Homework 2 of ECE/CS 584

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A1:

1. Satisfiability problem:

$$\exists \boldsymbol{x}, \boldsymbol{x} \in \mathcal{S} \wedge (y = f(\boldsymbol{x})) \wedge \left(y_i - \max_{\substack{1 \leqslant k \leqslant m \\ k \neq i}} y_k \leqslant 0 \right) \tag{1}$$

or equivalently

$$\exists \boldsymbol{x}, \boldsymbol{x} \in \mathcal{S} \wedge (y = f(\boldsymbol{x})) \wedge \bigvee_{\substack{k=1 \\ k \neq i}}^{m} (y_i - y_k \leqslant 0) \tag{2}$$

Corresponding optimization problem:

$$\min_{\boldsymbol{x} \in \mathcal{S}} g(\boldsymbol{x}) := y_i - \max_{\substack{1 \leqslant k \leqslant m \\ k \neq i}} y_k \tag{3}$$

or equivalently

$$\min_{\boldsymbol{x} \in \mathcal{S}} g_k(\boldsymbol{x}) := y_i - y_k,\ k \neq i \tag{4}$$

If $g(\boldsymbol{x})$ (or certain $g_k(\boldsymbol{x})$) becomes **non-positive** at the global minimum $g(\boldsymbol{x}^*)$ (or $g_k(\boldsymbol{x}^*)$), the requirement does not hold since $\boldsymbol{x}^*$ is a counter-example.

2. Satisfiability problem:

$$\exists \boldsymbol{x}, \boldsymbol{x} \in \mathcal{S} \wedge \left(y_j - \max_{\substack{1 \leqslant k \leqslant m \\ k \neq j}} y_k \geqslant 0 \right) \tag{5}$$

or equivalently

$$\exists \boldsymbol{x}, \boldsymbol{x} \in \mathcal{S} \wedge (y = f(\boldsymbol{x})) \wedge \bigwedge_{\substack{k=1 \\ k \neq j}}^{m} (y_j - y_k \geqslant 0) \tag{6}$$

Corresponding optimization problem:

$$\max_{\boldsymbol{x} \in \mathcal{S}} g(\boldsymbol{x}) := y_j - \max_{\substack{1 \leqslant k \leqslant m \\ k \neq j}} y_k \tag{7}$$

or equivalently

$$\max_{\boldsymbol{x} \in \mathcal{S}} g_k(\boldsymbol{x}) := y_j - y_k,\ k \neq j \tag{8}$$

If $g(\boldsymbol{x})$ (or all $g_k(\boldsymbol{x})$) becomes **non-negative** at the global maximum $g(\boldsymbol{x}^*)$ (or $g_k(\boldsymbol{x}^*)$), the requirement does not hold since $\boldsymbol{x}^*$ is a counter-example.

A2:

1. Firstly, we have

$$z_1^{(1)} = x_1 - x_2 + 1 \in [-1, 3],\ \ z_2^{(1)} = 2x_1 - 2x_2 + 1 \in [-3, 5] \tag{9}$$

Next, we have

$$\begin{aligned} \hat{z}_1^{(1)} = \text{ReLU}\left(z_1^{(1)}\right) \in [0, 3],\ \ \hat{z}_2^{(1)} = \text{ReLU}\left(z_2^{(1)}\right) \in [0, 5] \\ z_1^{(2)} = \hat{z}_1^{(1)} - \hat{z}_2^{(1)} + 2 \in [-3, 5],\ \ z_2^{(2)} = 2\hat{z}_1^{(1)} - 2\hat{z}_2^{(1)} + 2 \in [-8, 8] \end{aligned} \tag{10}$$

Finally, we have

$$\begin{aligned} \hat{z}_1^{(2)} = \text{ReLU}\left(z_1^{(2)}\right) \in [0, 5],\ \ \hat{z}_2^{(2)} = \text{ReLU}\left(z_2^{(2)}\right) \in [0, 8] \\ y = -\hat{z}_1^{(2)} - z_1^{(1)} + \hat{z}_2^{(2)} + z_2^{(1)} \in [-11, 14] \end{aligned} \tag{11}$$

Therefore, we get the lower bound of y is -11 by using interval bound propagation.

2. According to (9), it's clear that $|u_1^{(1)}| > |l_1^{(1)}|$ and $|u_2^{(1)}| > |l_2^{(1)}|$, so $\alpha_1^{(1)} = \alpha_2^{(1)} = 1$. Now using the approach of CROWN, we have

$$z_1^{(1)} \leqslant \text{ReLU}\left(z_1^{(1)}\right) \leqslant \frac{3}{4}z_1^{(1)} + \frac{3}{4},\ \ z_2^{(1)} \leqslant \text{ReLU}\left(z_2^{(1)}\right) \leqslant \frac{5}{8}z_2^{(1)} + \frac{15}{8} \tag{12}$$

Since

$$z_1^{(2)} = \hat{z}_1^{(1)} - \hat{z}_2^{(1)} + 2,\ \ z_2^{(2)} = 2\hat{z}_1^{(1)} - 2\hat{z}_2^{(1)} + 2 \tag{13}$$

we have

$$\begin{aligned} z_1^{(1)} - \frac{5}{8}z_2^{(1)} + \frac{1}{8} \leqslant z_1^{(2)} \leqslant \frac{3}{4}z_1^{(1)} - z_2^{(1)} + \frac{11}{4} \\ 2z_1^{(1)} - \frac{5}{4}z_2^{(1)} - \frac{7}{4} \leqslant z_2^{(2)} \leqslant \frac{3}{2}z_1^{(1)} - 2z_2^{(1)} + \frac{7}{2} \end{aligned} \tag{14}$$

Substituting $z_1^{(1)} = x_1 - x_2 + 1$ and $z_2^{(1)} = 2x_1 - 2x_2 + 1$, we have

$$\begin{aligned} -\frac{1}{4}x_1 + \frac{1}{4}x_2 + \frac{1}{2} \leqslant z_1^{(2)} \leqslant -\frac{5}{4}x_1 + \frac{5}{4}x_2 + \frac{5}{2} \\ -\frac{1}{2}x_1 + \frac{1}{2}x_2 - 1 \leqslant z_2^{(2)} \leqslant -\frac{5}{2}x_1 + \frac{5}{2}x_2 + 3 \end{aligned} \tag{15}$$

Thus

$$z_1^{(2)} \in [0, 5]\,,\ \ z_2^{(2)} \in [-2, 8] \tag{16}$$

3. According to (16), $z_1^{(2)}$ is stable, but $z_2^{(2)}$ is not. Since $|u_2^{(2)}| > |l_2^{(2)}|$, using the approach of CROWN, we have

$$z_2^{(2)} \leqslant \text{ReLU}\left(z_2^{(2)}\right) \leqslant \frac{4}{5}z_2^{(2)} + \frac{8}{5} \tag{17}$$

Since $y = -\hat{z}_1^{(2)} - z_1^{(1)} + \hat{z}_2^{(2)} + z_2^{(1)}$, now proceed step by step:

$$\begin{aligned}
y &\geqslant -z_1^{(2)} - z_1^{(1)} + z_2^{(2)} + z_2^{(1)} \\
&\geqslant -\frac{3}{4}z_1^{(1)} + z_2^{(1)} - \frac{11}{4} - z_1^{(1)} + 2z_1^{(1)} - \frac{5}{4}z_2^{(1)} - \frac{7}{4} + z_2^{(1)} \\
&= \frac{1}{4}z_1^{(1)} + \frac{3}{4}z_2^{(1)} - \frac{9}{2} \\
&= \frac{1}{4}x_1 - \frac{1}{4}x_2 + 1 + \frac{3}{2}x_1 - \frac{3}{2}x_2 + 1 - \frac{9}{2} \\
&= \frac{7}{4}x_1 - \frac{7}{4}x_2 - \frac{5}{2}
\end{aligned} \tag{18}$$

Therefore, the CROWN lower bound on the output y is -6.

4. We can use just $\alpha_1^{(1)}$, $\alpha_2^{(1)}$, and $\alpha_2^{(2)}$ to get the tightest possible lower bound. This is because we need only $\alpha_2^{(2)}$ to get the lower bound of $z_2^{(2)}$, and in the rest part, we need $\alpha_1^{(1)}$ and $\alpha_2^{(1)}$ to get the intermediate layer bounds. Specifically, suppose we have

$$\alpha_1^{(1)} z_1^{(1)} \leqslant \mathrm{ReLU}\left(z_1^{(1)}\right) \leqslant \frac{3}{4}z_1^{(1)} + \frac{3}{4},\ \alpha_2^{(1)} z_2^{(1)} \leqslant \mathrm{ReLU}\left(z_2^{(1)}\right) \leqslant \frac{5}{8}z_2^{(1)} + \frac{15}{8} \tag{19}$$

and

$$\alpha_1^{(2)} z_1^{(2)} \leqslant \mathrm{ReLU}\left(z_1^{(2)}\right) \leqslant k_1^{(2)} z_1^{(2)} + c_1^{(2)},\ \alpha_2^{(2)} z_2^{(2)} \leqslant \mathrm{ReLU}\left(z_2^{(2)}\right) \leqslant k_2^{(2)} z_2^{(2)} + c_2^{(2)} \tag{20}$$

where the value of $k_1^{(2)}$, $c_1^{(2)}$, $k_2^{(2)}$, and $c_2^{(2)}$ can be derived from the intermediate layer bounds, which are only related to $\alpha_1^{(1)}$ and $\alpha_2^{(1)}$. Subsequently, we have

$$\begin{aligned}
y &= -\hat{z}_1^{(2)} - z_1^{(1)} + \hat{z}_2^{(2)} + z_2^{(1)} \\
&\geqslant -k_1^{(2)} z_1^{(2)} - c_1^{(2)} - z_1^{(1)} + \alpha_2^{(2)} z_2^{(2)} + z_2^{(1)} \\
&= -k_1^{(2)}(\hat{z}_1^{(1)} - \hat{z}_2^{(1)} + 2) - c_1^{(2)} - z_1^{(1)} + \alpha_2^{(2)}(2\hat{z}_1^{(1)} - 2\hat{z}_2^{(1)} + 2) + z_2^{(1)}
\end{aligned} \tag{21}$$

Therefore, it's clear that getting the tightest CROWN lower bound of y can be an optimization problem like following:

$$\max_{\alpha_1^{(1)}, \alpha_2^{(1)}, \alpha_2^{(2)} \in [0,1]} \ \min_{x_1, x_2 \in [-1,1]} \ \mathrm{CROWNLowerBound}(\alpha_1^{(1)}, \alpha_2^{(1)}, \alpha_2^{(2)}, x_1, x_2) \tag{22}$$

This explains why we just need only $\alpha_1^{(1)}$, $\alpha_2^{(1)}$, and $\alpha_2^{(2)}$ to get the tightest CROWN lower bound.

A3:

1. Implementation see `mip.py`.

2. Implementation see `lp.py`.

3. Experimental results are in Table 1 and Table 2. Experimental logs can also be checked in the folder.

Table 1: Exact Solutions Found by MILP Method

Perturbation Size	0	0.001	0.003	0.01	0.03	0.1
Exact Solutions	11.93322	11.65533	11.08168	8.889835	2.877214	timeout
	14.64563	14.44137	14.01663	12.37658	7.69967	timeout
	9.964368	9.704725	9.163939	7.053752	1.337917	timeout
	9.421547	9.139847	8.586733	6.606274	0.702675	timeout
	16.29663	16.06381	15.59847	13.99572	9.506186	timeout
	11.35621	11.06384	10.47546	8.393649	2.232222	timeout
	21.63385	21.28212	20.57429	17.95548	10.75938	timeout
	12.16203	11.84295	11.19989	8.833205	2.427645	timeout
	10.91598	10.6624	10.15238	8.416098	3.226658	timeout

Table 2: Lower Bounds Found by LP Method

Perturbation Size	0	0.001	0.003	0.01	0.03	0.1
Lower Bounds	11.93322	11.64509	10.97531	8.243442	-4.31841	-65.2557
	14.64563	14.43426	13.91903	11.6801	0.467643	-69.5228
	9.964368	9.696616	9.042424	6.32135	-5.44882	-67.007
	9.421547	9.127076	8.491447	5.709146	-7.25529	-68.1426
	16.29663	16.05955	15.55909	13.39164	3.081971	-59.3878
	11.35621	11.05287	10.39308	7.621362	-5.5567	-81.4825
	21.63385	21.27357	20.46856	17.19302	2.704611	-72.9631
	12.16203	11.82792	11.06755	7.841307	-6.57479	-75.9695
	10.91598	10.65354	10.07684	7.705151	-4.18084	-69.7365

A4:

1. Completed.

2. Inspired by the way of constructing the upper bound for $\mathrm{ReLU}(z)$, the slope of one of the linear bounds for $\mathrm{hardtanh}(z)$ is equal to the line that connects both end points, i.e. $(l, \mathrm{hardtanh}(l))$ and $(u, \mathrm{hardtanh}(u))$. Since we can make the lower and upper bounds use the same slope, which is suggested in the problem statement, the slope of both linear bounds can be

$$\frac{\mathrm{hardtanh}(u) - \mathrm{hardtanh}(l)}{u - l} \tag{23}$$

We can easily verify that the expression of slope above can accommodate various different values of l and u, as illustrated in Figure 1.

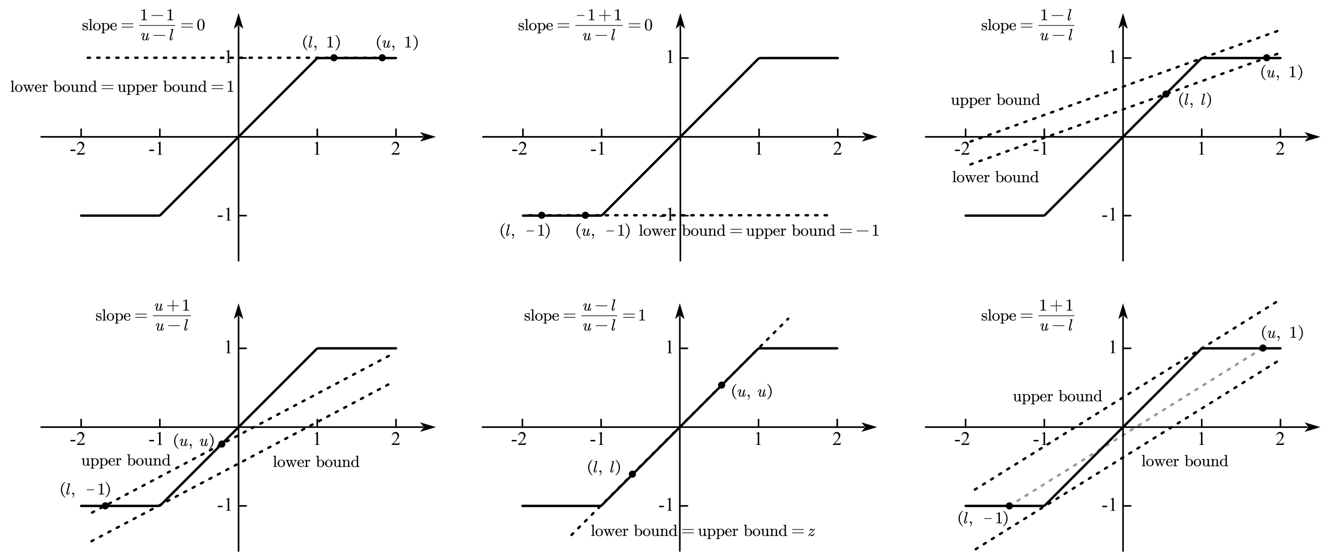

Figure 1

Then, we can work out the interception of the lower bound is

$$\operatorname{hardtanh}(u) - \frac{\operatorname{hardtanh}(u) - \operatorname{hardtanh}(l)}{u-l} \operatorname{hardtanh}(u) \tag{24}$$

and the interception of the upper bound is

$$\operatorname{hardtanh}(l) - \frac{\operatorname{hardtanh}(u) - \operatorname{hardtanh}(l)}{u-l} \operatorname{hardtanh}(l) \tag{25}$$

3. Implementation see `hardTanh_question.py`.

4. Noticed that

$$\operatorname{hardtanh}(z) = \operatorname{ReLU}(z+1) - \operatorname{ReLU}(z-1) - 1 \tag{26}$$

so it's not hard to find there are some cases can use the conclusion of the α-CROWN discussion about $\operatorname{ReLU}(z)$, as illustrated in Figure 2.

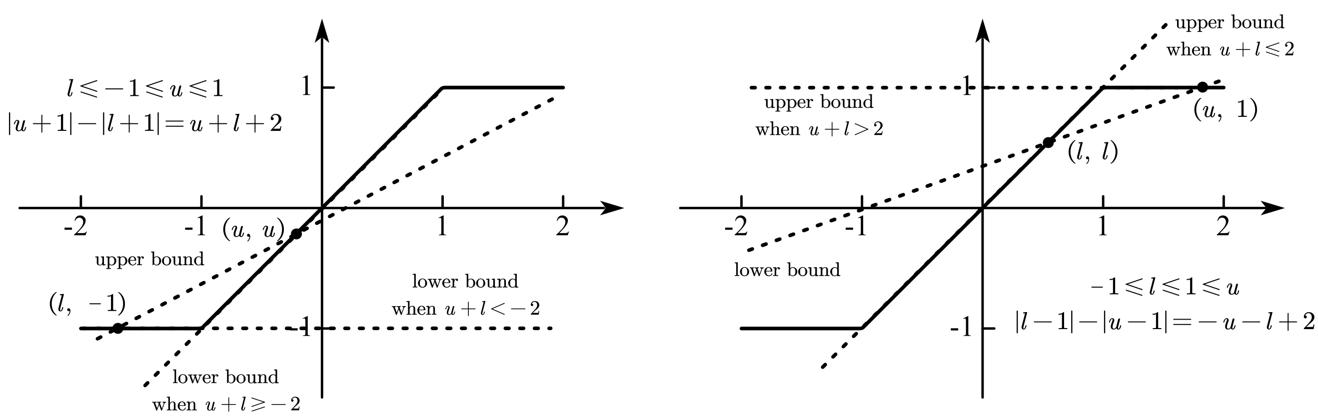

Figure 2: Two Cases Similar to $\operatorname{ReLU}(z)$

Now, we just need to focus on the most complicated case, which is $l < -1$ and $u > 1$.

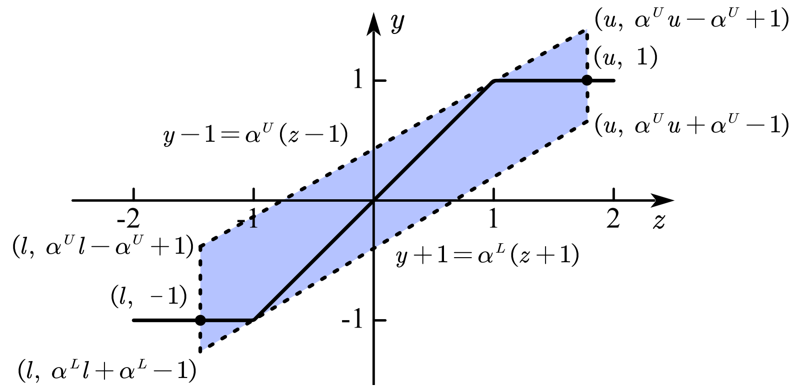

Figure 3

Suppose the linear bounds are

$$\alpha^L(z+1) - 1 \leqslant \text{hardtanh}\,(z) \leqslant \alpha^U(z-1) + 1,\ l \leqslant z \leqslant u \tag{27}$$

where

$$\begin{aligned} 0 \leqslant \alpha^L &\leqslant \frac{\text{hardtanh}\,(u) - \text{hardtanh}\,(l)}{u - \text{hardtanh}\,(l)} = \frac{2}{u+1} < 1 \\ 0 \leqslant \alpha^U &\leqslant \frac{\text{hardtanh}\,(u) - \text{hardtanh}\,(l)}{\text{hardtanh}\,(u) - l} = \frac{2}{1-l} < 1 \end{aligned} \tag{28}$$

Then the area of the region enclosed by lines $z = l$, $z = u$, the lower and the upper bound is

$$\text{Area} = \frac{u-l}{2}\left[(u+l-2)\alpha^U - (u+l+2)\alpha^L + 4\right] \tag{29}$$

Subsequently,

(a) when $u + l - 2 \leqslant 0$ and $-u - l - 2 \leqslant 0$, i.e. $-2 \leqslant u + l \leqslant 2$, to minimize the area, we should let $\alpha^L = \frac{2}{u+1}$ and $\alpha^U = \frac{2}{1-l}$;

(b) when $u + l - 2 \leqslant 0$ and $-u - l - 2 > 0$, i.e. $u + l > 2$, to minimize the area, we should let $\alpha^L = \frac{2}{u+1}$ and $\alpha^U = 0$;

(c) when $u + l - 2 > 0$ and $-u - l - 2 \leqslant 0$, i.e. $u + l < -2$, to minimize the area, we should let $\alpha^L = 0$ and $\alpha^U = \frac{2}{1-l}$;

(d) it impossible for both $u + l - 2 > 0$ and $-u - l - 2 > 0$ to hold simultaneously.

This implies

$$\alpha^L = \begin{cases} \frac{2}{u+1},\ u + l \geqslant -2 \\ 0,\ u + l < -2 \end{cases},\ \alpha^U = \begin{cases} \frac{2}{1-l},\ u + l \leqslant 2 \\ 0,\ u + l > 2 \end{cases},\ l < -1,\ u > 1 \tag{30}$$

In fact, the conclusion above is consistent with cases in Figure 2. What's more, it's not hard to check the conclusion is even consistent with other cases. Specifically, we have

$$\alpha^L = \begin{cases} \dfrac{\mathrm{hardtanh}\,(u) - \mathrm{hardtanh}\,(l)}{u - \mathrm{hardtanh}\,(l)}, & u + l \geqslant -2 \\ 0, & u + l < -2 \end{cases}$$
$$\alpha^U = \begin{cases} \dfrac{\mathrm{hardtanh}\,(u) - \mathrm{hardtanh}\,(l)}{\mathrm{hardtanh}\,(u) - l}, & u + l \leqslant 2 \\ 0, & u + l > 2 \end{cases} \tag{31}$$

Finally, we can work out the interception of the lower bound is

$$\begin{cases} \mathrm{hardtanh}\,(l) - \dfrac{\mathrm{hardtanh}\,(u) - \mathrm{hardtanh}\,(l)}{u - \mathrm{hardtanh}\,(l)}\mathrm{hardtanh}\,(l)\,, & u + l \geqslant -2 \\ \mathrm{hardtanh}\,(l)\,, & u + l < -2, \text{ (actually is -1, since } 2l < u + l < -2 \;\Rightarrow\; l < -1) \end{cases} \tag{32}$$

and the interception of the upper bound is

$$\begin{cases} \mathrm{hardtanh}\,(u) - \dfrac{\mathrm{hardtanh}\,(u) - \mathrm{hardtanh}\,(l)}{u - \mathrm{hardtanh}\,(l)}\mathrm{hardtanh}\,(u)\,, & u + l \leqslant 2 \\ \mathrm{hardtanh}\,(u)\,, & u + l > 2, \text{ (actually is 1, since } 2u > u + l > 2 \;\Rightarrow\; u > 1) \end{cases} \tag{33}$$

5. Implementation see `hardTanh_question_alpha.py`. Results for CROWN and α-CROWN is shown in Table 3 and Table 4 respectively. Experimental logs can also be checked in the folder.

Table 3: Lower and Upper CROWN Bounds

	Lower Bound	Upper Bound
f_0	-5.8888	7.9799
f_1	-8.4223	3.8257
f_2	-7.1542	6.6943
f_3	-4.233	10.6406
f_4	-12.0069	-0.582
f_5	-13.1308	2.7378
f_6	-15.1046	-1.7304
f_7	6.1154	21.6736
f_8	-6.8795	6.2323
f_9	-5.9975	6.5901

Table 4: Lower and Upper α-CROWN Bounds

	Lower Bound	Upper Bound
f_0	-5.2428	7.3142
f_1	-8.3839	2.5022
f_2	-7.0532	4.9316
f_3	-3.1677	9.9903
f_4	-11.7056	-1.1283
f_5	-12.3369	2.3594
f_6	-14.153	-2.3708
f_7	6.1764	20.4607
f_8	-6.1789	5.2903
f_9	-5.2493	5.474

It's clear that the α-CROWN bounds are tighter than CROWN Bounds.