Training Binarized Neural Networks using MIP and CP

Rodrigo Toro Icarte León Illanes Margarita P. Castro
Andre A. Cire Sheila A. McIlraith J. Christopher Beck

UNIVERSITY OF TORONTO
VECTOR INSTITUTE

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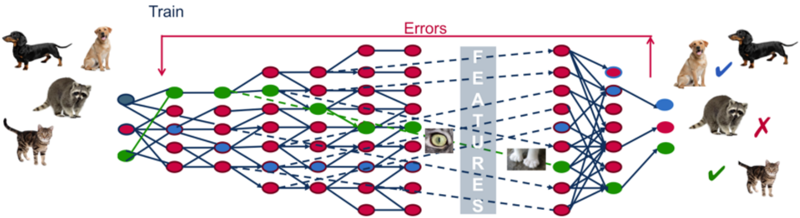
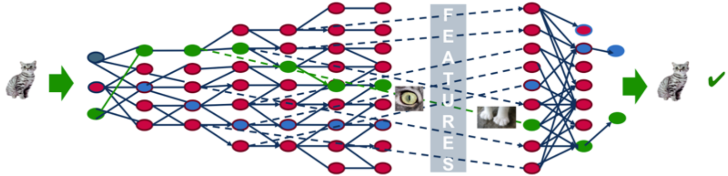
Binarized Neural Networks

Deep learning



Deep learning



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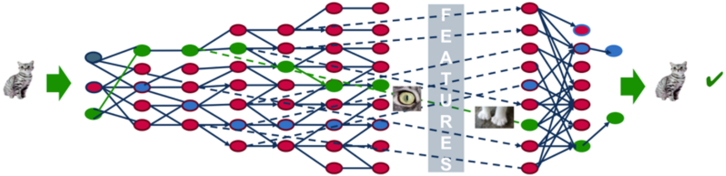

Binarized Neural Networks (BNNs)

- BNNs are NNs with binary weights and activations.
- Similar performance to standard deep learning.
- More efficient (w.r.t. energy and memory) at deploy time.

How to train BNNs

Supervised learning

Objective

Learn a function that maps inputs to outputs from examples.

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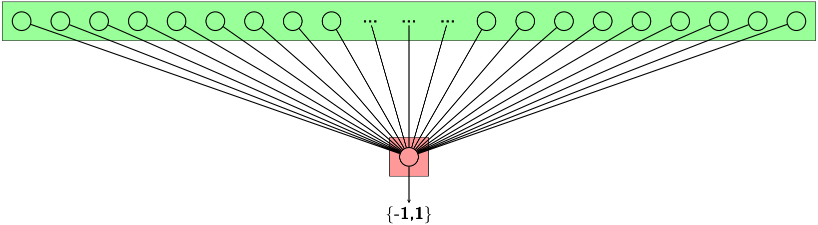
Learn a function that maps inputs to outputs from examples.

5 0 4 1 8 6 2 7 3 9

Example: Digit recognition.

The binarized perceptron



$$n = \begin{cases} +1 & \text{if } \sum_i w_i \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_i \in \{-1, 0, 1\}.$$

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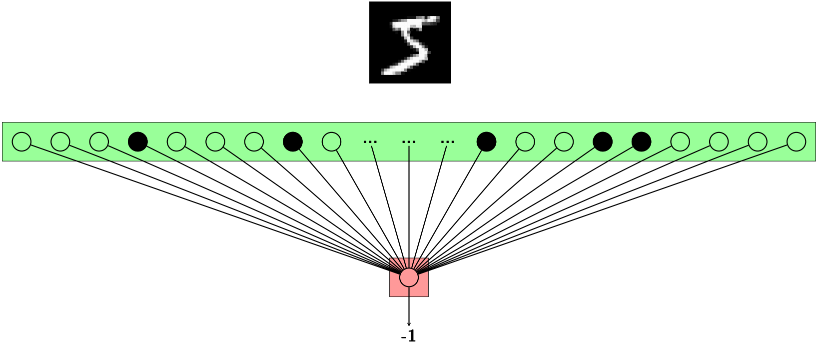

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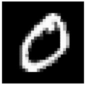

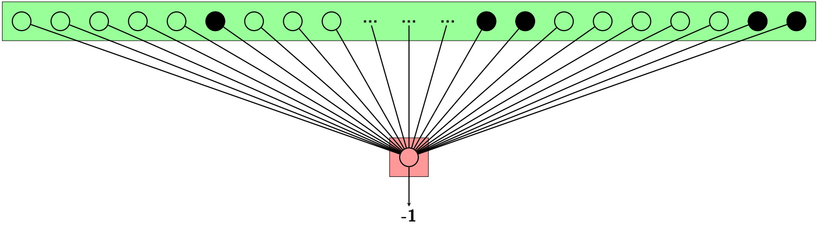

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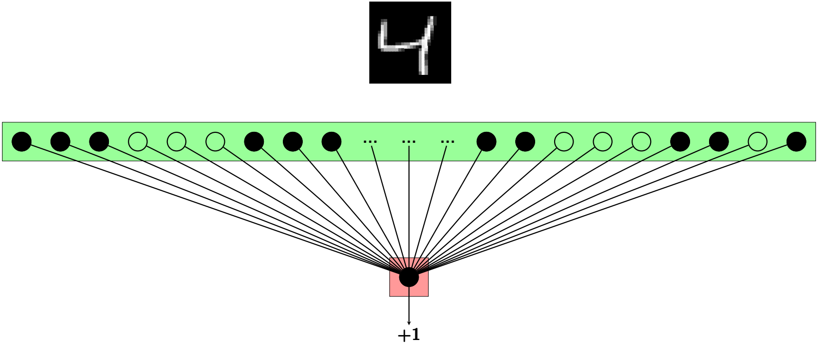

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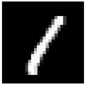

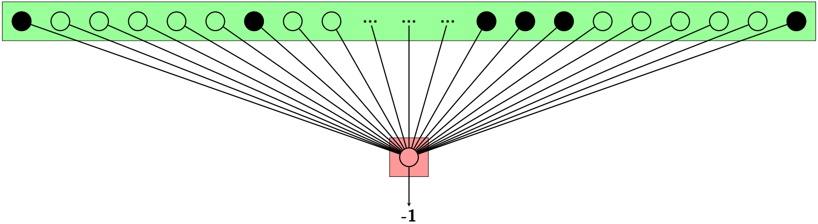

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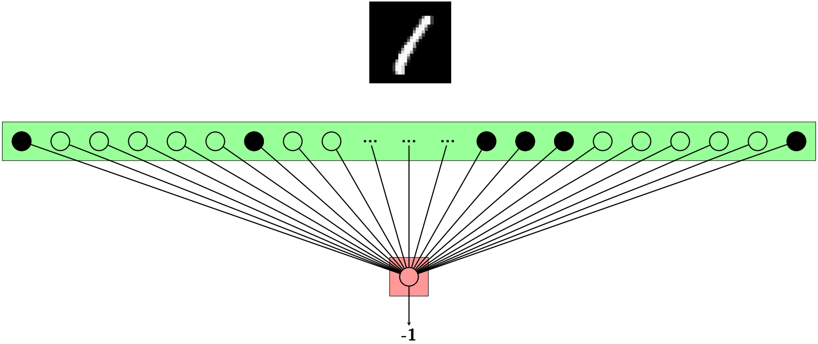
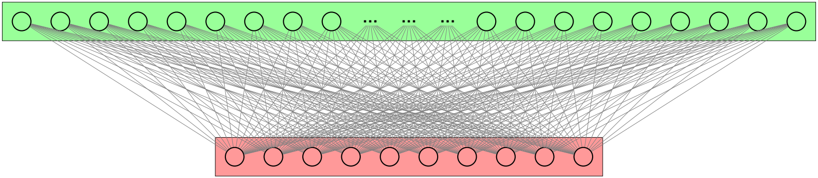


How can we use the perceptron for digit recognition?

The binarized perceptron



$$n_j = \begin{cases} +1 & \text{if } \sum_i w_{ij} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

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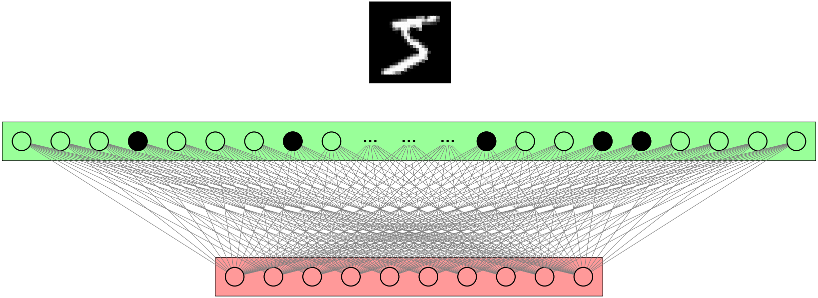

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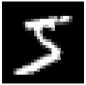
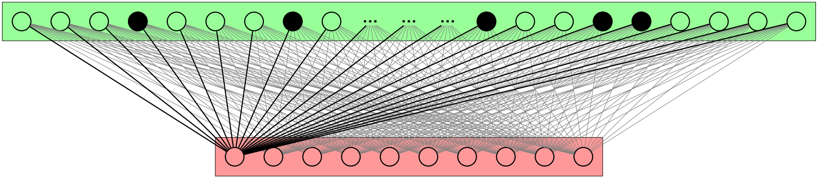
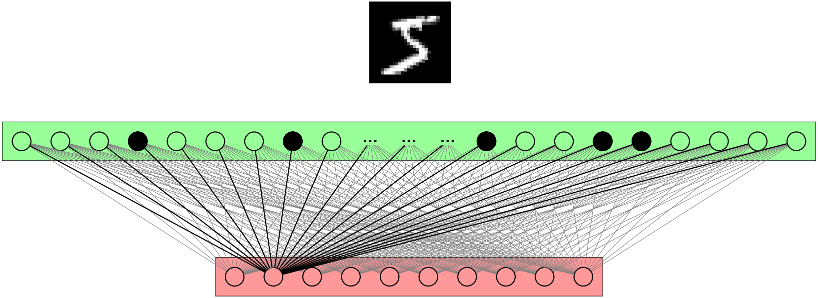




$$n_0 = \begin{cases} +1 & \text{if } \sum_i w_{i0} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

The binarized perceptron



$$n_1 = \begin{cases} +1 & \text{if } \sum_i w_{i1} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

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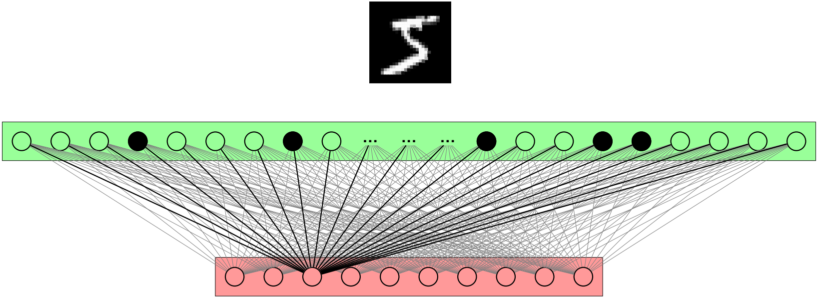

$$n_2 = \begin{cases} +1 & \text{if } \sum_i w_{i2} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

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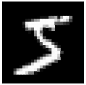
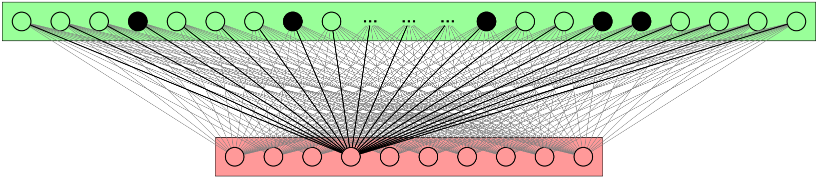
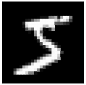
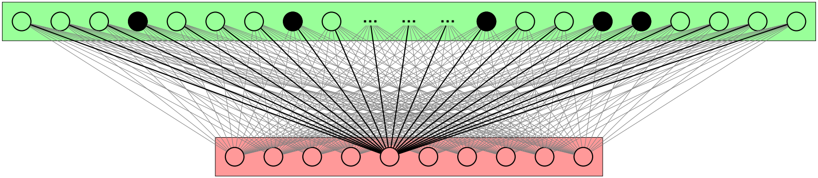




$$n_3 = \begin{cases} +1 & \text{if } \sum_i w_{i3} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

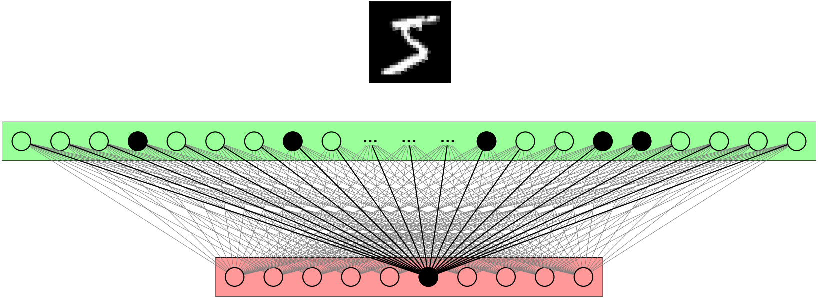
The binarized perceptron





$$n_4 = \begin{cases} +1 & \text{if } \sum_i w_{i4} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

The binarized perceptron



$$n_5 = \begin{cases} +1 & \text{if } \sum_i w_{i5} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

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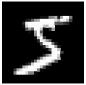
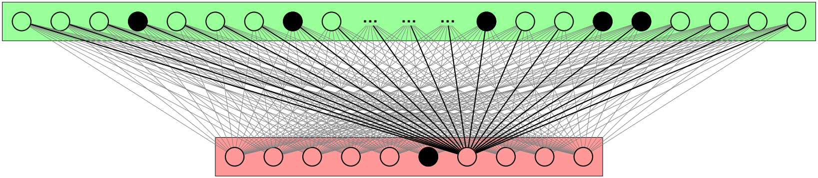
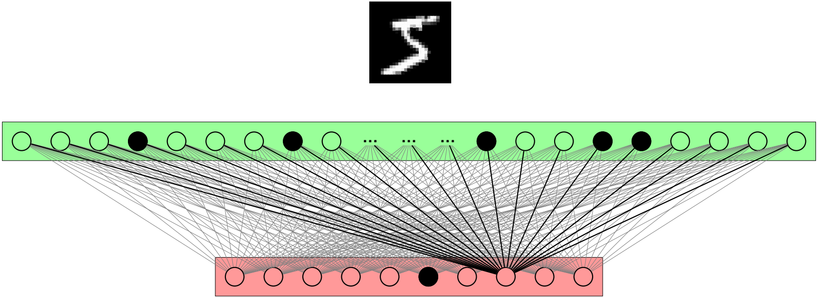




$$n_6 = \begin{cases} +1 & \text{if } \sum_i w_{i6} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$



$$n_7 = \begin{cases} +1 & \text{if } \sum_i w_{i7} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

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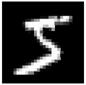

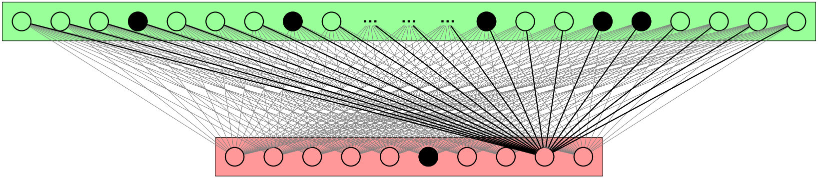

$$n_8 = \begin{cases} +1 & \text{if } \sum_i w_{i8} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$

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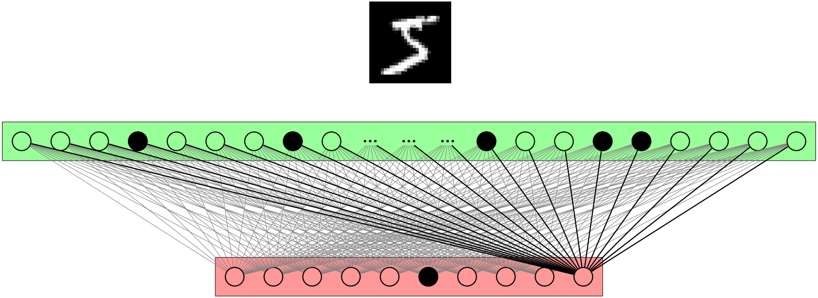
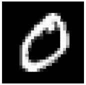
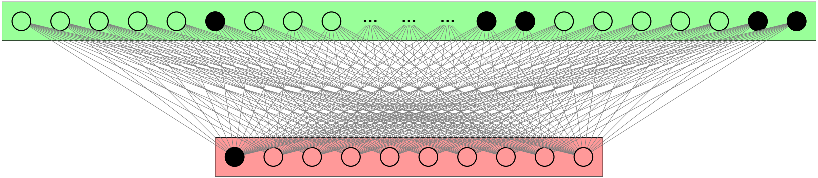


$$n_9 = \begin{cases} +1 & \text{if } \sum_i w_{i9} \cdot x_i \geq 0 \\ -1 & \text{otherwise} \end{cases}, \text{ where } w_{ij} \in \{-1, 0, 1\}.$$





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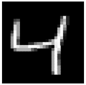

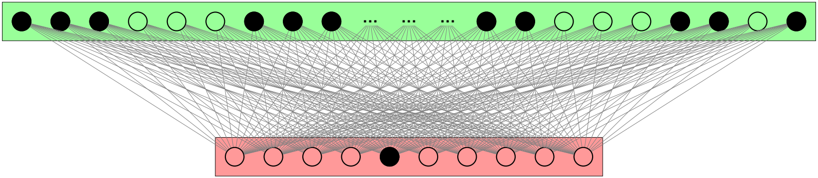

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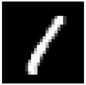

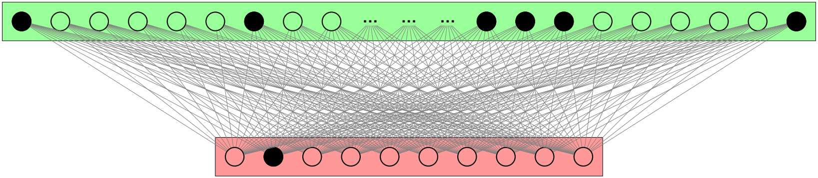

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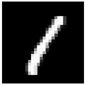
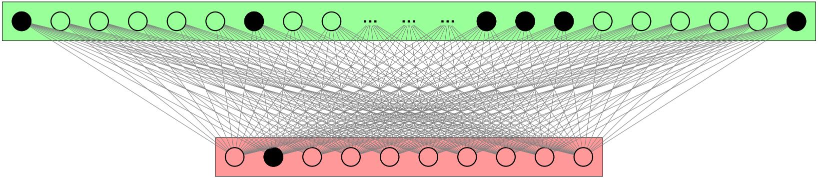
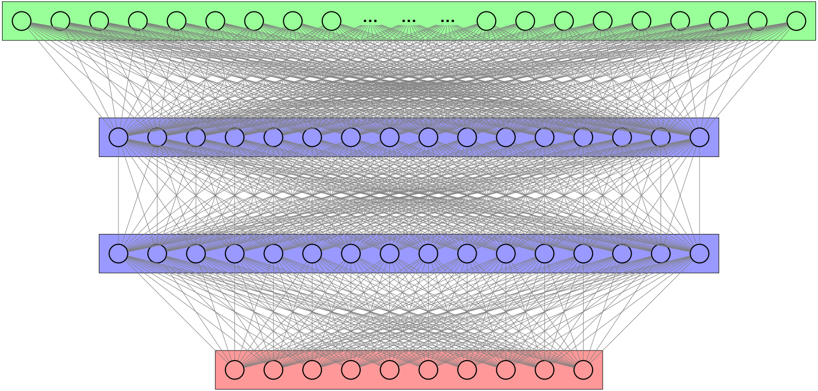




Problem: for most training sets, this problem is infeasible.

(Deep) binarized neural networks



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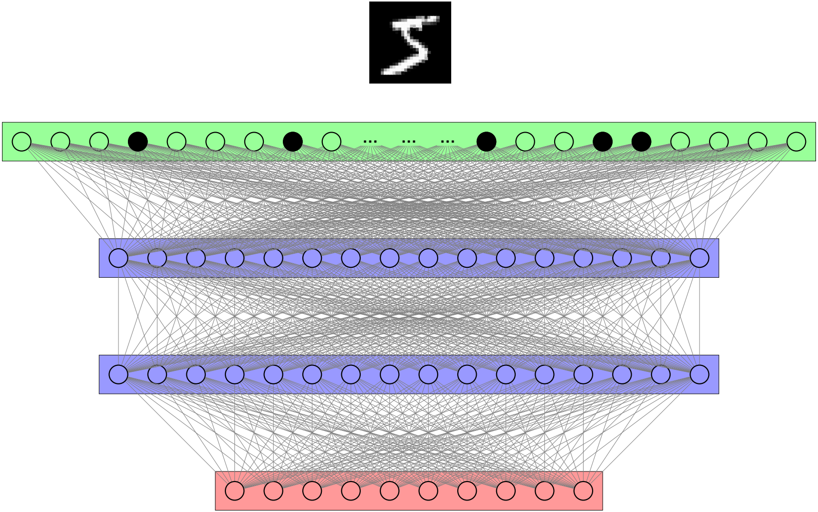

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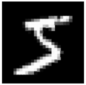

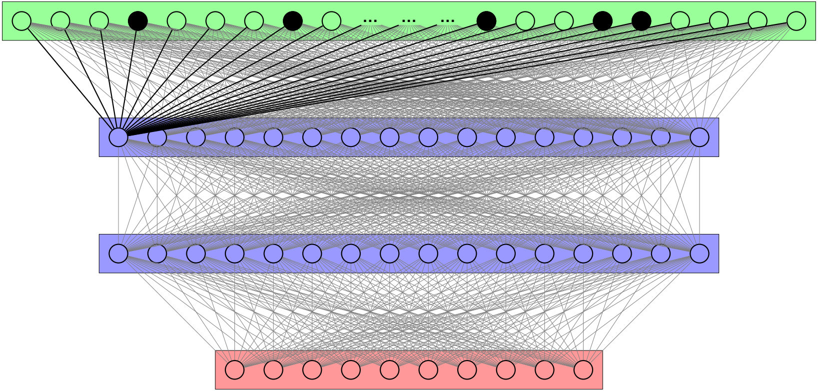

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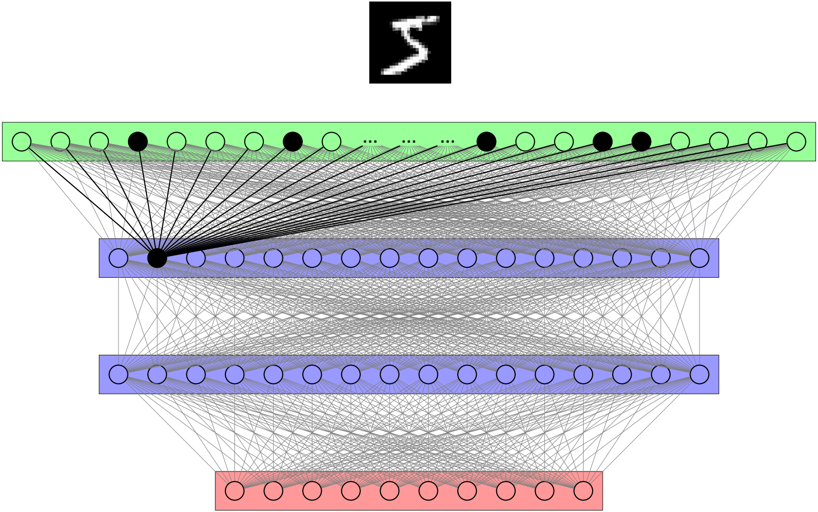

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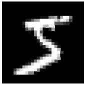

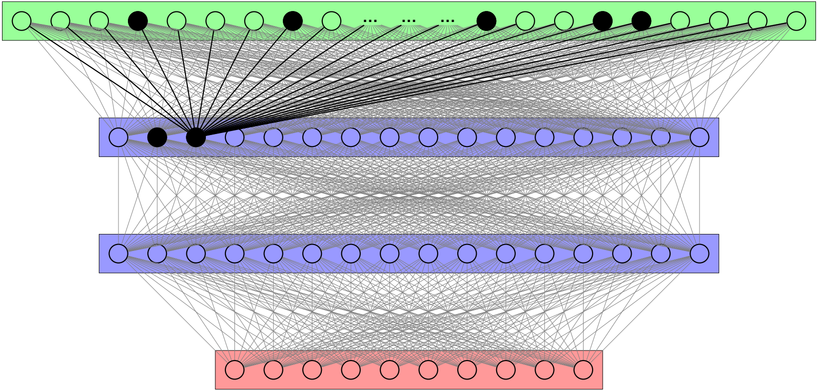

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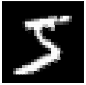

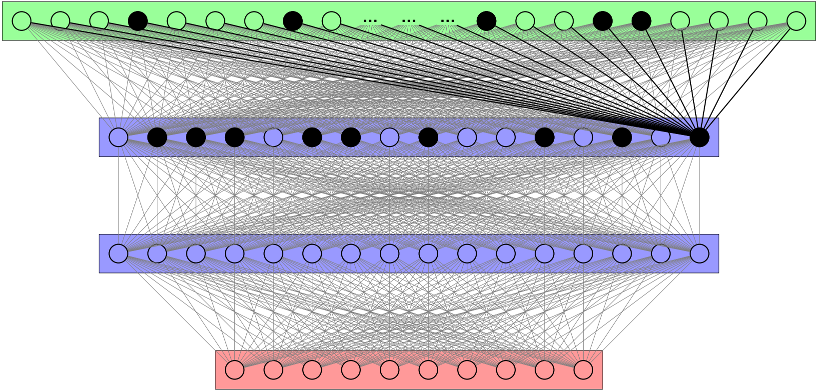

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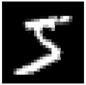

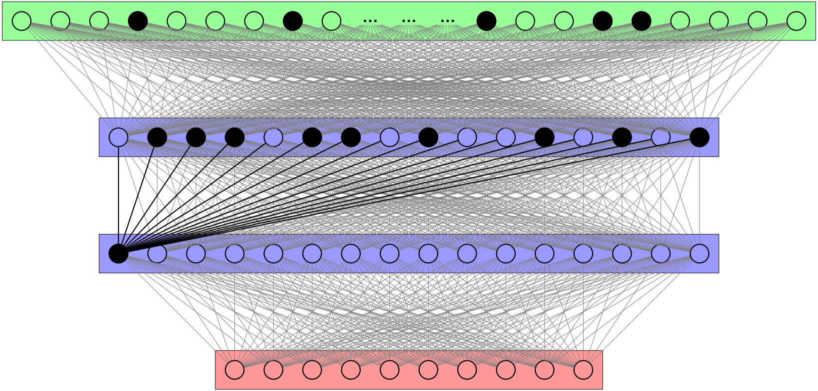

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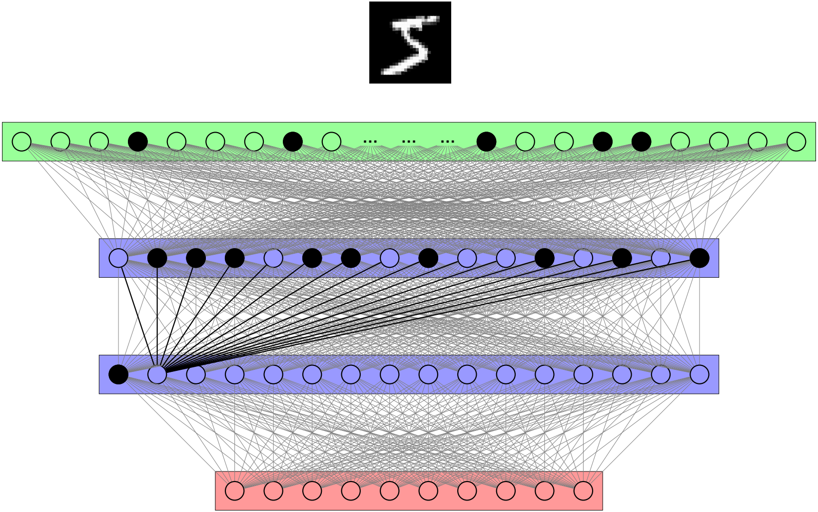

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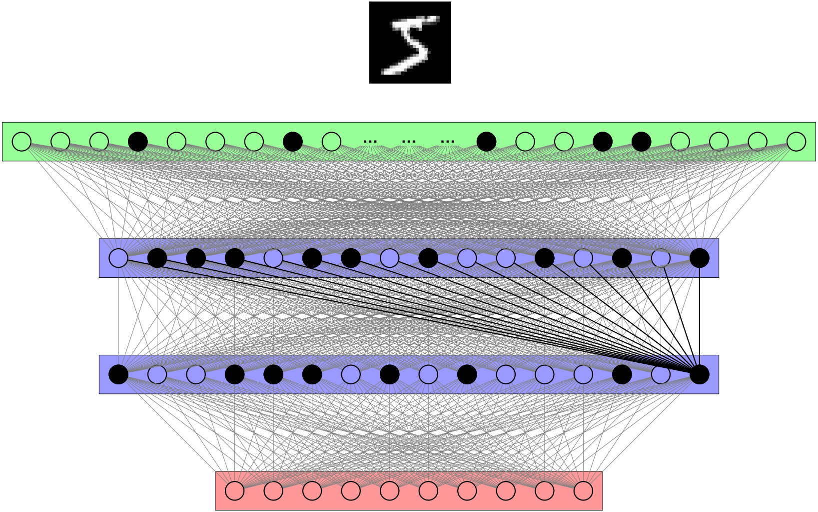

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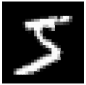

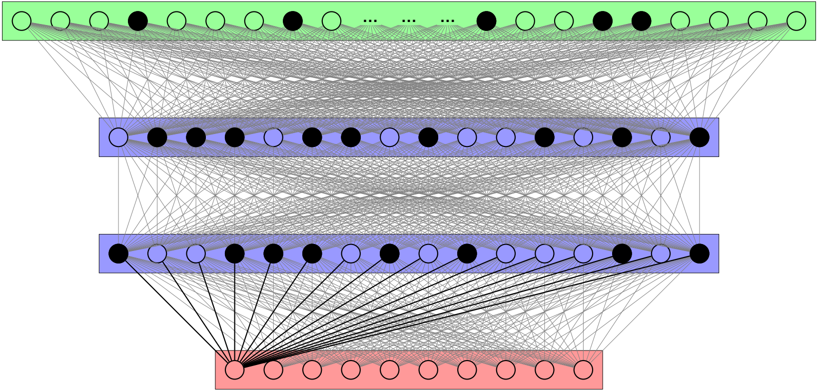

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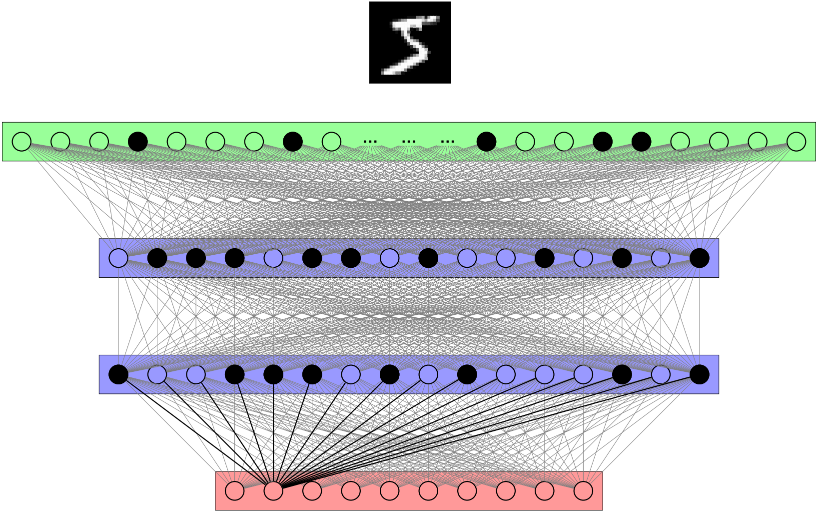

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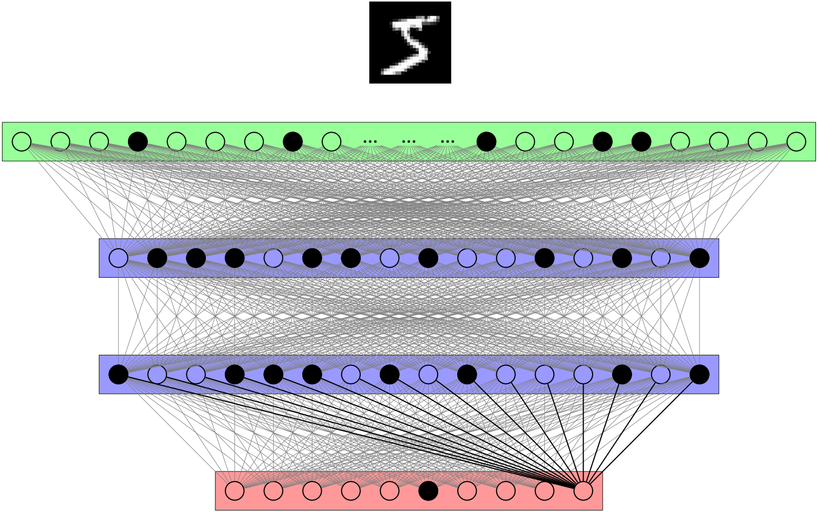

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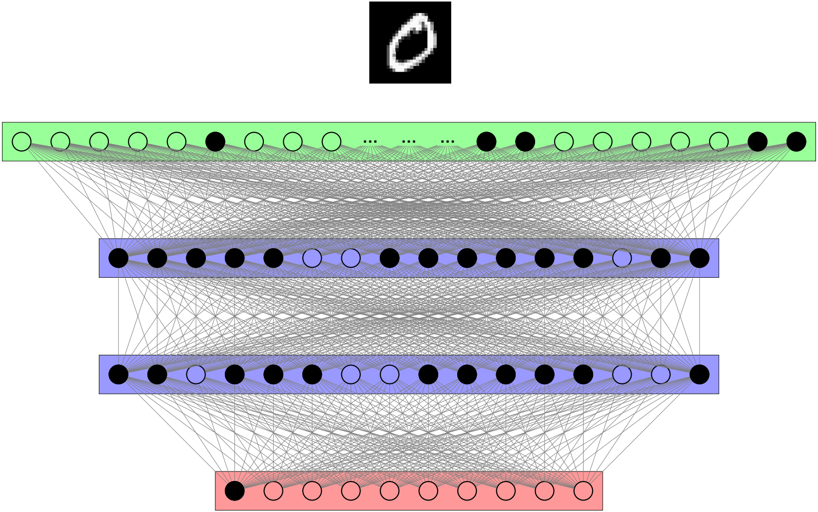

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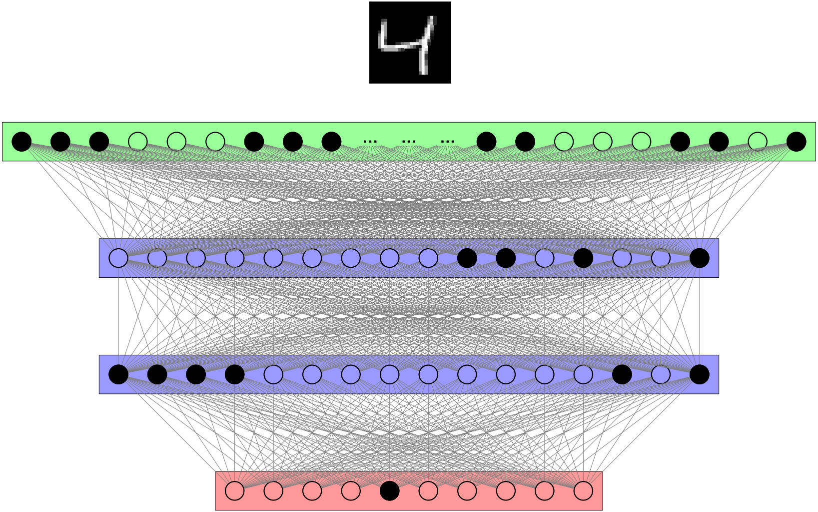

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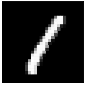

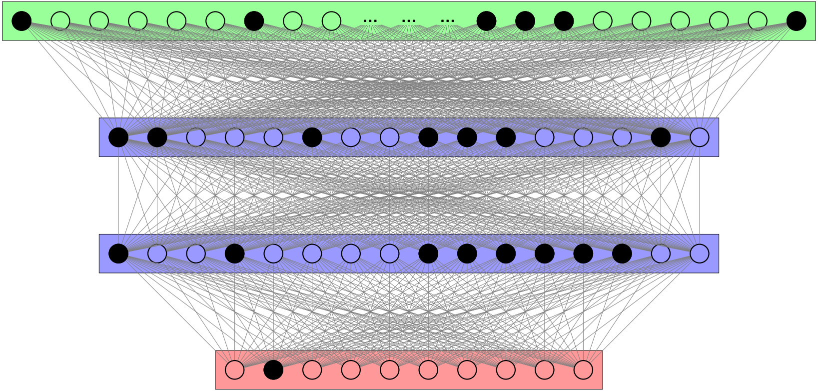

Formal definition

Any assignment to **W** defines a function $\mathcal{N}_{\mathbf{W}} : \mathbb{R}^{N_0} \rightarrow \{-1, 1\}^{N_L}$:

- $n_{0j} = x_j$ (first layer).
- $n_{\ell j} = 1$ if $\sum_i w_{i\ell j} \cdot n_{(\ell-1)i} \geq 0$; -1 otherwise.

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Training a BNN

Given $\mathcal{T} = \{(\mathbf{x}^1, \mathbf{y}^1), \ldots, (\mathbf{x}^T, \mathbf{y}^T)\}$, find **W** s.t. $\mathcal{N}_{\mathbf{W}}(\mathbf{x}^k) \approx \mathbf{y}^k \; \forall k$.

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Training a BNN

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How can we train a BNN?

Use gradient descent!

How to train binarized neural networks

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[To me] It feels like an odd hack to GD... but it works in practice.

About this work

Main contributions

1. Show that training BNNs is a discrete optimization problem.

2. Propose a MIP, CP, and MIP/CP hybrid model to train BNNs.

3. Run an extensive experimental comparison.

Code: `https://bitbucket.org/RToroIcarte/bnn`

Related Work

SAT and MIP have been used for generating adversarial examples and verifying properties of BNNs:

- e.g. Fischetti et al. (2017), Tjeng et al. (2017), Khalil et al. (2018), Narodytska (2018), Cheng et al. (2018), among others.

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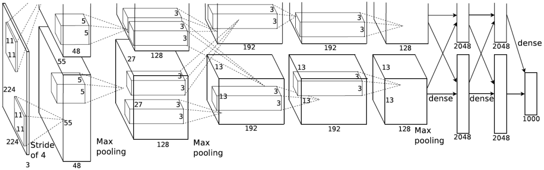
Model-based approaches can find provably optimal solutions, but they have two (fundamental) issues:

- Scalability.
- Overfitting.

Scalability

A rough estimation



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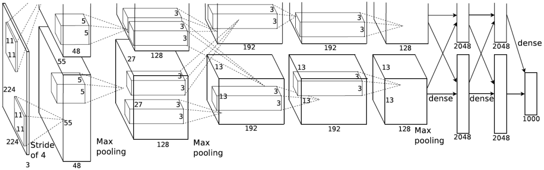

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- Neurons: 154K (input) – 707K (hidden) – 1K (output).
- Weights: 62.3 millions.
- ImageNet: 14 million examples.

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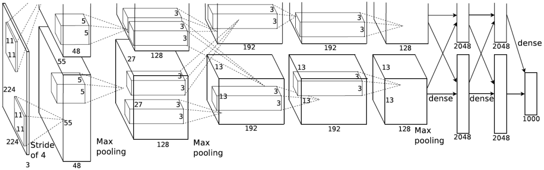

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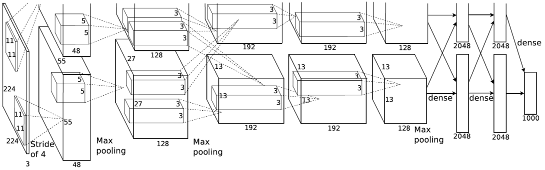

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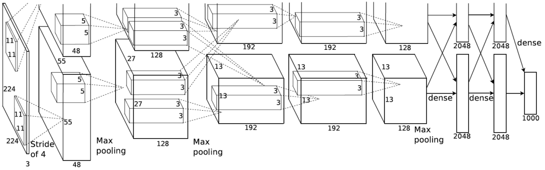

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$\approx 9.89 \cdot 10^{12}$ **decision variables!**

Fortunately, not all is about big data ;)

Few-shot learning

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We better classify them correctly!

Training BNNs: A feasibility perspective

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Objective: Find a BNN that fits the data.

Problem definition

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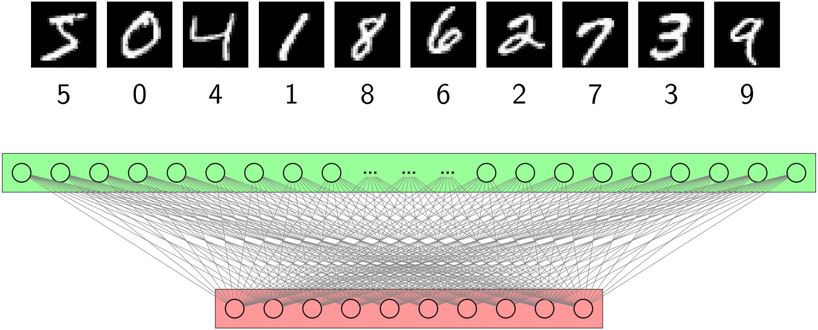
Let's start by formulating this problem as a MIP model.

MIP Model

5 0 4 1 8 6 2 7 3 9

MIP Model



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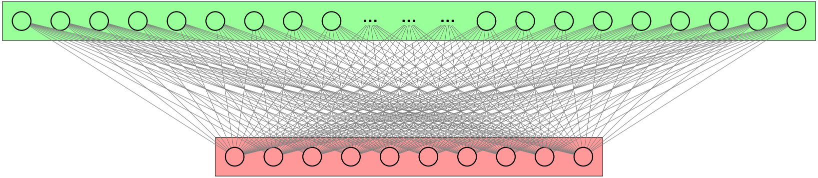

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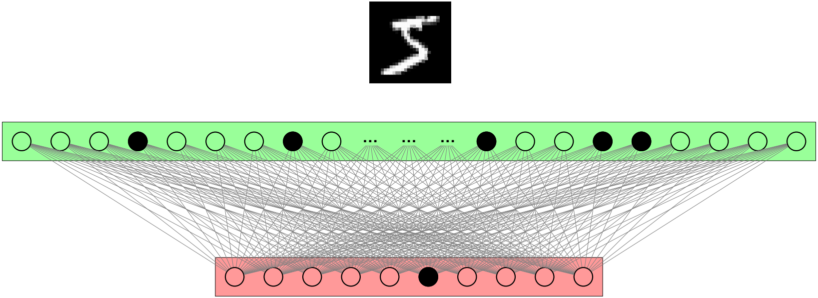

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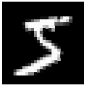
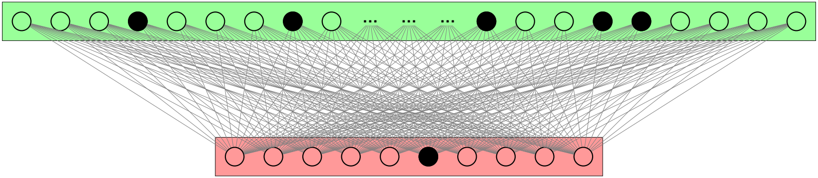
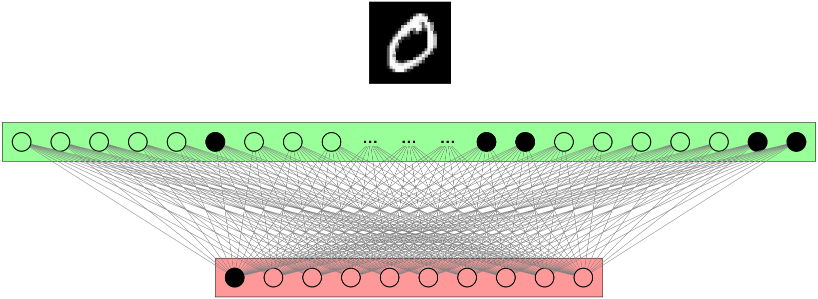




$$\sum_i w_{ij} \cdot x_i^0 \geq 0 \qquad\qquad j = 5$$

$$\sum_i w_{ij} \cdot x_i^0 < 0 \qquad\qquad j \neq 5$$

MIP Model



$$\sum_i w_{ij} \cdot x_i^1 \geq 0 \qquad\qquad j = 0$$

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MIP Model

$$w_{ij} \in \{-1, 0, 1\} \qquad \forall i \in N_0, j \in N_L$$

$$\sum_{i=1}^{N_0} x_i^k \cdot w_{ij} \geq 0 \qquad \forall j \in N_L, k \in T : y_j^k = 1$$

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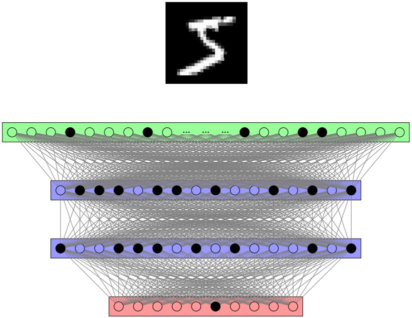
What if the BNN has hidden layers?

MIP Model



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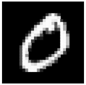

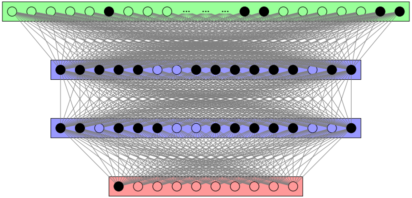

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We need to model the neuron activations using extra variables:

- $u_{\ell j}^{k}$ is 1 if neuron j in layer ℓ is *active* given $x^{k} \in \mathcal{T}$ and 0 o/w.
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MIP Model

$$
\begin{aligned}
&a^k_{\ell j} = \sum_{i \in N_{\ell-1}} c^k_{i\ell j} && \forall \ell \in \mathcal{L}, j \in N_\ell, k \in T \\
&a^k_{Lj} \geq 0 && \forall j \in N_L, k \in T : y^k_j = 1 \\
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&(u^k_{\ell j} = 1) \implies (a^k_{\ell j} \geq 0) && \forall \ell \in \mathcal{L}^{L-1}, j \in N_\ell, k \in T \\
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&c^k_{i1j} = x^k_i \cdot w_{i1j} && \forall i \in N_0, j \in N_1, k \in T \\
&(u^k_{\ell j} = 1) \implies (c^k_{i\ell j} = w_{i\ell j}) && \forall \ell \in \mathcal{L}_2, i \in N_{\ell-1}, j \in N_\ell, k \in T \\
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2. Everywhere I look, I see an implication constraint:

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CP model

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$$w_{i\ell j} \in \{-1, 0, 1\} \qquad \forall \ell \in \mathcal{L}, i \in N_{\ell-1}, j \in N_\ell$$

where $n_{\ell j}^k$ is a CP expression recursively defined as follows:

$$n_{0j}^k = x_j^k \qquad \forall j \in N_0, k \in T$$
$$n_{\ell j}^k = 2\left(\texttt{scal\_prod}(\mathbf{w}_{\ell j}, \mathbf{n}_{\ell-1}^k) \geq 0\right) - 1 \quad \forall \ell \in \mathcal{L} \setminus \{L\}, j \in N_\ell, k \in T$$

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A feasibility experiment

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Approaches:

- `GD`: Standard gradient-based approach.
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- A 100 small training sets sampled from MNIST.
- Each training set has from 1 to 10 examples per class.
- Zero, one, and two hidden layers with 16 neurons.

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- Zero, one, and two hidden layers with 16 neurons.

Question:

- Which approach solves more instances given a 2h time limit?

A feasibility experiment

	No hidden layers			One hidden layer			Two hidden layers		
$\lvert\mathcal{T}\rvert$	MIP	GD	CP	MIP	GD	CP	MIP	GD	CP
10	**10**	**10**	**10**	**10**	9.6	**10**	9	9.2	**10**
20	**10**	**10**	**10**	7	5.6	**10**	0	8.4	**10**
30	**10**	**10**	**10**	0	0.4	**9**	0	5.2	**10**
40	**10**	**10**	**10**	0	0	**8**	0	6.2	**10**
50	**10**	**10**	**10**	0	0	**8**	0	4.2	**10**
60	**10**	**10**	**10**	0	0	**7**	0	2.2	**10**
70	**10**	**10**	**10**	0	0	**3**	0	0	**10**
80	**10**	**10**	**10**	0	0	**3**	0	0	**10**
90	**10**	**10**	8	0	0	**1**	0	0	**8**
100	**10**	**10**	8	0	0	0	0	0	**6**

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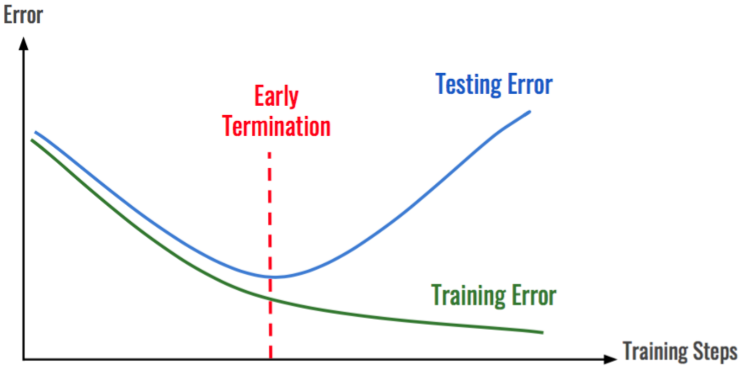

small training error $\neq$ small testing error

Towards finding solutions that generalize

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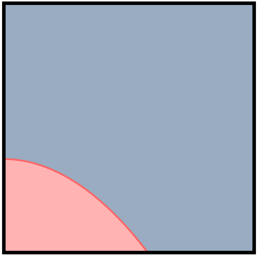

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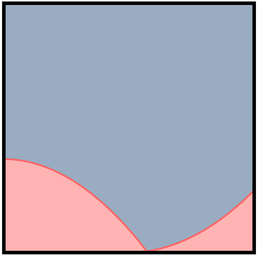

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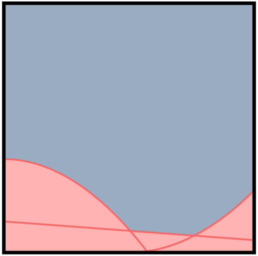

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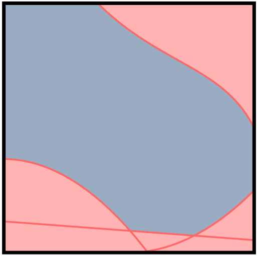

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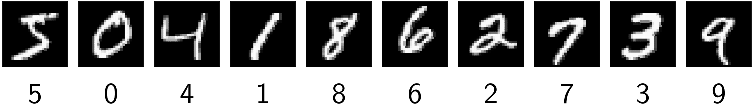

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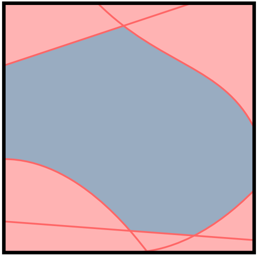
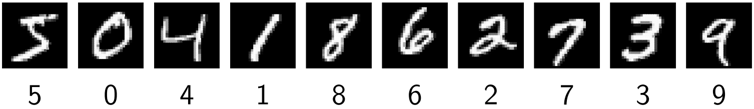


Towards finding solutions that generalize



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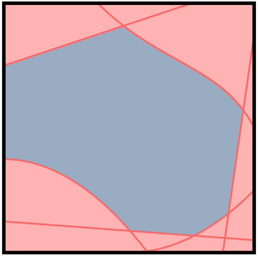

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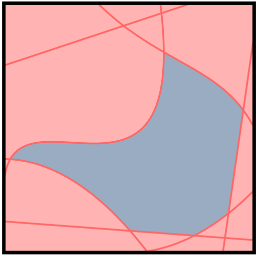

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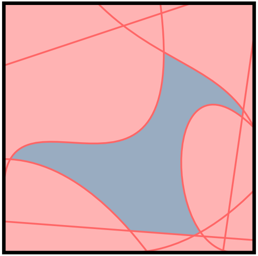

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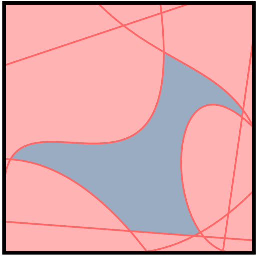

While most solutions overfit

... some generalize.

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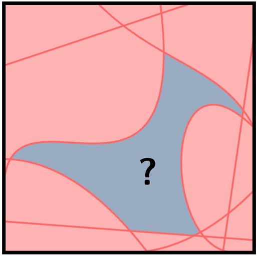

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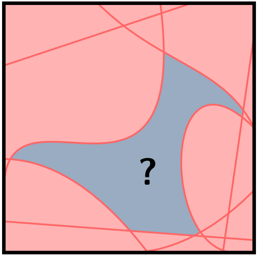

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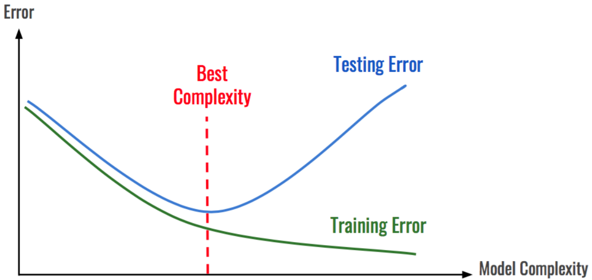
Two principles: simplicity & robustness.

The simplicity principle

The simplicity principle

Occam's razor: prefer the simplest BNN that fits the data.



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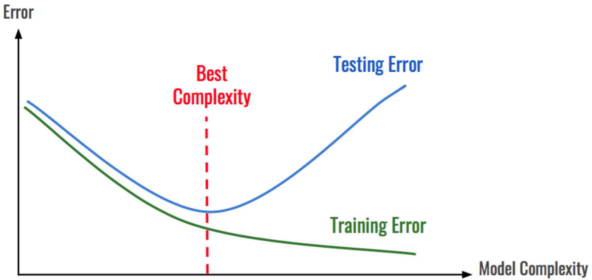


$$\min_{\mathbf{W}} \left\{ \sum_{w \in \mathbf{W}} |w| : \mathcal{N}_{\mathbf{W}}(\mathbf{x}) = \mathbf{y}, \forall (\mathbf{x}, \mathbf{y}) \in \mathcal{T},\ w \in \{-1, 0, 1\}, \forall w \in \mathbf{W} \right\}.$$

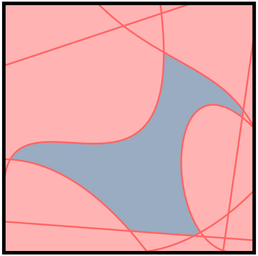
(min-weight)

The robustness principle

The robustness principle

Prefer robust solutions

BNNs that fit the data under small perturbations to their weights.



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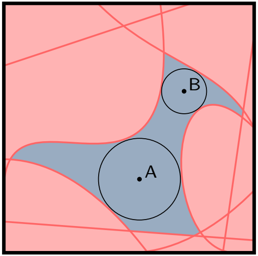

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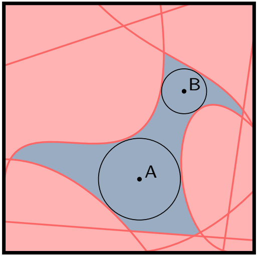

$$\max_{\mathbf{W}} \quad \sum_{\ell \in \mathcal{L}, j \in N_\ell} \min\{|a_{\ell j}(\mathbf{x})| : (\mathbf{x}, \mathbf{y}) \in \mathcal{T}\}$$

$$\text{s.t.} \quad \mathcal{N}_{\mathbf{W}}(\mathbf{x}) = \mathbf{y} \qquad \forall (\mathbf{x}, \mathbf{y}) \in \mathcal{T}$$

$$w \in \{-1, 0, 1\} \qquad \forall w \in \mathbf{W}$$

(max-margin)

An optimality experiment

An optimality experiment

Approaches:

- $\texttt{CP}_w$ and $\texttt{CP}_m$: min-weight and max-margin CP models.
- $\texttt{MIP}_w$ and $\texttt{MIP}_m$: min-weight and max-margin MIP models.

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Problem instances:

- Same 100 instances using 0, 1, or 2 hidden layers.

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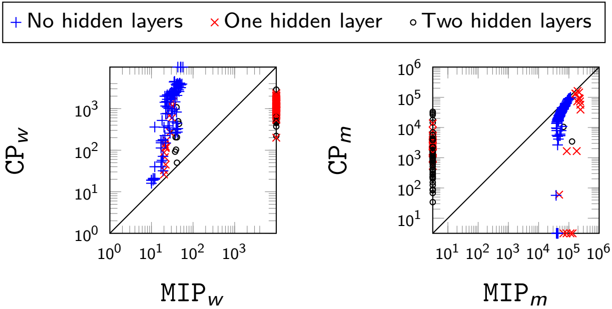
Question:

- Will MIP or CP find better solutions given a 2h time limit?

An optimality experiment



(a) Min-weight optimization (b) Max-margin optimization

CP/MIP hybrid methods

Idea: use CP to find feasible solutions and MIP to optimize them.

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Option 1: model `HW`

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Option 1: model `HW`

Use the CP solution as a warm-start for MIP.

Option 2: model `HA`

Use the CP solution to fix the activations of all neurons in the MIP model and search only over the weights.

CP/MIP hybrid methods

"This model is a nightmare for a MIP solver"

—Andre A. Ciré

1. It has (way too) many auxiliary variables:

$$u^k_{\ell j} \in \{0,1\} \qquad \forall \ell \in \mathcal{L}^{L-1}, j \in N_\ell, k \in T$$

$$c^k_{i\ell j} \in \mathbb{R} \qquad \forall \ell \in \mathcal{L}, i \in N_{\ell-1}, j \in N_\ell, k \in T$$

2. Everywhere I look, I see an implication constraint:

$$(u^k_{\ell j} = 1) \implies (a^k_{\ell j} \geq 0) \qquad \forall \ell \in \mathcal{L}^{L-1}, j \in N_\ell, k \in T$$

$$(u^k_{\ell j} = 0) \implies (a^k_{\ell j} \leq -\epsilon) \qquad \forall \ell \in \mathcal{L}^{L-1}, j \in N_\ell, k \in T$$

$$(u^k_{\ell j} = 1) \implies (c^k_{i\ell j} = w_{i\ell j}) \qquad \forall \ell \in \mathcal{L}_2, i \in N_{\ell-1}, j \in N_\ell, k \in T$$

$$(u^k_{\ell j} = 0) \implies (c^k_{i\ell j} = -w_{i\ell j}) \qquad \forall \ell \in \mathcal{L}_2, i \in N_{\ell-1}, j \in N_\ell, k \in T$$

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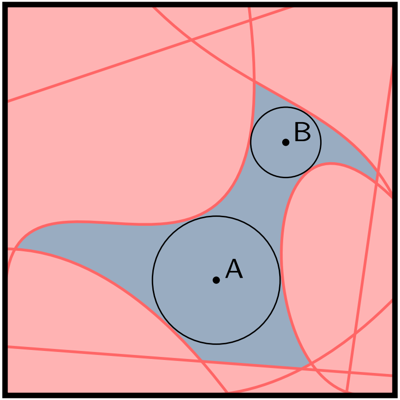

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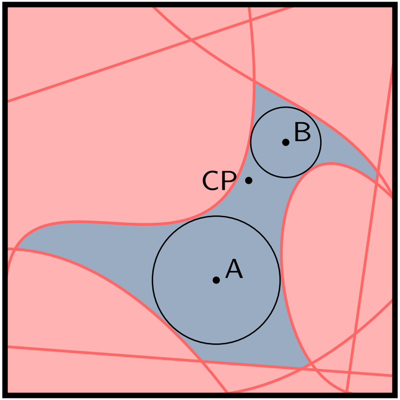

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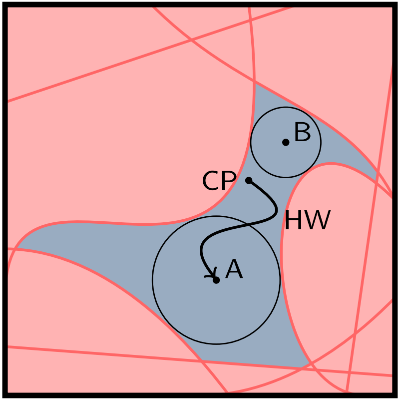

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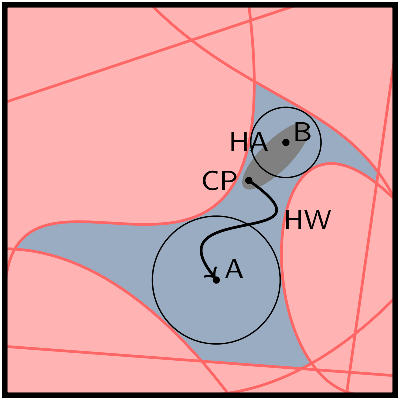

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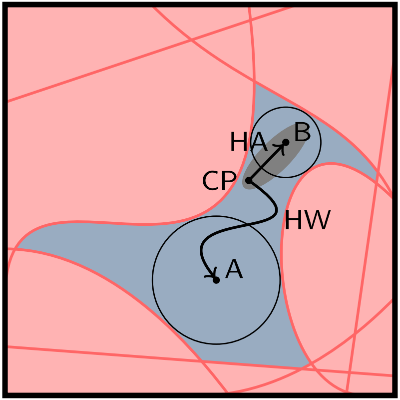

Results

A generalization experiment

Approaches:

- $\texttt{CP}_w$, $\texttt{CP}_m$, $\texttt{MIP}_w$, and $\texttt{MIP}_m$ as before.
- $\texttt{HW}_w$ and $\texttt{HW}_m$: min-weight and max-margin warm-start CP/MIP.
- $\texttt{HA}_w$ and $\texttt{HA}_m$: min-weight and max-margin fixed-activation CP/MIP.
- $\texttt{GD}_b$ and $\texttt{GD}_t$: Two versions of gradient descent.

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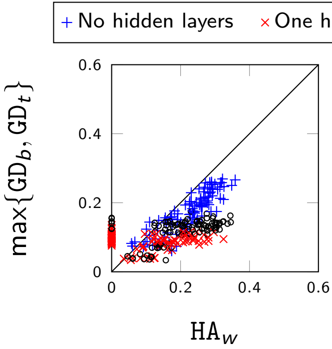
Question:

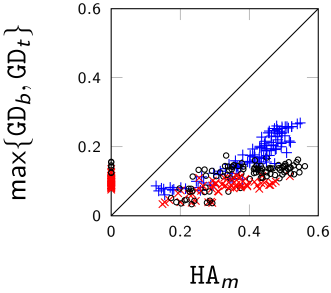
- Which model finds solutions that generalize better within 2h?

A generalization experiment

Test performance



(c) Min-weight optimization



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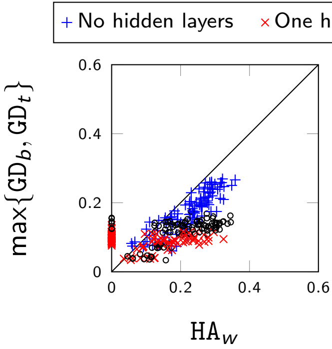
A generalization experiment

Test performance



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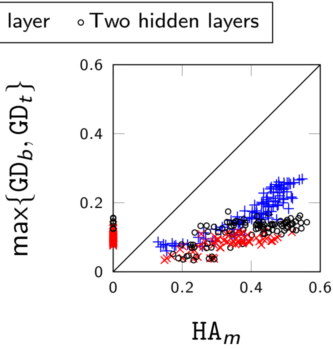

(f) Max-margin optimization

$\mathtt{HA}_m$ outperforms $\max\{\mathtt{GD}_b, \mathtt{GD}_t\}$ in **253 out of 300** experiments!

A generalization experiment

$\mathtt{HA}_m$ outperforms alternatives by a **large margin**!

A generalization experiment

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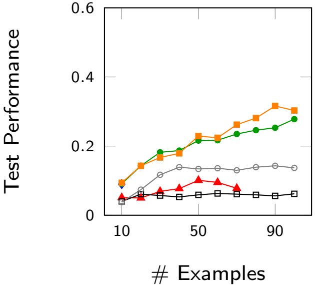
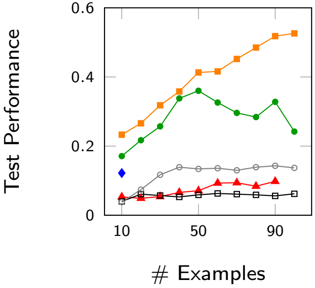


(i) 2 HL, min-weight



(j) 2 HL, max-margin

Concluding remarks

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Summary:

- Training BNNs is a discrete optimization problem.
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Thanks!