A MILP approach to a structured ensemble Binarized Neural Network

Matematica per l'Intelligenza Artificiale e il Machine Learning - Giovani ricercatori

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2022-11-24

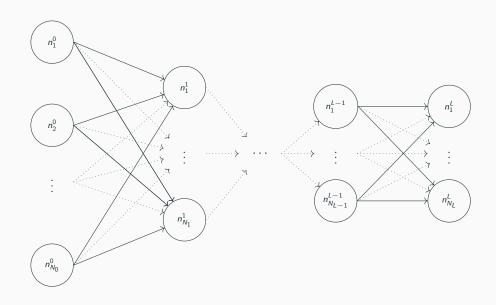


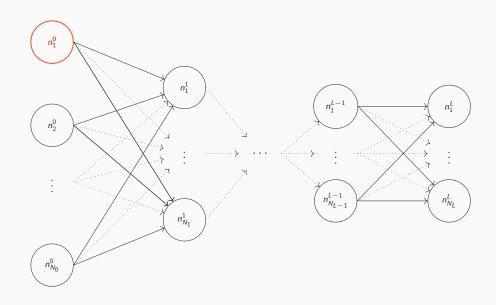


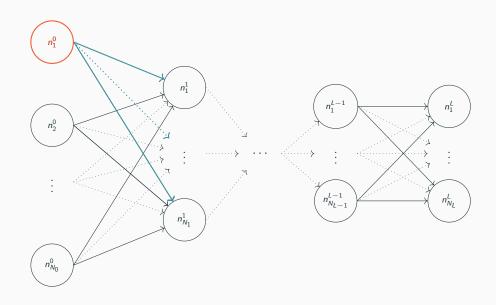
Overview

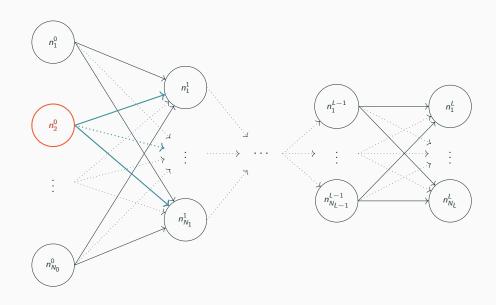
- 1. Introduction
- 2. Mathematical Models
- 3. Methodology
- 4. Computational Analysis
- 5. Conclusions

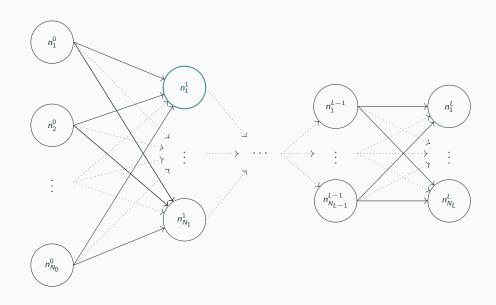
Introduction

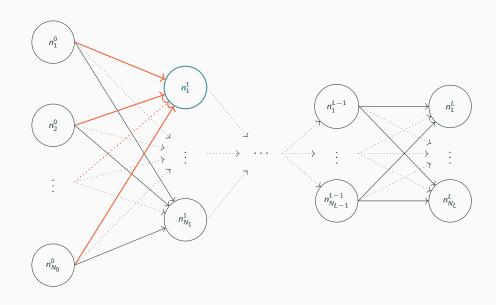


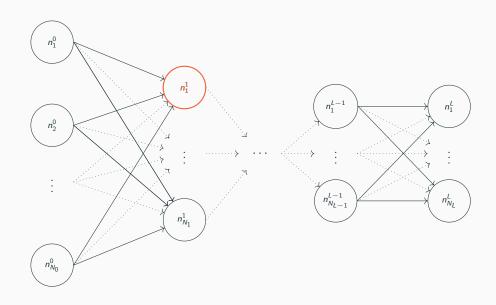


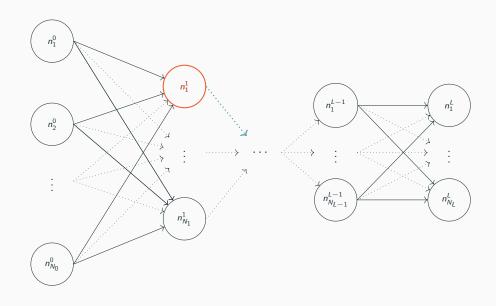












Binarized Neural Networks - BNNs

BNNs are getting increasing attention thanks to their compactness and versatility. In this kind of NN, every neuron $j \in N_l$ is connected to every neuron $i \in N_{l-1}$ by a weight $w_{ilj} \in \{-1,0,1\}$. Given a value x for input neurons, the preactivation $a_{lj}(x)$ of neuron $j \in N_l$ and the activation $p_j(x)$ are, respectively,

$$a_{lj}(x) = \sum_{i \in N_{l-1}} w_{ilj} \cdot p_{(l-1)i}(x) \quad \text{and} \quad p_{lj}(x) = \begin{cases} x_j & \text{if } l = 0, \\ +1 & \text{if } l > 0, a_{lj}(x) \ge 0, \\ -1 & \text{otherwise.} \end{cases}$$
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Recent works¹ show that this kind of networks are hard to train with GD-based algorithm in a context of few-shot learning. Instead, MILP approaches are being researched.

¹ Toro Icarte, R., Illanes, L., Castro, M.P., Cire, A.A., McIlraith, S.A. and Beck, J.C.: Training binarized neural networks using MIP and CP. In: Proceedings of CP'19. vol 11802, pp. 401–417. Springer (2019).

Mathematical Models

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(M-M) Max-Margin: a way of finding robust BNNs by maximizing the margins of their neurons. Intuitively, neurons with larger margins requires bigger changes on their inputs and weights to change their activation values;¹

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- (M-W) Min-Weight: a way of finding simple BNNs by minimizing the number of connections;¹

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- (M-M) Max-Margin: a way of finding robust BNNs by maximizing the margins of their neurons. Intuitively, neurons with larger margins requires bigger changes on their inputs and weights to change their activation values;¹
- (M-W) Min-Weight: a way of finding simple BNNs by minimizing the number of connections; 1
- (S-M) Sat-Margin: a way of finding BNNs by maximizing the number of correct predictions. At the same time each correctly predicted sample is confidently predicted.²

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²Thorbjarnarson, T., Yorke-Smith, N.: On Training Neural Networks with Mixed Integer Programming. arXiv preprint arXiv:2009.03825 (2020).

$$\max_{\mathbf{c},\mathbf{u},\mathbf{w},\mathbf{m}} \qquad \sum_{l \in \mathcal{L}} \sum_{j \in N_l} m_{lj} \tag{2}$$

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s.t.
$$\sum_{i \in \mathcal{N}_{L-1}} c_{iLj}^k \ge m_{Lj} \qquad \forall j \in \mathcal{N}_L, k \in \mathcal{T} : y_j^k = 1, \qquad (3)$$

$$\sum_{i \in \mathcal{N}_{L-1}} c_{iLj}^k \le -\epsilon - m_{Lj} \qquad \forall j \in \mathcal{N}_L, k \in \mathcal{T} : y_j^k = -1, \qquad (4)$$

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$$u_{lj}^{k} = 1 \implies \sum_{i \in \mathcal{N}_{l-1}} c_{ilj}^{k} \geq m_{lj} \qquad \forall l \in \mathcal{L}^{L-1}, j \in \mathcal{N}_{l}, k \in \mathcal{T}, \qquad (5)$$

$$u_{lj}^{k} = 0 \implies \sum_{i \in \mathcal{N}_{l-1}} c_{ilj}^{k} \leq -\epsilon - m_{lj} \qquad \forall l \in \mathcal{L}^{L-1}, j \in \mathcal{N}_{l}, k \in \mathcal{T}, \qquad (6)$$

$$c_{i1j}^{k} = x_{i}^{k} \cdot w_{i1j} \qquad \forall i \in N_{0}, j \in N_{1}, k \in T,$$

$$c_{ilj}^{k} - w_{ilj} + 2u_{(l-1)i}^{k} \leq 2 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$

$$c_{ilj}^{k} + w_{ilj} - 2u_{(l-1)i}^{k} \leq 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$

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$$c_{ilj}^{k} + w_{ilj} - 2u_{(l-1)i}^{k} \leq 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (9)$$

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$$c_{ilj}^{k} + w_{ilj} + 2u_{(l-1)i}^{k} \geq 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (11)$$

$$w_{ilj} \in \{-1, 0, 1\} \qquad \forall l \in \mathcal{L}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (13)$$

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$$m_{lj} \in \mathbb{R}_{\geq 0} \qquad \forall l \in \mathcal{L}, j \in N_{l}. \qquad (16)$$

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$$\min_{\mathbf{c},\mathbf{u},\mathbf{w},\mathbf{v}} \qquad \sum_{l \in \mathcal{L}} \sum_{i \in N_{l-1}} \sum_{j \in N_l} v_{ilj} \tag{17}$$

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s.t.
$$\sum_{i \in N_{L-1}} c_{iLj}^{k} \geq 0 \qquad \forall j \in N_{L}, k \in T : y_{j}^{k} = 1, \tag{18}$$

$$\sum_{i \in N_{L-1}} c_{iLj}^{k} \leq -0 - \epsilon \qquad \forall j \in N_{L}, k \in T : y_{j}^{k} = -1, \tag{19}$$

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$$u_{lj}^{k} = 1 \implies \sum_{i \in N_{l-1}} c_{ilj}^{k} \geq 0 \qquad \forall l \in \mathcal{L}^{l-1}, j \in N_{l}, k \in T, \tag{20}$$

$$u_{lj}^{k} = 0 \implies \sum_{i \in N_{l-1}} c_{ilj}^{k} \leq -0 - \epsilon \qquad \forall l \in \mathcal{L}^{l-1}, j \in N_{l}, k \in T, \tag{21}$$

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$$c_{i1j}^{k} = x_{i}^{k} \cdot w_{i1j} \qquad \forall i \in N_{0}, j \in N_{1}, k \in T,$$

$$c_{ilj}^{k} - w_{ilj} + 2u_{(l-1)i}^{k} \leq 2 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$
(22)

$$c_{ilj}^{k} + w_{ilj} - 2u_{(l-1)i}^{k} \le 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$
 (24)

$$c_{ilj}^{k} - w_{ilj} - 2u_{(l-1)i}^{k} \ge -2$$
 $\forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$ (25)

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$$c_{ilj}^{k} + w_{ilj} \leq w_{ilj} \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$

$$w_{ilj} \leq w_{ilj} \leq w_{ilj} \qquad \forall l \in \mathcal{L}, i \in N_{l-1}, j \in N_{l},$$

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$$c_{i1j}^{k} = x_{i}^{k} \cdot w_{i1j} \qquad \forall i \in N_{0}, j \in N_{1}, k \in T, \qquad (22)$$

$$c_{iij}^{k} - w_{ilj} + 2u_{(l-1)i}^{k} \leq 2 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (23)$$

$$c_{ilj}^{k} + w_{ilj} - 2u_{(l-1)i}^{k} \leq 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (24)$$

$$c_{ilj}^{k} - w_{ilj} - 2u_{(l-1)i}^{k} \geq -2 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (25)$$

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$$- v_{ilj} \leq w_{ilj} \leq v_{ilj} \qquad \forall l \in \mathcal{L}, i \in N_{l-1}, j \in N_{l}, \qquad (27)$$

$$w_{ilj} \in \{-1, 0, 1\} \qquad \forall l \in \mathcal{L}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (29)$$

$$c_{ilj}^{k} \in \{0, 1\} \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (30)$$

$$c_{ilj}^{k} \in \{-1, 0, 1\} \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (31)$$

 $\forall I \in \mathcal{L}, i \in N_{I-1}, j \in N_I$.

Toro lcarte, R., Illanes, L., Castro, M.P., Cire, A.A., McIlraith, S.A. and Beck, J.C.: Training binarized neural networks using MIP and CP. In: Proceedings of CP'19. vol 11802, pp. 401–417. Springer (2019).

(32)

$$\max_{\mathbf{c},\mathbf{u},\mathbf{w},\hat{\mathbf{y}},\mathbf{q}} \qquad \sum_{k \in T} \sum_{j \in N_L} q_j^k \tag{33}$$

$$\max_{\mathbf{c},\mathbf{u},\mathbf{w},\hat{\mathbf{y}},\mathbf{q}} \qquad \sum_{k \in \mathcal{T}} \sum_{j \in \mathcal{N}_{L}} q_{j}^{k} \qquad (33)$$

$$q_{j}^{k} = 1 \implies \hat{y}_{j}^{k} \cdot y_{j}^{k} \ge 1/2 \qquad \forall j \in \mathcal{N}_{L}, k \in \mathcal{T}, \qquad (34)$$

$$q_{j}^{k} = 0 \implies \hat{y}_{j}^{k} \cdot y_{j}^{k} \le 1/2 - \epsilon \qquad \forall j \in \mathcal{N}_{L}, k \in \mathcal{T}, \qquad (35)$$

$$q_{j}^{k} \in \{0,1\} \qquad \forall j \in \mathcal{N}_{L}, k \in \mathcal{T}, \qquad (36)$$

$$\hat{y}_{j}^{k} = \frac{2}{\mathcal{N}_{L-1} + 1} \sum_{i \in \mathcal{N}_{L-1}} c_{iL_{j}}^{k} \qquad \forall j \in \mathcal{N}_{L}, k \in \mathcal{T}, \qquad (37)$$

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$$q_j^k \in \{0,1\} \qquad \forall j \in N_L, k \in T, \qquad (36)$$

$$\hat{y}_j^k = \frac{2}{N_{L-1} + 1} \sum_{i \in N_{L-1}} c_{iLj}^k \qquad \forall j \in N_L, k \in T, \qquad (37)$$

$$u_{lj}^k = 1 \implies \sum_{i \in N_{l-1}} c_{ilj}^k \ge 0 \qquad \forall l \in \mathcal{L}^{L-1}, j \in N_l, k \in T, \qquad (38)$$

$$u_{lj}^k = 0 \implies \sum_{i \in N_{l-1}} c_{ilj}^k \le -\epsilon \qquad \forall l \in \mathcal{L}^{L-1}, j \in N_l, k \in T, \qquad (39)$$

$$c_{i1j}^{k} = x_{i}^{k} \cdot w_{i1j} \qquad \forall i \in N_{0}, j \in N_{1}, k \in T,$$

$$c_{ilj}^{k} - w_{ilj} + 2u_{(l-1)i}^{k} \leq 2 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$

$$c_{ilj}^{k} + w_{ilj} - 2u_{(l-1)i}^{k} \leq 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$

$$c_{ilj}^{k} - w_{ilj} - 2u_{(l-1)i}^{k} \geq -2 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T,$$

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$$c_{iij}^{k} - w_{ilj} + 2u_{(l-1)i}^{k} \leq 2 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (41)$$

$$c_{ilj}^{k} + w_{ilj} - 2u_{(l-1)i}^{k} \leq 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (42)$$

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$$c_{ilj}^{k} + w_{ilj} + 2u_{(l-1)i}^{k} \geq 0 \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (44)$$

$$w_{ilj} \in \{-1, 0, 1\} \qquad \forall l \in \mathcal{L}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (45)$$

$$u_{lj}^{k} \in \{0, 1\} \qquad \forall l \in \mathcal{L}^{l-1}, j \in N_{l}, k \in T, \qquad (46)$$

$$c_{i1j}^{k} \in [-\mathfrak{b}, \mathfrak{b}] \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (47)$$

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Sat-Margin

$$c_{i1j}^{k} = x_{i}^{k} \cdot w_{i1j} \qquad \forall i \in N_{0}, j \in N_{1}, k \in T, \qquad (40)$$

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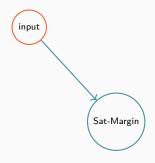
$$c_{ilj}^{k} \in [-\mathfrak{b}, \mathfrak{b}] \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T, \qquad (47)$$

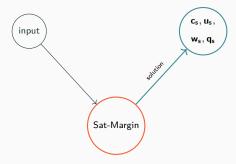
$$c_{ilj}^{k} \in \{-1, 0, 1\} \qquad \forall l \in \mathcal{L}_{2}, i \in N_{l-1}, j \in N_{l}, k \in T. \qquad (48)$$

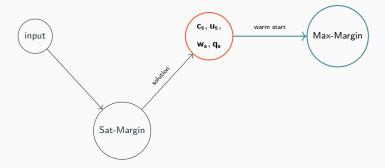
Thorbjarnarson, T., Yorke-Smith, N.: On Training Neural Networks with Mixed Integer Programming. arXiv preprint arXiv:2009.03825 (2020).

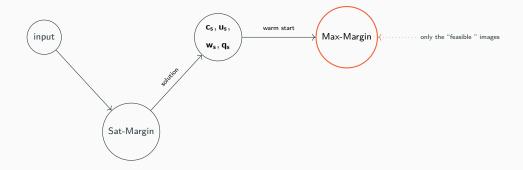
Methodology

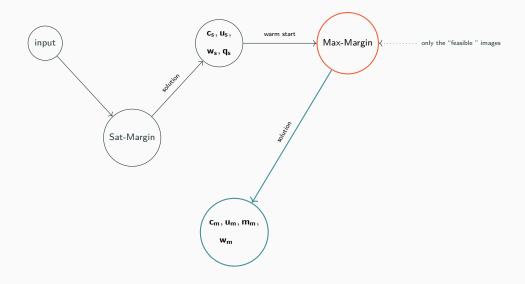


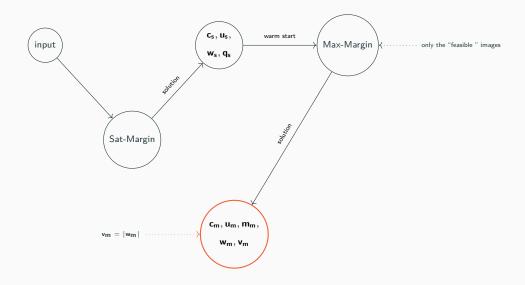


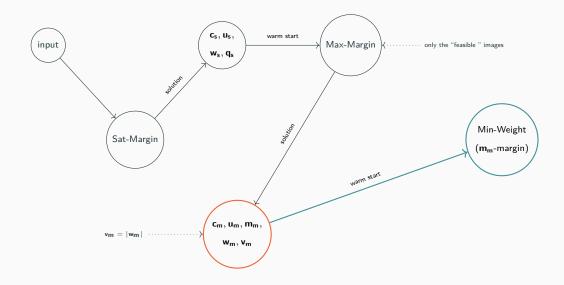


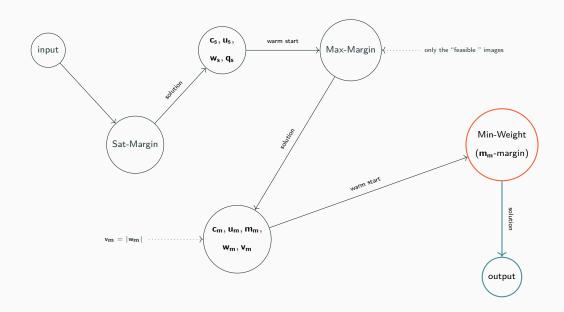


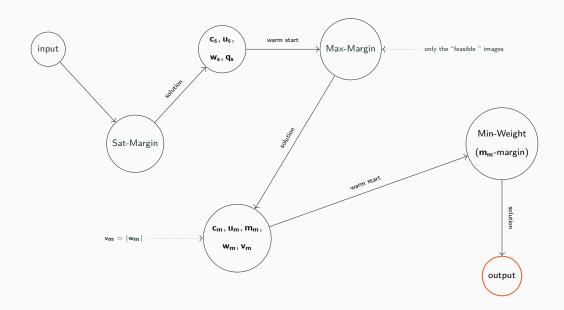












Suppose we have a labelling problem and that our set of labels is $\mathcal{I}.$

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We set a parameter $1 < k \le n = |\mathcal{I}|$.

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When testing an input, we feed it to our list of networks $(\mathcal{N}_{\mathcal{J}})_{\mathcal{J} \in \mathcal{P}(\mathcal{I})_k}$ and we obtain a list of labels $(\mathfrak{e}_{\mathcal{J}})_{\mathcal{J} \in \mathcal{P}(\mathcal{I})_k}$.

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We then apply a majority voting system.

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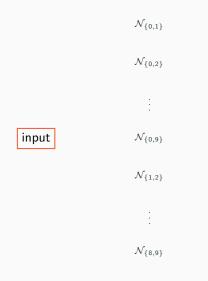
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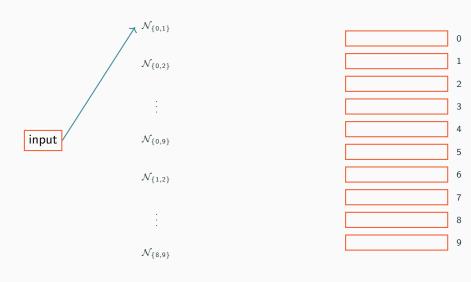
We then apply a majority voting system.

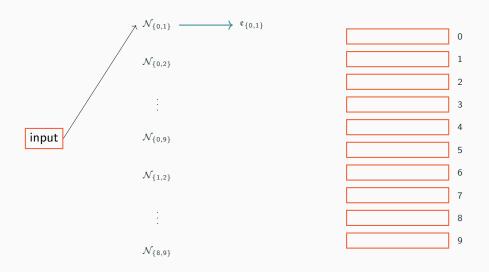
For the sake of simplicty, suppose $\mathcal{I}=\{0,1,\ldots,9\}$ and k=2. So every \mathcal{J} is a set of type $\{i,j\},\ i,j\in\{0,1,\ldots,9\},\ i\neq j$. We denote with $\mathfrak{e}_{\{i,j\}}$ the output of the network $\mathcal{N}_{\{i,j\}}$ and with $\hat{\mathfrak{e}}_{\{i,j\}}$ the only element of the set $\{i,j\}\setminus\mathfrak{e}_{\{i,j\}}$.

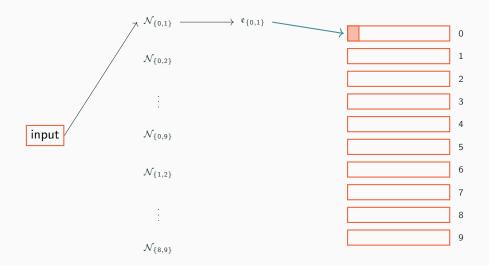
input

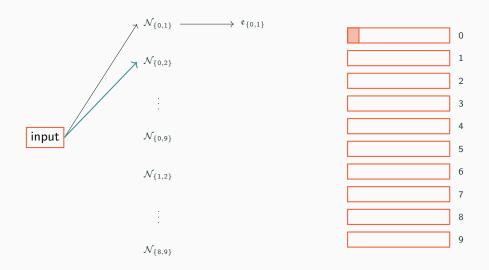


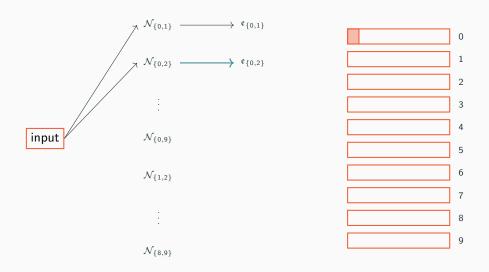


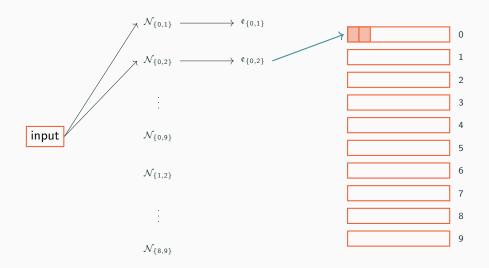


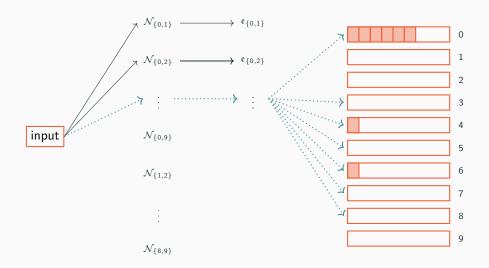


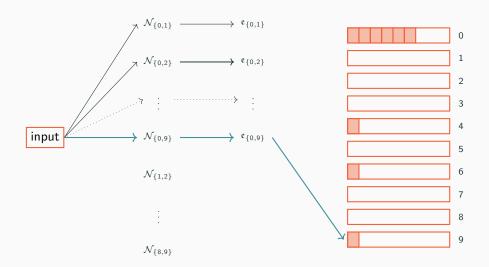


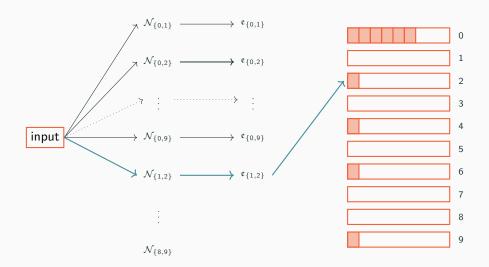


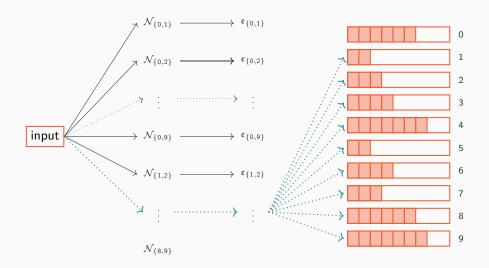


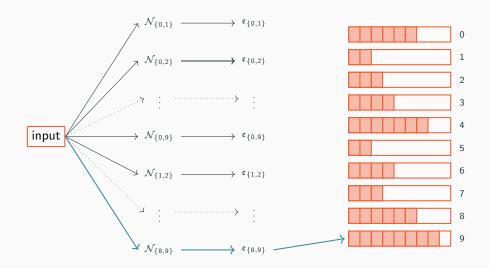


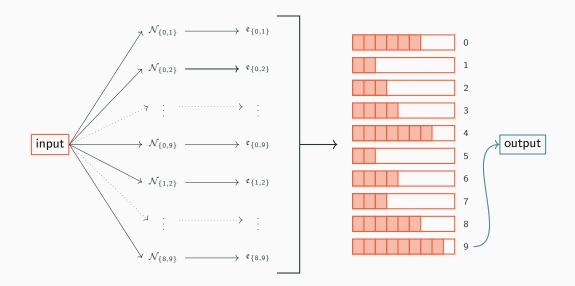












What about ex-aequo?

For every $k \in \{0, 1, \dots, 9\}$ we define

$$C_k = \{\{i,j\} \in \mathcal{P}(\{0,1,\ldots,9\})_2 \mid \mathfrak{e}_{\{i,j\}} = k\}$$

and we say that a label k is a dominant label if $|C_k| \ge |C_l|$ for every $l \in \{0, 1, \dots, 9\}$.

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(a) there exists one $k \in \{0, 1, ..., 9\}$ such that $|C_k| > |C_l|$ for every $l \in \{0, 1, ..., 9\} \setminus \{k\}$ (there exists exactly one dominant label) \implies our input is labelled as k;

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- (b) there exist $k_1, k_2 \in \{0, 1, \dots, 9\}, k_1 \neq k_2$, such that $|C_{k_1}| = |C_{k_2}| > |C_l|$ for every $l \in \{0, 1, \dots, 9\} \setminus \{k_1, k_2\}$ (there exist exactly two dominant labels) \implies our input is labelled as $\mathfrak{e}_{\{k_1, k_2\}}$;

What about ex-aequo?

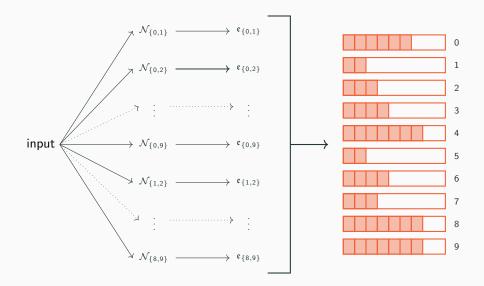
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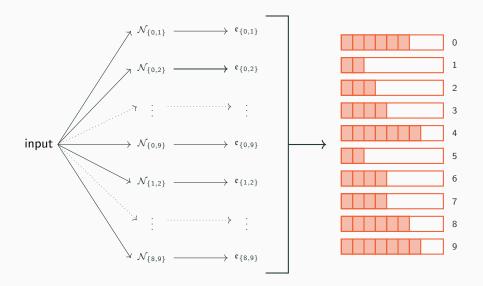
and we say that a label k is a dominant label if $|C_k| \ge |C_l|$ for every $l \in \{0, 1, ..., 9\}$. Then we can have three possible outcomes:

- (a) there exists one $k \in \{0, 1, ..., 9\}$ such that $|C_k| > |C_l|$ for every $l \in \{0, 1, ..., 9\} \setminus \{k\}$ (there exists exactly one dominant label) \implies our input is labelled as k;
- (b) there exist $k_1, k_2 \in \{0, 1, \dots, 9\}, k_1 \neq k_2$, such that $|C_{k_1}| = |C_{k_2}| > |C_I|$ for every $I \in \{0, 1, \dots, 9\} \setminus \{k_1, k_2\}$ (there exist exactly two dominant labels) \implies our input is labelled as $\mathfrak{e}_{\{k_1, k_2\}}$;
- (c) there exist three or more dominant labels \implies our input is labelled as -1.

Majority voting - Example 2



Majority voting - Example 3



As a consequence of our labelling system, when testing an input seven different cases can show up:

(0) there exists exactly one dominant label and it is the correct one;

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- (1) there exist exactly two dominant labels k_1, k_2 and $\mathfrak{e}_{\{k_1, k_2\}}$ is the correct one;

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- (1) there exist exactly two dominant labels k_1, k_2 and $\mathfrak{e}_{\{k_1, k_2\}}$ is the correct one;
- (2) there exist exactly two dominant labels k_1, k_2 and $\hat{\mathfrak{e}}_{\{k_1, k_2\}}$ is the correct one;

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- (2) there exist exactly two dominant labels k_1, k_2 and $\hat{\mathfrak{e}}_{\{k_1, k_2\}}$ is the correct one;
- (3) there exist three or more dominant labels and one of them is the correct one;

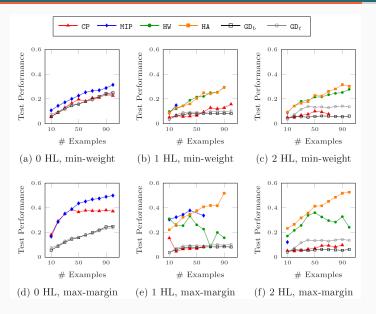
- (0) there exists exactly one dominant label and it is the correct one;
- (1) there exist exactly two dominant labels k_1, k_2 and $\mathfrak{e}_{\{k_1, k_2\}}$ is the correct one;
- (2) there exist exactly two dominant labels k_1, k_2 and $\hat{\mathfrak{e}}_{\{k_1, k_2\}}$ is the correct one;
- (3) there exist three or more dominant labels and one of them is the correct one;
- (4) there exist three or more dominant labels but none of them is the correct one;

- (0) there exists exactly one dominant label and it is the correct one;
- (1) there exist exactly two dominant labels k_1, k_2 and $\mathfrak{e}_{\{k_1, k_2\}}$ is the correct one;
- (2) there exist exactly two dominant labels k_1, k_2 and $\hat{\mathfrak{e}}_{\{k_1, k_2\}}$ is the correct one;
- (3) there exist three or more dominant labels and one of them is the correct one;
- (4) there exist three or more dominant labels but none of them is the correct one;
- (5) there exist exactly two dominant labels k_1, k_2 but neither $\mathfrak{e}_{\{k_1, k_2\}}$ nor $\hat{\mathfrak{e}}_{\{k_1, k_2\}}$ is the correct one;

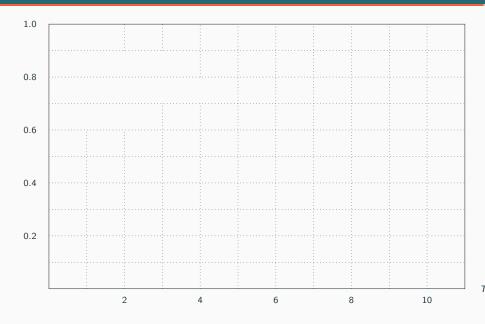
- (0) there exists exactly one dominant label and it is the correct one;
- (1) there exist exactly two dominant labels k_1, k_2 and $\mathfrak{e}_{\{k_1, k_2\}}$ is the correct one;
- (2) there exist exactly two dominant labels k_1, k_2 and $\hat{\mathfrak{e}}_{\{k_1, k_2\}}$ is the correct one;
- (3) there exist three or more dominant labels and one of them is the correct one;
- (4) there exist three or more dominant labels but none of them is the correct one;
- (5) there exist exactly two dominant labels k_1, k_2 but neither $\mathfrak{e}_{\{k_1, k_2\}}$ nor $\hat{\mathfrak{e}}_{\{k_1, k_2\}}$ is the correct one;
- (6) there exists exactly one dominant label but it is not the correct one.

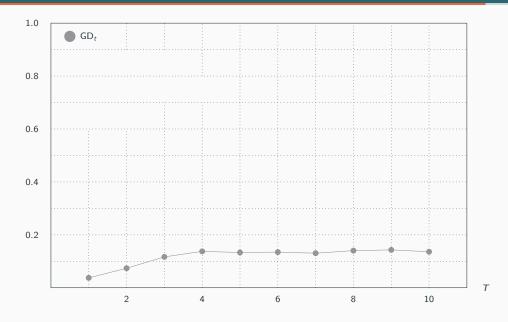
Computational Analysis

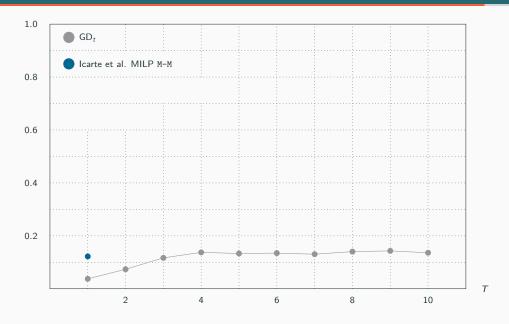
Some previous results

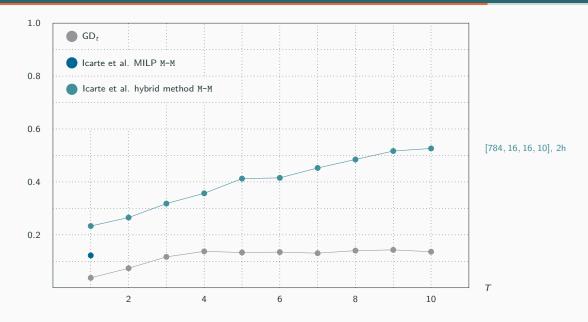


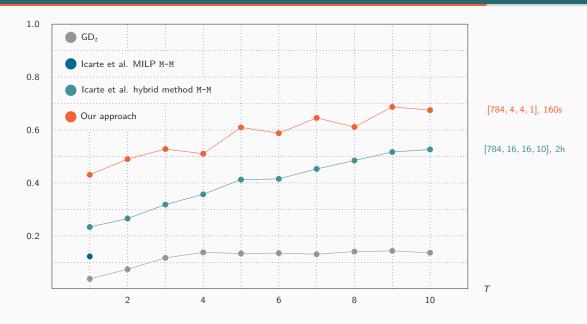
Toro Icarte, R., Illanes, L., Castro, M.P., Cire, A.A., McIlraith, S.A. and Beck, J.C.: Training binarized neural networks using MIP and CP. In: Proceedings of CP'19. vol 11802, pp. 401–417. Springer (2019).











Bigger tests

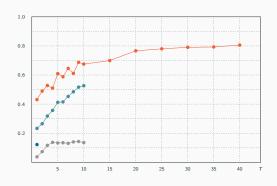
Structure:

networks architecture: [784, 10, 3, 1];

time limit for each network: 290s + 290s + 20s;

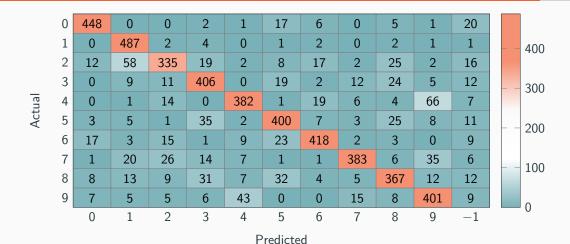
tested images: 5000.

Т	%Correct	%Incorrect	%-1	Feas. S-M	% w M-M	% w M-W
10	67.56	29.94	2.50	20	51.59	25.46
15	69.94	26.96	3.10	30	53.25	26.32
20	76.62	21.18	2.20	40	52.73	21.95
25	78.00	20.20	1.80	50	53.86	22.92
30	79.04	19.06	1.90	60	57.58	23.51
35	79.28	19.02	1.70	70	57.36	23.92
40	80.56	17.38	2.06	80	58.97	25.65



Т	%Status 0	%Status 1	%Status 2	%Status 3	%Status 4	%Status 5	%Status 6
10	65.82	1.74	1.52	2.20	0.30	2.16	26.26
15	68.46	1.48	1.18	2.58	0.52	2.12	23.66
20	74.76	1.86	1.12	1.72	0.48	1.56	18.50
25	76.64	1.36	1.34	1.46	0.34	1.78	17.08
30	77.68	1.36	1.40	1.56	0.34	1.54	16.12
35	77.66	1.62	1.36	1.54	0.16	1.26	16.40
40	78.60	1.96	1.66	1.90	0.16	1.80	13.92

Confusion matrix



 $Networks\ architecture:\ [784,10,3,1];$

time limit for each network: 290s + 290s + 20s;

training images per digit: 40;

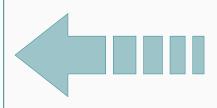
tested images: 5000.

Conclusions

Final Remarks & Future Perspectives

Different approaches from the literature and how to model them with MILPs;

- a way of combining these approaches to preserve feasibility, robustness, and simplicity;
- a structured ensemble method with its majority voting system.

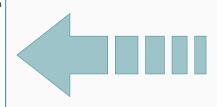


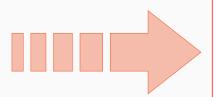
Final Remarks & Future Perspectives

Different approaches from the literature and how to model them with MILPs;

a way of combining these approaches to preserve feasibility, robustness, and simplicity;

a structured ensemble method with its majority voting system.





Apply a dimensionality reduction method to use more data or data with bigger dimensions;

alternative model formulations to improve the solver performances;

study the theoretical framework.

That's all Folks!

Any Questions?

You can also send me an e-mail at

 $\verb|ambrogiomaria.bernardelli01@universitadipavia.it|$