A Proof of Theorem 3.2

Given an m-layer neural network function $f : \mathbb{R}^{n_0} \rightarrow \mathbb{R}^{n_m}$ with pre-activation bounds $\mathbf{l}^{(k)}$ and $\mathbf{u}^{(k)}$ for $\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)$ and $\forall k \in [m-1]$, let the pre-activation inputs for the i-th neuron at layer $m-1$ be $\mathbf{y}_i^{(m-1)} := \mathbf{W}_{i,:}^{(m-1)} \Phi_{m-2}(\mathbf{x}) + \mathbf{b}_i^{(m-1)}$. The j-th output of the neural network is the following:

$$
\begin{aligned}
f_j(\mathbf{x}) &= \sum_{i=1}^{n_{m-1}} \mathbf{W}_{j,i}^{(m)} [\Phi_{m-1}(\mathbf{x})]_i + \mathbf{b}_j^{(m)}, && (5) \\
&= \sum_{i=1}^{n_{m-1}} \mathbf{W}_{j,i}^{(m)} \sigma(\mathbf{y}_i^{(m-1)}) + \mathbf{b}_j^{(m)}, \\
&= \underbrace{\sum_{\mathbf{W}_{j,i}^{(m)} \geq 0} \mathbf{W}_{j,i}^{(m)} \sigma(\mathbf{y}_i^{(m-1)})}_{F_1} + \underbrace{\sum_{\mathbf{W}_{j,i}^{(m)} < 0} \mathbf{W}_{j,i}^{(m)} \sigma(\mathbf{y}_i^{(m-1)})}_{F_2} + \mathbf{b}_j^{(m)}. && (6)
\end{aligned}
$$

Assume the activation function $\sigma(y)$ is bounded by two linear functions $h_{U,i}^{(m-1)}, h_{L,i}^{(m-1)}$ in Definition 3.1, we have

$$
h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) \leq \sigma(\mathbf{y}_i^{(m-1)}) \leq h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}).
$$

Thus, if the associated weight $\mathbf{W}_{j,i}^{(m)}$ to the i-th neuron is non-negative (the terms in F_1 bracket), we have

$$
\mathbf{W}_{j,i}^{(m)} \cdot h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) \leq \mathbf{W}_{j,i}^{(m)} \sigma(\mathbf{y}_i^{(m-1)}) \leq \mathbf{W}_{j,i}^{(m)} \cdot h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}); \tag{7}
$$

otherwise (the terms in F_2 bracket), we have

$$
\mathbf{W}_{j,i}^{(m)} \cdot h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) \leq \mathbf{W}_{j,i}^{(m)} \sigma(\mathbf{y}_i^{(m-1)}) \leq \mathbf{W}_{j,i}^{(m)} \cdot h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}). \tag{8}
$$

Upper bound. Let $f_j^{U,m-1}(\mathbf{x})$ be an upper bound of $f_j(\mathbf{x})$. To compute $f_j^{U,m-1}(\mathbf{x})$, (6), (7) and (8) are the key equations. Precisely, for the $\mathbf{W}_{j,i}^{(m)} \geq 0$ terms in (6), the upper bound is the right-hand-side (RHS) in (7); and for the $\mathbf{W}_{j,i}^{(m)} < 0$ terms in (6), the upper bound is the RHS in (8). Thus, we obtain:

$$
\begin{aligned}
& f_j^{U,m-1}(\mathbf{x}) \\
&= \sum_{\mathbf{W}_{j,i}^{(m)} \geq 0} \mathbf{W}_{j,i}^{(m)} \cdot h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) + \sum_{\mathbf{W}_{j,i}^{(m)} < 0} \mathbf{W}_{j,i}^{(m)} \cdot h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) + \mathbf{b}_j^{(m)}, && (9) \\
&= \sum_{\mathbf{W}_{j,i}^{(m)} \geq 0} \mathbf{W}_{j,i}^{(m)} \alpha_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)} + \beta_{U,i}^{(m-1)}) + \sum_{\mathbf{W}_{j,i}^{(m)} < 0} \mathbf{W}_{j,i}^{(m)} \alpha_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)} + \beta_{L,i}^{(m-1)}) + \mathbf{b}_j^{(m)}, && (10) \\
&= \sum_{i=1}^{n_{m-1}} \mathbf{W}_{j,i}^{(m)} \lambda_{j,i}^{(m-1)}(\mathbf{y}_i^{(m-1)} + \mathbf{\Delta}_{i,j}^{(m-1)}) + \mathbf{b}_j^{(m)}, && (11) \\
&= \sum_{i=1}^{n_{m-1}} \mathbf{\Lambda}_{j,i}^{(m-1)}\Big(\sum_{r=1}^{n_{m-2}} \mathbf{W}_{i,r}^{(m-1)} [\Phi_{m-2}(\mathbf{x})]_r + \mathbf{b}_i^{(m-1)} + \mathbf{\Delta}_{i,j}^{(m-1)}\Big) + \mathbf{b}_j^{(m)}, && (12) \\
&= \sum_{i=1}^{n_{m-1}} \mathbf{\Lambda}_{j,i}^{(m-1)}\Big(\sum_{r=1}^{n_{m-2}} \mathbf{W}_{i,r}^{(m-1)} [\Phi_{m-2}(\mathbf{x})]_r\Big) + \sum_{i=1}^{n_{m-1}} \mathbf{\Lambda}_{j,i}^{(m-1)}(\mathbf{b}_i^{(m-1)} + \mathbf{\Delta}_{i,j}^{(m-1)}) + \mathbf{b}_j^{(m)}, && (13) \\
&= \sum_{r=1}^{n_{m-2}} \left(\sum_{i=1}^{n_{m-1}} \mathbf{\Lambda}_{j,i}^{(m-1)} \mathbf{W}_{i,r}^{(m-1)} \right) [\Phi_{m-2}(\mathbf{x})]_r + \left(\sum_{i=1}^{n_{m-1}} \mathbf{\Lambda}_{j,i}^{(m-1)}(\mathbf{b}_i^{(m-1)} + \mathbf{\Delta}_{i,j}^{(m-1)}) + \mathbf{b}_j^{(m)} \right), && (14) \\
&= \sum_{r=1}^{n_{m-2}} \tilde{\mathbf{W}}_{j,r}^{(m-1)} [\Phi_{m-2}(\mathbf{x})]_r + \tilde{\mathbf{b}}_j^{(m-1)}. && (15)
\end{aligned}
$$

From (9) to (10), we replace $h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)})$ and $h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)})$ by their definitions; from (10) to (11), we use variables $\lambda_{j,i}^{(m-1)}$ and $\mathbf{\Delta}_{j,i}^{(m-1)}$ to denote the slopes in front of $\mathbf{y}_i^{(m-1)}$ and the intercepts in the parentheses:

$$\lambda_{j,i}^{(m-1)} = \begin{cases} \alpha_{U,i}^{(m-1)} & \text{if } \mathbf{W}_{j,i}^{(m)} \geq 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m)}\mathbf{W}_{:,i}^{(m)} \geq 0); \\ \alpha_{L,i}^{(m-1)} & \text{if } \mathbf{W}_{j,i}^{(m)} < 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m)}\mathbf{W}_{:,i}^{(m)} < 0); \end{cases} \tag{16}$$

$$\mathbf{\Delta}_{i,j}^{(m-1)} = \begin{cases} \beta_{U,i}^{(m-1)} & \text{if } \mathbf{W}_{j,i}^{(m)} \geq 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m)}\mathbf{W}_{:,i}^{(m)} \geq 0); \\ \beta_{L,i}^{(m-1)} & \text{if } \mathbf{W}_{j,i}^{(m)} < 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m)}\mathbf{W}_{:,i}^{(m)} < 0). \end{cases} \tag{17}$$

From (11) to (12), we replace $\mathbf{y}_i^{(m-1)}$ with its definition and let $\mathbf{\Lambda}_{j,i}^{(m-1)} := \mathbf{W}_{j,i}^{(m)}\lambda_{j,i}^{(m-1)}$. We further let $\mathbf{\Lambda}_{j,:}^{(m)} = \mathbf{e}_j^\top$ (the standard unit vector with the only non-zero jth element equal to 1), and thus we can rewrite the conditions of $\mathbf{W}_{j,i}^{(m)}$ in (16) and (17) as $\mathbf{\Lambda}_{j,:}^{(m)}\mathbf{W}_{:,i}^{(m)}$. From (12) to (13), we collect the constant terms that are not related to $\mathbf{x}$. From (13) to (14), we swap the summation order of i and r, and the coefficients in front of $[\Phi_{m-2}(x)]_r$ can be combined into a new equivalent weight $\tilde{\mathbf{W}}_{j,r}^{(m-1)}$ and the constant term can combined into a new equivalent bias $\tilde{\mathbf{b}}_j^{(m-1)}$ in (15):

$$\tilde{\mathbf{W}}_{j,r}^{(m-1)} = \sum_{i=1}^{n_{m-1}} \mathbf{\Lambda}_{j,i}^{(m-1)}\mathbf{W}_{i,r}^{(m-1)} = \mathbf{\Lambda}_{j,:}^{(m-1)}\mathbf{W}_{:,r}^{(m-1)},$$

$$\tilde{\mathbf{b}}_{j}^{(m-1)} = \sum_{i=1}^{n_{m-1}} \mathbf{\Lambda}_{j,i}^{(m-1)}(\mathbf{b}_i^{(m-1)} + \mathbf{\Delta}_{i,j}^{(m-1)}) + \mathbf{b}_j^{(m)} = \mathbf{\Lambda}_{j,:}^{(m-1)}(\mathbf{b}^{(m-1)} + \mathbf{\Delta}_{:,j}^{(m-1)}) + \mathbf{b}_j^{(m)}.$$

Notice that after defining the new equivalent weight $\tilde{\mathbf{W}}_{j,r}^{(m-1)}$ and equivalent bias $\tilde{\mathbf{b}}_j^{(m-1)}$, $f_j^{U,m-1}(\mathbf{x})$ in (15) and $f_j(\mathbf{x})$ in (5) are in the same form. Thus, we can repeat the above procedure again to obtain an upper bound of $f_j^{U,m-1}(\mathbf{x})$, i.e. $f_j^{U,m-2}(\mathbf{x})$:

$$\begin{aligned} \mathbf{\Lambda}_{j,i}^{(m-2)} &= \tilde{\mathbf{W}}_{j,i}^{(m-1)}\lambda_{j,i}^{(m-2)} \\ &= \mathbf{\Lambda}_{j,:}^{(m-1)}\mathbf{W}_{:,i}^{(m-1)}\lambda_{j,i}^{(m-2)} \\ \tilde{\mathbf{W}}_{j,r}^{(m-2)} &= \mathbf{\Lambda}_{j,:}^{(m-2)}\mathbf{W}_{:,r}^{(m-2)} \\ \tilde{\mathbf{b}}_{j}^{(m-2)} &= \mathbf{\Lambda}_{j,:}^{(m-2)}(\mathbf{b}^{(m-2)} + \mathbf{\Delta}_{:,j}^{(m-2)}) + \tilde{\mathbf{b}}_j^{(m-1)} \end{aligned}$$

$$\lambda_{j,i}^{(m-2)} = \begin{cases} \alpha_{U,i}^{(m-2)} & \text{if } \tilde{\mathbf{W}}_{j,i}^{(m-1)} \geq 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m-1)}\mathbf{W}_{:,i}^{(m-1)} \geq 0); \\ \alpha_{L,i}^{(m-2)} & \text{if } \tilde{\mathbf{W}}_{j,i}^{(m-1)} < 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m-1)}\mathbf{W}_{:,i}^{(m-1)} < 0); \end{cases}$$

$$\mathbf{\Delta}_{i,j}^{(m-2)} = \begin{cases} \beta_{U,i}^{(m-2)} & \text{if } \tilde{\mathbf{W}}_{j,i}^{(m-1)} \geq 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m-1)}\mathbf{W}_{:,i}^{(m-1)} \geq 0); \\ \beta_{L,i}^{(m-2)} & \text{if } \tilde{\mathbf{W}}_{j,i}^{(m-1)} < 0 \quad (\iff \mathbf{\Lambda}_{j,:}^{(m-1)}\mathbf{W}_{:,i}^{(m-1)} < 0). \end{cases}$$

and repeat again iteratively until obtain the final upper bound $f_j^{U,1}(\mathbf{x})$, where $f_j(\mathbf{x}) \leq f_j^{U,m-1}(\mathbf{x}) \leq f_j^{U,m-2}(\mathbf{x}) \leq \ldots \leq f_j^{U,1}(\mathbf{x})$. We let $f_j(\mathbf{x})$ denote the final upper bound $f_j^{U,1}(\mathbf{x})$, and we have

$$f_j^U(\mathbf{x}) = \mathbf{\Lambda}_{j,:}^{(0)}\mathbf{x} + \sum_{k=1}^{m} \mathbf{\Lambda}_{j,:}^{(k)}(\mathbf{b}^{(k)} + \mathbf{\Delta}_{:,j}^{(k)})$$

and ($\odot$ is the Hadamard product)

$$\mathbf{\Lambda}_{j,:}^{(k-1)} = \begin{cases} \mathbf{e}_j^\top & \text{if } k = m+1; \\ (\mathbf{\Lambda}_{j,:}^{(k)}\mathbf{W}^{(k)}) \odot \lambda_{j,:}^{(k-1)} & \text{if } k \in [m]. \end{cases}$$

and $\forall i \in [n_k]$,

$$\lambda_{j,i}^{(k)} = \begin{cases} \alpha_{U,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Lambda}_{j,:}^{(k+1)}\mathbf{W}_{:,i}^{(k+1)} \geq 0; \\ \alpha_{L,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Lambda}_{j,:}^{(k+1)}\mathbf{W}_{:,i}^{(k+1)} < 0; \\ 1 & \text{if } k = 0. \end{cases}$$

$$\mathbf{\Delta}_{i,j}^{(k)} = \begin{cases} \beta_{U,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Lambda}_{j,:}^{(k+1)} \mathbf{W}_{:,i}^{(k+1)} \geq 0; \\ \beta_{L,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Lambda}_{j,:}^{(k+1)} \mathbf{W}_{:,i}^{(k+1)} < 0; \\ 0 & \text{if } k = m. \end{cases}$$

Lower bound. The above derivations of upper bound can be applied similarly to deriving lower bounds of $f_j(\mathbf{x})$, and the only difference is now we need to use the LHS of (7) and (8) (rather than RHS when deriving upper bound) to bound the two terms in (6). Thus, following the same procedure in deriving the upper bounds, we can iteratively unwrap the activation functions and obtain a final lower bound $f_j^{L,1}(\mathbf{x})$, where $f_j(\mathbf{x}) \geq f_j^{L,m-1}(\mathbf{x}) \geq f_j^{L,m-2}(\mathbf{x}) \geq \ldots \geq f_j^{L,1}(\mathbf{x})$. Let $f_j^L(\mathbf{x}) = f_j^{L,1}(\mathbf{x})$, we have:

$$f_j^L(\mathbf{x}) = \mathbf{\Omega}_{j,:}^{(0)} \mathbf{x} + \sum_{k=1}^{m} \mathbf{\Omega}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Theta}_{:,j}^{(k)})$$

$$\mathbf{\Omega}_{j,:}^{(k-1)} = \begin{cases} \mathbf{e}_j^\top & \text{if } k = m+1; \\ (\mathbf{\Omega}_{j,:}^{(k)} \mathbf{W}^{(k)}) \odot \omega_{j,:}^{(k-1)} & \text{if } k \in [m]. \end{cases}$$

and $\forall i \in [n_k]$,

$$\omega_{j,i}^{(k)} = \begin{cases} \alpha_{L,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Omega}_{j,:}^{(k+1)} \mathbf{W}_{:,i}^{(k+1)} \geq 0; \\ \alpha_{U,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Omega}_{j,:}^{(k+1)} \mathbf{W}_{:,i}^{(k+1)} < 0; \\ 1 & \text{if } k = 0. \end{cases}$$

$$\mathbf{\Theta}_{i,j}^{(k)} = \begin{cases} \beta_{L,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Omega}_{j,:}^{(k+1)} \mathbf{W}_{:,i}^{(k+1)} \geq 0; \\ \beta_{U,i}^{(k)} & \text{if } k \in [m-1],\ \mathbf{\Omega}_{j,:}^{(k+1)} \mathbf{W}_{:,i}^{(k+1)} < 0; \\ 0 & \text{if } k = m. \end{cases}$$

Indeed, $\lambda_{j,i}^{(k)}$ and $\omega_{j,i}^{(k)}$ only differs in the conditions of selecting $\alpha_{U,i}^{(k)}$ or $\alpha_{L,i}^{(k)}$; similarly for $\mathbf{\Delta}_{i,j}^{(k)}$ and $\mathbf{\Theta}_{i,j}^{(k)}$.

B Proof of Corollary 3.3

Definition B.1 (Dual norm)**.** *Let $\|\cdot\|$ be a norm on $\mathbb{R}^n$. The associated dual norm, denoted as $\|\cdot\|_*$, is defined as*

$$\|\mathbf{a}\|_* = \{\sup_{\mathbf{y}} \mathbf{a}^\top \mathbf{y} \mid \|\mathbf{y}\| \leq 1\}.$$

Global upper bound. Our goal is to find a *global* upper and lower bound for the m-th layer network output $f_j(\mathbf{x}), \forall \mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)$. By Theorem 3.2, for $\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)$, we have $f_j^L(\mathbf{x}) \leq f_j(\mathbf{x}) \leq f_j^U(\mathbf{x})$ and $f_j^U(\mathbf{x}) = \mathbf{\Lambda}_{j,:}^{(0)} \mathbf{x} + \sum_{k=1}^m \mathbf{\Lambda}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Delta}_{:,j}^{(k)})$. Thus define $\gamma_j^U := \max_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} f_j^U(\mathbf{x})$, and we have

$$f_j(\mathbf{x}) \leq f_j^U(\mathbf{x}) \leq \max_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} f_j^U(\mathbf{x}) = \gamma_j^U,$$

since $\forall \mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)$. In particular,

$$\begin{aligned} \max_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} f_j^U(\mathbf{x}) &= \max_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} \left[\mathbf{\Lambda}_{j,:}^{(0)} \mathbf{x} + \sum_{k=1}^m \mathbf{\Lambda}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Delta}_{:,j}^{(k)}) \right] \\ &= \left[\max_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} \mathbf{\Lambda}_{j,:}^{(0)} \mathbf{x} \right] + \sum_{k=1}^m \mathbf{\Lambda}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Delta}_{:,j}^{(k)}) \qquad (18) \\ &= \epsilon \left[\max_{\mathbf{y} \in \mathbb{B}_p(\mathbf{0}, 1)} \mathbf{\Lambda}_{j,:}^{(0)} \mathbf{y} \right] + \mathbf{\Lambda}_{j,:}^{(0)} \mathbf{x_0} + \sum_{k=1}^m \mathbf{\Lambda}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Delta}_{:,j}^{(k)}) \qquad (19) \\ &= \epsilon \|\mathbf{\Lambda}_{j,:}^{(0)}\|_q + \mathbf{\Lambda}_{j,:}^{(0)} \mathbf{x_0} + \sum_{k=1}^m \mathbf{\Lambda}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Delta}_{:,j}^{(k)}). \qquad (20) \end{aligned}$$

From (18) to (19), let $\mathbf{y} := \frac{\mathbf{x}-\mathbf{x_0}}{\epsilon}$, and thus $\mathbf{y} \in \mathbb{B}_p(\mathbf{0}, 1)$. From (19) to (20), apply Definition B.1 and use the fact that ℓ_q norm is dual of ℓ_p norm for $p, q \in [1, \infty]$.

Global lower bound. Similarly, let $\gamma_j^L := \min_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} f_j^L(\mathbf{x})$, we have

$$f_j(\mathbf{x}) \geq f_j^L(\mathbf{x}) \geq \min_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} f_j^L(\mathbf{x}) = \gamma_j^L.$$

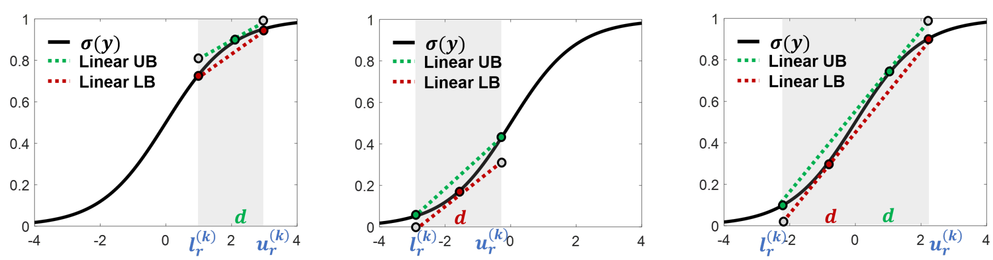
Since $f_j^L(\mathbf{x}) = \mathbf{\Omega}_{j,:}^{(0)} \mathbf{x} + \sum_{k=1}^{m} \mathbf{\Omega}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Theta}_{:,j}^{(k)})$, we can derive γ_j^L (similar to the derivation of γ_j^U) below:

$$\begin{aligned}
\min_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} f_j^L(\mathbf{x}) &= \min_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} \left[\mathbf{\Omega}_{j,:}^{(0)} \mathbf{x} + \sum_{k=1}^{m} \mathbf{\Omega}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Theta}_{:,j}^{(k)}) \right] \\
&= \left[\min_{\mathbf{x} \in \mathbb{B}_p(\mathbf{x_0}, \epsilon)} \mathbf{\Omega}_{j,:}^{(0)} \mathbf{x} \right] + \sum_{k=1}^{m} \mathbf{\Omega}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Theta}_{:,j}^{(k)}) \\
&= -\epsilon \left[\max_{\mathbf{y} \in \mathbb{B}_p(\mathbf{0}, 1)} -\mathbf{\Omega}_{j,:}^{(0)} \mathbf{y} \right] + \mathbf{\Omega}_{j,:}^{(0)} \mathbf{x_0} + \sum_{k=1}^{m} \mathbf{\Omega}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Theta}_{:,j}^{(k)}) \\
&= -\epsilon \| \mathbf{\Omega}_{j,:}^{(0)} \|_q + \mathbf{\Omega}_{j,:}^{(0)} \mathbf{x_0} + \sum_{k=1}^{m} \mathbf{\Omega}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Theta}_{:,j}^{(k)}).
\end{aligned}$$

Thus, we have

$$\begin{aligned}
&\text{(global upper bound)} \quad \gamma_j^U = \epsilon \| \mathbf{\Lambda}_{j,:}^{(0)} \|_q + \mathbf{\Lambda}_{j,:}^{(0)} \mathbf{x_0} + \sum_{k=1}^{m} \mathbf{\Lambda}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Delta}_{:,j}^{(k)}), \\
&\text{(global lower bound)} \quad \gamma_j^L = -\epsilon \| \mathbf{\Omega}_{j,:}^{(0)} \|_q + \mathbf{\Omega}_{j,:}^{(0)} \mathbf{x_0} + \sum_{k=1}^{m} \mathbf{\Omega}_{j,:}^{(k)} (\mathbf{b}^{(k)} + \mathbf{\Theta}_{:,j}^{(k)}),
\end{aligned}$$

C Illustration of linear upper and lower bounds on sigmoid activation function.



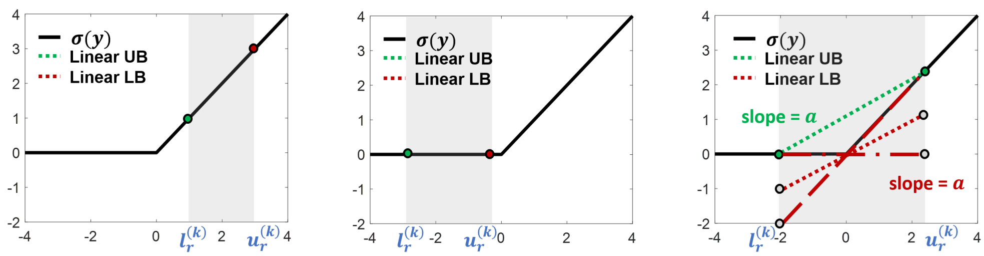
(a) $r \in \mathcal{S}_k^+$ (b) $r \in \mathcal{S}_k^-$ (c) $r \in \mathcal{S}_k^\pm$

Figure 3: The linear upper and lower bounds for $\sigma(y) = $ sigmoid

D $f_j^U(\mathbf{x})$ and $f_j^L(\mathbf{x})$ by Quadratic approximation

Upper bound. Let $f_j^U(\mathbf{x})$ be an upper bound of $f_j(\mathbf{x})$. To compute $f_j^U(\mathbf{x})$ with quadratic approximations, we can still apply (7) and (8) except that $h_{U,r}^{(k)}(y)$ and $h_{L,r}^{(k)}(y)$ are replaced by the following quadratic functions:

$$h_{U,r}^{(k)}(y) = \eta_{U,r}^{(k)} y^2 + \alpha_{U,r}^{(k)} (y + \beta_{U,r}^{(k)}), \; h_{L,r}^{(k)}(y) = \eta_{L,r}^{(k)} y^2 + \alpha_{L,r}^{(k)} (y + \beta_{L,r}^{(k)}).$$



(a) $r \in \mathcal{S}_k^+$ (b) $r \in \mathcal{S}_k^-$ (c) $r \in \mathcal{S}_k^\pm$

Figure 4: The linear upper and lower bounds for $\sigma(y) = $ ReLU. For the cases (a) and (b), the linear upper bound and lower bound are exactly the function $\sigma(y)$ in the region (grey-shaded). For (c), we plot three out of many choices of lower bound, and they are $h_{L,r}^{(k)}(y) = 0$ (dashed-dotted), $h_{L,r}^{(k)}(y) = y$ (dashed), and $h_{L,r}^{(k)}(y) = \frac{\mathbf{u}_r^{(k)}}{\mathbf{u}_r^{(k)} - \mathbf{l}_r^{(k)}} y$ (dotted).

Therefore,

$$\begin{aligned}
f_j^U(\mathbf{x}) &= \sum_{\mathbf{W}_{j,i}^{(m)} \geq 0} \mathbf{W}_{j,i}^{(m)} \cdot h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) + \sum_{\mathbf{W}_{j,i}^{(m)} < 0} \mathbf{W}_{j,i}^{(m)} \cdot h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) + \mathbf{b}_j^{(m)}, &(21)\\
&= \sum_{i=1}^{n_{m-1}} \mathbf{W}_{j,i}^{(m)} \left(\tau_{j,i}^{(m-1)} \mathbf{y}_i^{(m-1)2} + \lambda_{j,i}^{(m-1)} (\mathbf{y}_i^{(m-1)} + \mathbf{\Delta}_{i,j}^{(m-1)}) \right) + \mathbf{b}_j^{(m)}, &(22)\\
&= \mathbf{y}^{(m-1)\top} \mathrm{diag}(\mathbf{q}_{U,j}^{(m-1)}) \mathbf{y}^{(m-1)} + \mathbf{\Lambda}_{j,:}^{(m-1)} \mathbf{y}^{(m-1)} + \mathbf{W}_{j,:}^{(m)} \mathbf{\Delta}_{:,j}^{(m-1)}, &(23)\\
&= \Phi_{m-2}(\mathbf{x})^\top \mathbf{Q}_U^{(m-1)} \Phi_{m-2}(\mathbf{x}) + 2\mathbf{p}_U^{(m-1)} \Phi_{m-2}(\mathbf{x}) + s_U^{(m-1)}. &(24)
\end{aligned}$$

From (21) to (22), we replace $h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)})$ and $h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)})$ by their definitions and let

$$(\tau_{j,i}^{(m-1)}, \lambda_{j,i}^{(m-1)}, \mathbf{\Delta}_{i,j}^{(m-1)}) = \begin{cases} (\eta_{U,i}^{(m-1)}, \alpha_{U,i}^{(m-1)}, \beta_{U,i}^{(m-1)}) & \text{if } \mathbf{W}_{j,i}^{(m)} \geq 0; \\ (\eta_{L,i}^{(m-1)}, \alpha_{L,i}^{(m-1)}, \beta_{L,i}^{(m-1)}) & \text{if } \mathbf{W}_{j,i}^{(m)} < 0. \end{cases}$$

From (22) to (23), we let $\mathbf{q}_{U,j}^{(m-1)} = \mathbf{W}_{j,:}^{(m)} \odot \tau_{j,i}^{(m-1)}$, and write in the matrix form. From (23) to (24), we substitute $\mathbf{y}^{(m-1)}$ by its definition: $\mathbf{y}^{(m-1)} = \mathbf{W}^{(m-1)} \Phi_{(m-2)}(\mathbf{x}) + \mathbf{b}^{(m-1)}$ and then collect the quadratic terms, linear terms and constant terms of $\Phi_{(m-2)}(\mathbf{x})$, where

$$\begin{aligned}
\mathbf{Q}_U^{(m-1)} &= \mathbf{W}^{(m-1)\top} \mathrm{diag}(\mathbf{q}_{U,j}^{(m-1)}) \mathbf{W}^{(m-1)},\\
\mathbf{p}_U^{(m-1)} &= \mathbf{b}^{(m-1)\top} \odot \mathbf{q}_{U,j}^{(m-1)} + \mathbf{\Lambda}_{j,:}^{(m-1)},\\
s_U^{(m-1)} &= \mathbf{p}_U^{(m-1)} \mathbf{b}^{(m-1)} + \mathbf{W}_{j,:}^{(m)} \mathbf{\Delta}_{:,j}^{(m-1)}.
\end{aligned}$$

Lower bound. Similar to the above derivation, we can simply swap $h_{U,r}^{(k)}$ and $h_{L,r}^{(k)}$ and obtain lower bound $f_j^L(\mathbf{x})$:

$$\begin{aligned}
f_j^L(\mathbf{x}) &= \sum_{\mathbf{W}_{j,i}^{(m)} < 0} \mathbf{W}_{j,i}^{(m)} \cdot h_{U,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) + \sum_{\mathbf{W}_{j,i}^{(m)} \geq 0} \mathbf{W}_{j,i}^{(m)} \cdot h_{L,i}^{(m-1)}(\mathbf{y}_i^{(m-1)}) + \mathbf{b}_j^{(m)},\\
&= \Phi_{m-2}(\mathbf{x})^\top \mathbf{Q}_L^{(m-1)} \Phi_{m-2}(\mathbf{x}) + 2\mathbf{p}_L^{(m-1)} \Phi_{m-2}(\mathbf{x}) + s_L^{(m-1)},
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{Q}_L^{(m-1)} &= \mathbf{W}^{(m-1)\top} \mathrm{diag}(\mathbf{q}_{L,j}^{(m-1)}) \mathbf{W}^{(m-1)}, \quad \mathbf{q}_{L,j}^{(m-1)} = \mathbf{W}_{j,:}^{(m)} \odot \nu_{j,i}^{(m-1)}; &(25)\\
\mathbf{p}_U^{(m-1)} &= \mathbf{b}^{(m-1)\top} \odot \mathbf{q}_{U,j}^{(m-1)} + \mathbf{\Lambda}_{j,:}^{(m-1)}, \quad \mathbf{p}_L^{(m-1)} = \mathbf{b}^{(m-1)\top} \odot \mathbf{q}_{L,j}^{(m-1)} + \mathbf{\Omega}_{j,:}^{(m-1)}; &(26)\\
s_U^{(m-1)} &= \mathbf{p}_U^{(m-1)} \mathbf{b}^{(m-1)} + \mathbf{W}_{j,:}^{(m)} \mathbf{\Delta}_{:,j}^{(m-1)}, \quad s_L^{(m-1)} = \mathbf{p}_L^{(m-1)} \mathbf{b}^{(m-1)} + \mathbf{W}_{j,:}^{(m)} \mathbf{\Theta}_{:,j}^{(m-1)}, &(27)
\end{aligned}$$

and

$$(\nu_{j,i}^{(m-1)}, \omega_{j,i}^{(m-1)}, \mathbf{\Theta}_{i,j}^{(m-1)}) = \begin{cases} (\eta_{L,i}^{(m-1)}, \alpha_{L,i}^{(m-1)}, \beta_{L,i}^{(m-1)}) & \text{if } \mathbf{W}_{j,i}^{(m)} \geq 0; \\ (\eta_{U,i}^{(m-1)}, \alpha_{U,i}^{(m-1)}, \beta_{U,i}^{(m-1)}) & \text{if } \mathbf{W}_{j,i}^{(m)} < 0. \end{cases} \quad (28)$$

E Additional Experimental Results

E.1 Results on CROWN-Ada

Table 6: Comparison of our proposed certified lower bounds for ReLU with adaptive lower bounds (CROWN-Ada), Fast-Lin and Fast-Lip and Op-nrom. LP-full and Reluplex cannot finish within a reasonable amount of time for all the networks reported here. We also include Op-norm, where we directly compute the operator norm (for example, for $p = 2$ it is the spectral norm) for each layer and use their products as a global Lipschitz constant and then compute the robustness lower bound. CLEVER is an estimated robustness lower bound, and attacking algorithms (including CW [6] and EAD [32]) provide upper bounds of the minimum adversarial distortion. For each norm, we consider the robustness against three targeted attack classes: the runner-up class (with the second largest probability), a random class and the least likely class. It is clear that CROWN-Ada notably improves the lower bound comparing to Fast-Lin, especially for larger and deeper networks, the improvements can be up to 28%.

Networks			Lower bounds and upper bounds (Avg.)							Time per Image (Avg.)		
			Lower Bounds (certified)				improvements	Uncertified		Lower Bounds		
Config	p	Target	[20]		[3]	Our algorithm	over	[27]	Attacks	[20]		Our bound
			Fast-Lin	Fast-Lip	Op norm	CROWN-Ada	Fast-Lin	CLEVER	CW/EAD	Fast-Lin	Fast-Lip	CROWN-Ada
MNIST $2 \times [1024]$	∞	runner-up	0.02256	0.01802	0.00159	0.02467	+9.4%	0.0447	0.0856	163 ms	179 ms	128 ms
		rand	0.03083	0.02512	0.00263	0.03353	+8.8%	0.0708	0.1291	176 ms	213 ms	166 ms
		least	0.03854	0.03128	0.00369	0.04221	+9.5%	0.0925	0.1731	176 ms	251 ms	143 ms
	2	runner-up	0.46034	0.42027	0.24327	0.50110	+8.9%	0.8104	1.1874	154 ms	184 ms	110 ms
		rand	0.63299	0.59033	0.40201	0.68506	+8.2%	1.2841	1.8779	141 ms	212 ms	133 ms
		least	0.79263	0.73133	0.56509	0.86377	+9.0%	1.6716	2.4556	152 ms	291 ms	116 ms
	1	runner-up	2.78786	3.46500	0.20601	3.01633	+8.2%	4.5970	9.5295	159 ms	989 ms	136 ms
		rand	3.88241	5.10000	0.35957	4.17760	+7.6%	7.4186	17.259	168 ms	1.15 s	157 ms
		least	4.90809	6.36600	0.48774	5.33261	+8.6%	9.9847	23.933	179 ms	1.37 s	144 ms
MNIST $3 \times [1024]$	∞	runner-up	0.01830	0.01021	0.00004	0.02114	+15.5%	0.0509	0.1037	805 ms	1.28 s	1.33 s
		rand	0.02216	0.01236	0.00007	0.02576	+16.2%	0.0717	0.1484	782 ms	859 ms	1.37 s
		least	0.02432	0.01384	0.00009	0.02835	+16.6%	0.0825	0.1777	792 ms	684 ms	1.37 s
	2	runner-up	0.35867	0.22120	0.06626	0.41295	+15.1%	0.8402	1.3513	732 ms	1.06 s	1.26 s
		rand	0.43892	0.26980	0.10233	0.50841	+15.8%	1.2441	2.0387	711 ms	696 ms	1.26 s
		least	0.48361	0.30147	0.13256	0.56167	+16.1%	1.4401	2.4916	723 ms	655 ms	1.25 s
	1	runner-up	2.08887	1.80150	0.00734	2.39443	+14.6%	4.8370	10.159	685 ms	2.36 s	1.15 s
		rand	2.59898	2.25950	0.01133	3.00231	+15.5%	7.2177	17.796	743 ms	2.69 s	1.25 s
		least	2.87560	2.50000	0.01499	3.33231	+15.9%	8.3523	22.395	729 ms	3.08 s	1.31 s
MNIST $4 \times [1024]$	∞	runner-up	0.00715	0.00219	0.00001	0.00861	+20.4%	0.0485	0.08635	1.54 s	3.42 s	3.23 s
		rand	0.00823	0.00264	0.00001	0.00997	+21.1%	0.0793	0.1303	1.53 s	2.17 s	3.57 s
		least	0.00899	0.00304	0.00001	0.01096	+21.9%	0.1028	0.1680	1.74 s	2.00 s	3.87 s
	2	runner-up	0.16338	0.05244	0.11015	0.19594	+19.9%	0.8689	1.2422	1.79 s	2.58 s	3.52 s
		rand	0.18891	0.06487	0.17734	0.22811	+20.8%	1.4231	1.8921	1.78 s	1.96 s	3.79 s
		least	0.20671	0.07440	0.23710	0.25119	+21.5%	1.8864	2.4451	1.98 s	2.01 s	4.01 s
	1	runner-up	1.33794	0.58480	0.00114	1.58151	+18.2%	5.2685	10.079	1.87 s	1.93 s	3.34 s
		rand	1.57649	0.72800	0.00183	1.88217	+19.4%	8.9764	17.200	1.80 s	2.04 s	3.54 s
		least	1.73874	0.82800	0.00244	2.09157	+20.3%	11.867	23.910	1.94 s	2.40 s	3.72 s
CIFAR $5 \times [2048]$	∞	runner-up	0.00137	0.00020	0.00000	0.00167	+21.9%	0.0062	0.00950	18.2 s	38.2 s	33.1 s
		rand	0.00170	0.00030	0.00000	0.00212	+24.7%	0.0147	0.02351	19.6 s	48.2 s	36.7 s
		least	0.00188	0.00036	0.00000	0.00236	+25.5%	0.0208	0.03416	20.4 s	50.5 s	38.6 s
	2	runner-up	0.06122	0.00948	0.00156	0.07466	+22.0%	0.2712	0.3778	24.2 s	39.4 s	41.0 s
		rand	0.07654	0.01417	0.00333	0.09527	+24.5%	0.6399	0.9497	26.0 s	31.2 s	42.5 s
		least	0.08456	0.01778	0.00489	0.10588	+25.2%	0.9169	1.4379	25.0 s	33.2 s	44.4 s
	1	runner-up	0.93836	0.22632	0.00000	1.13799	+21.3%	4.0755	7.6529	24.7 s	45.1 s	40.5 s
		rand	1.18928	0.31984	0.00000	1.47393	+23.9%	9.7145	21.643	25.7 s	36.2 s	44.0 s
		least	1.31904	0.38887	0.00001	1.64452	+24.7%	12.793	34.497	26.0 s	31.7 s	44.9 s
CIFAR $6 \times [2048]$	∞	runner-up	0.00075	0.00005	0.00000	0.00094	+25.3%	0.0054	0.00770	27.6 s	64.7 s	47.3 s
		rand	0.00090	0.00007	0.00000	0.00114	+26.7%	0.0131	0.01866	28.1 s	72.3 s	49.3 s
		least	0.00095	0.00008	0.00000	0.00122	+28.4%	0.0199	0.02868	28.1 s	76.3 s	49.4 s
	2	runner-up	0.03462	0.00228	0.00476	0.04314	+24.6%	0.2394	0.2979	37.0 s	60.7 s	65.8 s
		rand	0.04129	0.00331	0.01079	0.05245	+27.0%	0.5860	0.7635	40.0 s	56.8 s	71.5 s
		least	0.04387	0.00385	0.01574	0.05615	+28.0%	0.8756	1.2111	40.0 s	56.3 s	72.5 s
	1	runner-up	0.59636	0.05647	0.00000	0.73727	+23.6%	3.3569	6.0112	37.2 s	65.6 s	66.8 s
		rand	0.72178	0.08212	0.00000	0.91201	+26.4%	8.2507	17.160	39.5 s	53.5 s	71.6 s
		least	0.77179	0.09397	0.00000	0.98331	+27.4%	12.603	28.958	40.7 s	42.1 s	72.5 s
CIFAR $7 \times [1024]$	∞	runner-up	0.00119	0.00006	0.00000	0.00148	+24.4%	0.0062	0.0102	8.98 s	20.1 s	16.2 s
		rand	0.00134	0.00008	0.00000	0.00169	+26.1%	0.0112	0.0218	8.98 s	20.3 s	16.7 s
		least	0.00141	0.00010	0.00000	0.00179	+27.0%	0.0148	0.0333	8.81 s	22.1 s	17.4 s
	2	runner-up	0.05279	0.00308	0.00020	0.06569	+24.4%	0.2661	0.3943	12.7 s	20.9 s	20.7 s
		rand	0.05937	0.00407	0.00029	0.07496	+26.3%	0.5145	0.9730	12.6 s	18.7 s	21.8 s
		least	0.06249	0.00474	0.00038	0.07943	+27.1%	0.6253	1.3709	12.9 s	20.7 s	22.2 s
	1	runner-up	0.76648	0.07028	0.00000	0.95204	+24.2%	4.815	7.9987	12.8 s	21.0 s	21.9 s
		rand	0.86468	0.09239	0.00000	1.09067	+26.1%	8.630	22.180	13.2 s	19.8 s	22.4 s
		least	0.91127	0.10639	0.00000	1.15687	+27.0%	11.44	31.529	13.3 s	17.6 s	22.9 s

E.2 Results on CROWN-general

Table 7: Comparison of certified lower bounds by CROWN-Ada on ReLU networks and CROWN-general on networks with tanh, sigmoid and arctan activations. CIFAR models with sigmoid activations achieve much worse accuracy than other networks and are thus excluded. For each norm, we consider the robustness against three targeted attack classes: the runner-up class (with the second largest probability), a random class and the least likely class.

Network			Certified Bounds by CROWN-general			Average Computation Time (sec)		
	ℓ_p norm	target	tanh	sigmoid	arctan	tanh	sigmoid	arctan
MNIST $3 \times [1024]$	ℓ_∞	runner-up	0.0164	0.0225	0.0169	0.3374	0.3213	0.3148
		random	0.0230	0.0325	0.0240	0.3185	0.3388	0.3128
		least	0.0306	0.0424	0.0314	0.3129	0.3586	0.3156
	ℓ_2	runner-up	0.3546	0.4515	0.3616	0.3139	0.3110	0.3005
		random	0.5023	0.6552	0.5178	0.3044	0.3183	0.2931
		least	0.6696	0.8576	0.6769	0.3869	0.3495	0.2676
	ℓ_1	runner-up	2.4600	2.7953	2.4299	0.2940	0.3339	0.3053
		random	3.5550	4.0854	3.5995	0.3277	0.3306	0.3109
		least	4.8215	5.4528	4.7548	0.3201	0.3915	0.3254
MNIST $4 \times [1024]$	ℓ_∞	runner-up	0.0091	0.0162	0.0107	1.6794	1.7902	1.7099
		random	0.0118	0.0212	0.0136	1.7783	1.7597	1.7667
		least	0.0147	0.0243	0.0165	1.8908	1.8483	1.7930
	ℓ_2	runner-up	0.2086	0.3389	0.2348	1.6416	1.7606	1.8267
		random	0.2729	0.4447	0.3034	1.7589	1.7518	1.6945
		least	0.3399	0.5064	0.3690	1.8206	1.7929	1.8264
	ℓ_1	runner-up	1.8296	2.2397	1.7481	1.5506	1.6052	1.6704
		random	2.4841	2.9424	2.3325	1.6149	1.7015	1.6847
		least	3.1261	3.3486	2.8881	1.7762	1.7902	1.8345
MNIST $5 \times [1024]$	ℓ_∞	runner-up	0.0060	0.0150	0.0062	3.9916	4.4614	3.7635
		random	0.0073	0.0202	0.0077	3.5068	4.4069	3.7387
		least	0.0084	0.0230	0.0091	3.9076	4.6283	3.9730
	ℓ_2	runner-up	0.1369	0.3153	0.1426	4.1634	4.3311	4.1039
		random	0.1660	0.4254	0.1774	4.1468	4.1797	4.0898
		least	0.1909	0.4849	0.2096	4.5045	4.4773	4.5497
	ℓ_1	runner-up	1.1242	2.0616	1.2388	4.4911	3.9944	4.4436
		random	1.3952	2.8082	1.5842	4.4543	4.0839	4.2609
		least	1.6231	3.2201	1.9026	4.4674	4.5508	4.5154
CIFAR-10 $5 \times [2048]$	ℓ_∞	runner-up	0.0005	-	0.0006	37.3918	-	37.1383
		random	0.0008	-	0.0009	38.0841	-	37.9199
		least	0.0010	-	0.0011	39.1638	-	39.4041
	ℓ_2	runner-up	0.0219	-	0.0256	47.4896	-	48.3390
		random	0.0368	-	0.0406	54.0104	-	52.7471
		least	0.0460	-	0.0497	55.8924	-	56.3877
	ℓ_1	runner-up	0.3744	-	0.4491	46.4041	-	47.1640
		random	0.6384	-	0.7264	54.2138	-	51.6295
		least	0.8051	-	0.8955	56.2512	-	55.6069
CIFAR-10 $6 \times [2048]$	ℓ_∞	runner-up	0.0004	-	0.0003	59.5020	-	58.2473
		random	0.0006	-	0.0006	59.7220	-	58.0388
		least	0.0006	-	0.0007	60.8031	-	60.9790
	ℓ_2	runner-up	0.0177	-	0.0163	78.8801	-	72.1884
		random	0.0254	-	0.0251	84.2228	-	83.1202
		least	0.0294	-	0.0306	86.2997	-	86.9320
	ℓ_1	runner-up	0.3043	-	0.2925	78.7486	-	70.2496
		random	0.4406	-	0.4620	89.7717	-	83.7972
		least	0.5129	-	0.5665	87.2094	-	86.6502
CIFAR-10 $7 \times [1024]$	ℓ_∞	runner-up	0.0006	-	0.0005	20.8612	-	20.5169
		random	0.0008	-	0.0007	21.4550	-	21.2134
		least	0.0008	-	0.0008	21.3406	-	21.1804
	ℓ_2	runner-up	0.0260	-	0.0225	27.9442	-	27.0240
		random	0.0344	-	0.0317	30.3782	-	29.8086
		least	0.0376	-	0.0371	30.7492	-	30.7321
	ℓ_1	runner-up	0.3826	-	0.3648	28.1898	-	27.1238
		random	0.5087	-	0.5244	29.6373	-	30.5106
		least	0.5595	-	0.6171	31.3457	-	30.6481