{i} = \left(k_{i}^{\text{BN}} \sum_{j=1}^{n} W_{ij}^{\text{bin}} x_{j} + b_{i}^{\text{BN}} \ge 0\right)$$

$$= \left(k_{i}^{\text{BN}} \left(\sum_{j=1}^{n} l_{ij}(x_{j}) + b_{i}^{\text{SAT}}\right) + b_{i}^{\text{BN}} \ge 0\right)$$

$$= \left(\sum_{j=1}^{n} l_{ij}(x_{j}) \gtrless \left[b_{i}(k^{\text{BN}}, W^{\text{bin}}, b^{\text{BN}})\right]\right)$$
(4)

where:

$$l_{ij}(x_j) = \begin{cases} x_j & \text{if } W_{ij}^{\text{bin}} = 1\\ 0 & \text{if } W_{ij}^{\text{bin}} = 0\\ \neg x_j & \text{if } W_{ij}^{\text{bin}} = -1 \end{cases}$$

$$b_i^{\text{SAT}} = \sum_{j=1}^n \min\left(W_{ij}^{\text{bin}}, 0\right)$$

$$b_i(k^{\text{BN}}, W^{\text{bin}}, b^{\text{BN}}) = -\frac{b_i^{\text{BN}}}{k_i^{\text{BN}}} - b_i^{\text{SAT}}$$

$$\left(x \gtrsim y\right) = \begin{cases} x \geq y & \text{if } k_i^{\text{BN}} > 0\\ x \leq y & \text{if } k_i^{\text{BN}} < 0 \end{cases}$$

$$[x] = \begin{cases} \begin{bmatrix} x \\ x \end{bmatrix} & \text{if } k_i^{\text{BN}} > 0\\ x \end{bmatrix}$$

2 Experimental details

Experimental environment We conduct our experiments on a workstation equipped with two GPUs (NVIDIA Titan RTX and NVIDIA GeForce RTX 2070 SUPER), 128 GiB of RAM and an AMD Ryzen Threadripper 2970WX 24-core processor. We use the PyTorch [3] framework to train all the networks.

Training method We train the networks using the Adam optimizer [2] for 200 epochs with a minibatch size of 128, with the exception of the undefended conv-small networks on CIFAR10 which is trained for only 90 epochs to avoid overfitting. Due to fluctuations of test accuracy between epochs, we select from the last three epochs the model with the highest natural test accuracy or PGD accuracy on the first 40 training minibatches. The mean and variance statistics of batch normalization layers are recomputed on the whole training set after training finishes. Learning rate is initially 1e-4 and decayed to half on epoch 150. We use PGD with adaptive gradient cancelling to train robust networks, where the perturbation bound ϵ is increased linearly from 0 to the desired value in the first 100 epochs and the number of PGD iteration steps grows linearly from 0 to 10 in the first 50 epochs.

The parameter α in adaptive gradient cancelling is chosen to maximize the PGD attack success rate evaluated on 40 minibatches of training data sampled at the first epoch. Candidate values of α are between 0.6 to 3.0 with a step of 0.4. Note that α is a global parameter shared by all neurons.

We do not use any data augmentation techniques for training. Due to limited computing resource and significant differences between the settings we considered, data in this paper are reported based on one evaluation run.

Weight initialization All weights for the convolutional or fully connected layers are initialized from a Gaussian distribution with standard deviation 0.01, and the mask weights M_W in BinMask are enforced to be positive by taking the absolute value during initialization.

Table 1.	Verification	time with	varvina	nerturbation	hounde	Time	limit ic	120 seconds.
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Dataset	Network	Mean Solve Time			Solver Timeout			Mean Build+Solve Time		
Training ϵ		$\epsilon = \epsilon_0$	$\epsilon=\epsilon_1$	$\epsilon=\epsilon_2$	$\epsilon = \epsilon_0$	$\epsilon=\epsilon_1$	$\epsilon = \epsilon_2$	$\epsilon = \epsilon_0$	$\epsilon=\epsilon_1$	$\epsilon = \epsilon_2$
$\begin{array}{l} \text{MNIST} \\ \epsilon = 0.1 \end{array}$	conv-small conv-large	0.0004 0.0025	0.0021 0.0129	0.0713 0.1269	0	0	0.01% 0.01%	0.0162 0.1115	0.0180 0.1197	0.0876 0.2254
$\begin{array}{c} \hline \text{MNIST} \\ \epsilon = 0.3 \end{array}$	conv-small	0.0004 0.0010	0.0004 0.0018	0.0006 0.0039	0	0	0	0.0147 0.1162	0.0155 0.1142	0.0146 0.1179
$\begin{array}{c} \hline \text{CIFAR10} \\ \epsilon = 2/255 \end{array}$	conv-small	0.0013 0.0097	0.0017 0.0136	0.0025 0.0141	0	0	0	0.0271 0.1750	0.0298 0.1947	0.0366 0.1918
CIFAR10 $\epsilon = 8/255$	conv-small conv-large	0.0009 0.0087	0.0011 0.0084	0.0014 0.0090	0	0	0	0.0236 0.1704	0.0284 0.1696	0.0327 0.1781

Other hyperparameters The input quantization step s is set to be 0.61 for training on the MNIST dataset, and $0.064 \approx 16.3/255$ for CIFAR10, which are chosen to be slightly greater than twice the largest perturbation bound we consider for each dataset. The CBD loss is applied on conv-large networks only and η is set to be $5\mathrm{e}{-4}$ unless otherwise stated. We apply a weight decay of $1\mathrm{e}{-7}$ on the binarized mask weight M_W of BinMask for conv-small and conv-large networks, and the weight decay is $1\mathrm{e}{-5}$ for the MNIST-MLP network. PGD accuracies reported for the test set are evaluated with 100 steps of PGD iterations.

3 Adversarial robustness against varying perturbation bounds

We run the verifier with varying perturbation bounds and present the time in Table 1 and the accuracy in Table 2. The bounds are set to be $\epsilon_0=0.1$, $\epsilon_1=0.2$, and $\epsilon_2=0.3$ for MNIST and $\epsilon_0=2/255$, $\epsilon_1=5/255$, and $\epsilon_2=8/255$ for CIFAR10. We note a few interesting discoveries:

- 1. For the same network, the verification becomes slower for larger perturbation bounds. This behavior is expected because a larger bound corresponds to a larger input perturbation space, which makes the verification problem harder to solve.
- 2. For the same bound used in verification, verification is faster for a more robust network that is trained with a larger perturbation bound. One plausible explanation is that robust networks are less sensitive to input changes, and they naturally allow the solver to learn simpler clauses that describe relationships between neurons. Another factor is that stronger adversarial training usually (but not always) induces more sparse weights as can be seen in Table 2.
- 3. The gap between PGD accuracy and verifiable accuracy for a fixed test perturbation bound gets narrower as the training perturbation becomes stronger. More interestingly, when tested against perturbations of ϵ_0 , although the network has higher verifiable accuracy when it is trained with stronger perturbations, its PGD accuracy even gets lower (comparing PGD accuracy with $\epsilon=\epsilon_0$ in Table 2). Such phenomenon suggests that PGD accuracy is not always positively correlated with verfiable accuracy and the adversarial training algorithm could be further improved.

4 Ablation study

We conduct comprehensive experiments to study the effectiveness of our proposed methods — namely BinMask, CBD loss, and native handling of the reified cardinality constraints in the MiniSatCS verifier — under different settings. We apply various combinations of ternary quantization, BinMask, and CBD loss during training, and verify the networks using multiple solvers. The experimental results are presented in Table 3 and Table 4.

For each dataset, we train the conv-small and conv-large networks under two training settings: undefended (i.e., $\epsilon=0$) and adversarial training with a large perturbation bound ($\epsilon=0.3$ for MNIST and $\epsilon=8/255$ for CFAR10). We tune the weight decay coefficient of ternary quantization so that the total sparsity is close to that of BinMask or BinMask+CBD. All BinMask networks have the same

Table 2: Verifiable accuracy with varying perturbation bounds.

Dataset	Network	Test Accuracy	PGD A	dversarial A	ccuracy	Ver	ifiable Accu	racy	Sparsity
Training ϵ			$\epsilon = \epsilon_0$	$\epsilon = \epsilon_1$	$\epsilon = \epsilon_2$	$\epsilon = \epsilon_0$	$\epsilon = \epsilon_1$	$\epsilon = \epsilon_2$	
$\begin{array}{l} \text{MNIST} \\ \epsilon = 0.1 \end{array}$	conv-small	97.44%	93.47%	86.22%	70.68%	89.29%	66.49%	25.45%	90%
	conv-large	97.46%	95.47%	92.56%	86.98%	91.68%	75.35%	40.14%	91%
$\begin{array}{c} \text{MNIST} \\ \epsilon = 0.3 \end{array}$	conv-small	94.31%	91.74%	87.43%	80.70%	90.24%	82.14%	66.42%	94%
	conv-large	96.36%	94.82%	92.19%	87.90%	93.71%	88.55%	77.59%	87%
CIFAR10 $\epsilon = 2/255$	conv-small conv-large	46.58% 47.35%	33.70% 38.22%	18.85% 28.20%	9.32% 19.60%	26.13% 30.49%	8.26% 13.30%	2.39% 4.98%	94% 85%
CIFAR10 $\epsilon = 8/255$	conv-small	37.75%	33.88%	29.02%	24.60%	32.18%	24.82%	18.93%	96%
	conv-large	35.00%	32.45%	29.17%	26.41%	31.20%	26.39%	22.55%	98%

Table 3: Comparison of methods on 40 randomly chosen MNIST test images with solving time limit of 3600 seconds.

$\epsilon_{ ext{train}}$	Network Architecture	Training Method	Test Accuracy	Sparsity	Solver	Mean Solve Time	Median Solve Time	Timeout	Verifiable Accuracy
		Ternary	97.59%	81%	MiniSatCS	756.288	4.281	15%	0%
	conv-small	BinMask	97.35%	84%	MiniSatCS MiniSat Z3	0.002 2.249 0.089	0.002 1.142 0.089	0 0 0	52% 52% 52%
					RoundingSat	0.048	0.042	0	52%
0		Ternary	99.07%	86%	MiniSatCS	2522.082	3600.002	68%	0%
		Ternary+CBD	95.58%	87%	MiniSatCS	886.007	21.711	20%	0%
	conv-large	Ternary+10xCBD	92.91%	78%	MiniSatCS	342.097	4.742	5%	2%
		BinMask	98.94%	86%	MiniSatCS	2595.032	3600.001	70%	2%
		BinMask+CBD	96.88%	89%	MiniSatCS MiniSat Z3 RoundingSat	0.664 225.861 146.567 33.922	0.028 18.761 0.997 0.702	0 0 0	70% 70% 70% 70%
		Ternary (wd0)	94.72%	80%	MiniSatCS	186.935	0.105	5%	30%
		Ternary (wd1)	89.53%	93%	MiniSatCS	0.005	0.002	0	35%
	conv-small	BinMask	94.31%	94%	MiniSatCS MiniSat Z3 RoundingSat MiniSat-CN	0.001 0.060 0.040 0.021 0.034	0.001 0.024 0.040 0.031 0.008	0 0 0 0	52% 52% 52% 52% 52%
0.3		Ternary	96.89%	91%	MiniSatCS	2828.479	3600.001	78%	0%
	conv-large	Ternary+CBD	81.33%	80%	MiniSatCS MiniSat Z3 RoundingSat	0.034 173.877 2.093 2.941	0.020 23.527 1.840 1.642	0 0 0 0	42% 42% 42% 42%
	3	BinMask	98.88%	82%	MiniSatCS	2442.698	3600.001	65%	5%
		BinMask+CBD	96.26%	87%	MiniSatCS MiniSat Z3 RoundingSat MiniSat-CN	0.005 0.242 0.530 0.088 0.388	0.005 0.045 0.540 0.104 0.076	0 0 0 0	52% 52% 52% 52% 52%

weight decay of 1e-7, except for the undefended conv-large networks on CIFAR10 which have a larger weight decay of 2.5e-6 due to the low sparsity under the default setting.

We consider the following questions for ablation study:

Q: Does native handling of reified cardinality constraints always facilitate the SAT solving?

A: Yes. We compare the solving time of MiniSatCS, MiniSat, Z3, and RoundingSat on both network architectures trained on both datasets. The sequential counters encoding is used for MiniSat, and we also evaluate MiniSat-CN that uses the cardinality networks encoding on a few cases, but it

Table 4: Comparison of methods on 40 randomly chosen CIFAR10 test images with solving time limit of 3600 seconds.

$\epsilon_{\mathrm{train}}$	Network Architecture	Training Method	Test Accuracy	Sparsity	Solver	Mean Solve Time	Median Solve Time	Timeout	Verifiable Accuracy
			54.78%	82%	MiniSatCS MiniSat	0.267 327.303	0.006 50.036	0 7%	0% 0%
		Ternary			7.3	411.638	117.604	5%	0%
	conv-small				RoundingSat	0.361	0.098	0	0%
	COMV DMGII				MiniSatCS	0.003	0.003	0	0%
		BinMask	55.22%	79%	MiniSat	3.981	3.577	0	0%
0		Dilliviask	33.22 70	1970	Z3	0.590	0.376	0	0%
					RoundingSat	0.081	0.077	0	0%
		Ternary	69.25%	89%	MiniSatCS	823.370	1.860	20%	0%
	conv-large	BinMask	67.46%	94%	MiniSatCS	300.404	3.201	5%	0%
		BinMask+CBD	63.18%	88%	MiniSatCS	1.415	0.048	0	0%
					MiniSat	168.079	69.471	0	0%
					Z3	3515.386	3600.121	92%	0%
					RoundingSat	19.162	0.858	0	0%
		Ternary	32.59%	95%	MiniSatCS	0.002	0.002	0	15%
	conv-small	BinMask	37.75%	96%	MiniSatCS	0.001	0.002	0	18%
					MiniSat	0.070	0.082	0	18%
					Z3	0.050	0.052	0	18%
					RoundingSat	0.033	0.043	0	18%
8/255		Ternary	34.60%	94%	MiniSatCS	241.572	0.047	5%	10%
		Ternary	34.00%	94%	RoundingSat	516.767	1.154	12%	10%
		BinMask	53.91%	88%	MiniSatCS	206.037	0.052	5%	0%
	conv-large	DIIIIVIASK	33.91%	88%	RoundingSat	301.062	0.546	7%	0%
		BinMask+CBD		-	MiniSatCS	0.009	0.011	0	20%
			38.75%	87%	MiniSat	0.224	0.267	0	20%
		DIMINIONACIDE	30.1370	0170	Z3	0.768	0.795	0	20%
					RoundingSat	0.218	0.126	0	20%

is not consistently better than MiniSat. Our solver MiniSatCS, extended from MiniSat with native handling of reified cardinality constraints, delivers a speedup of mean solving time by a factor of between 1.35 to 5104.94 times compared all other solvers in all cases, and the average speedup is 40.21. The speedup of median solving time of MiniSatCS compared to others is 8.93 to 75289.76. Note that although the encoding complexity of MiniSat-CN is $O(n\log^2 b)$ which is asymptotically better than O(nb) of MiniSat, the low cardinality bounds in our networks make such asymptotic comparison inaccurate. Also note that MiniSatCS is constantly faster than all other solvers, and no solver is constantly the second fastest (RoundingSat is usually faster than Z3 and MiniSat, but it is slower than Z3 in the Ternary+CBD setting with the adversarially trained conv-large network on MNIST).

Q: How fast do BinMask networks verify compared to ternary quantization networks?

A: For the conv-small networks, BinMask networks verify significantly faster than ternary networks with similar sparsity, especially in the undefended training setting. For the conv-large networks without the CBD loss, neither of them constantly verifies faster than the other. We note that for the conv-large networks, BinMask still produces more balanced layer-wise sparsities, which are, for example, $[9\%\ 21\%\ 21\%\ 28\%\ 90\%\ 87\%\ 41\%]$ and $[84\%\ 61\%\ 65\%\ 61\%\ 87\%\ 86\%\ 70\%]$ for the undefended ternary and BinMask networks on MNIST respectively. Their verification speeds are both slow because the high cardinality bounds dominate verification complexity, which are 115.3 and 119.4 on average for each neuron in the two networks respectively.

Q: How accurate are BinMask networks compared to ternary quantization networks?

A: Interestingly, ternary quantization networks have slightly higher test accuracy in most of the undefended training cases, but BinMask networks have both higher test accuracy and verifiable accuracy when trained adversarially. We highlight the comparison of Ternary (wd0), Ternary (wd1), and BinMask on the adversarially trained conv-small network in Table 3. The wd0 ternary

network has a weaker weight decay to match the accuracy with the BinMask network, but it verifies much slower and has lowered verifiable accuracy. The wd1 ternary network is trained with a stronger weight decay to match the sparsity of the BinMask network, but it has much lower test accuracy and also verifies slower. Our results suggest that BinMask not only reduces verification complexity, but also regularizes model capacity to make it more robust.

Q: Does the CBD loss reduce cardinality bound and speed up verification for ternary quantization networks?

A: Yes, but less effectively. We train conv-large networks on MNIST with ternary quantization and CBD loss as the Ternary+CBD networks shown in Table 3. The CBD loss induces denser networks with ternary quantization, and the weight decay of Ternary+CBD networks is increased by five times compared to Ternary networks to maintain comparable sparsity. The average cardinality bound of the undefended Ternary+CBD network is 4.3, compared to 115.3 of the Ternary network. Although the Ternary+CBD and BinMask+CBD networks achieve similar average cardinality bounds (4.3 vs 3.8), the ternary network has much higher maximal cardinality bound (146.3 vs 22.3). Therefore, the verification time of Ternary+CBD is significantly improved over Ternary but is still longer than that of the BinMask+CBD network. Ternary+10xCBD is obtained by increasing the CBD loss coefficient η by ten times on Ternary+CBD, which has a lower average cardinality bound of 3.2, but the maximal cardinality bound is not decreased (157.7) and its test accuracy is much worse. The adversarially trained Ternary+CBD network has a lower maximal cardinality bound of 73.1, which also verifies faster. Ternary quantization networks with the CBD loss suffer from a larger decline of test accuracy compared to BinMask networks. Our results suggest that lower cardinality bound reduces verification complexity, and the BinMask formulation makes it easier to optimize for lower cardinality bounds.

Q: Do other solvers benefit from more balanced layer-wise sparsities and/or lower cardinality bounds?

A: Yes. We evaluate MiniSat, Z3, and RoundingSat on a relatively easy to verify ternary network (undefended conv-small on CIFAR10 in Table 4). The results show that all the solvers achieve significant speedup on the corresponding BinMask network, although Z3 benefits more from BinMask than MiniSat and RoundingSat. We also try MiniSat and Z3 on the easiest-to-verify conv-large network trained with only BinMask (i.e., the one adversarially trained on CIFAR10), but MiniSat fails due to out of memory error, and Z3 always exceeds the one hour time limit (data not shown in the table). With BinMask+CBD they both verify much faster. RoundingSat also benefits from BinMask and BinMask+CBD in this setting as shown in the table. Note that the ternary network has lower test accuracy and higher overall sparsity, but still verifies slower for all the solvers. Our results suggest that our two strategies, which are inducing more balanced layer-wise sparsity and lower cardinality bounds, both reduce the complexity of the verification problem and facilitate all the solvers that we have considered.

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