A Appendix

This is the appendix for "Semialgebraic Representation of Monotone Deep Equilibrium Models and Applications to Certification".

A.1 Proof of Lemma 1

Definition 1 ***(Clarke's generalized Jacobian) [10]*** *Let $f : \mathbb{R}^n \to \mathbb{R}^m$ be a locally Lipschitz vector-valued function, denote by Ω_f any zero measure set such that f is differentiable outside Ω_f. For $\mathbf{x} \notin \Omega_f$, denote by $\mathcal{J}_f(\mathbf{x})$ the* Jacobian matrix *of f evaluated at $\mathbf{x}$. For any $\mathbf{x} \in \mathbb{R}^n$, the* generalized Jacobian*, or* Clarke Jacobian*, of f evaluated at $\mathbf{x}$, denoted by $\mathcal{J}_f^C(\mathbf{x})$, is defined as the convex hull of all $m \times n$ matrices obtained as the limit of a sequence of the form $\mathcal{J}_f(\mathbf{x}_i)$ with $\mathbf{x}_i \to \mathbf{x}$ and $\mathbf{x}_i \notin \Omega_f$. Symbolically, one has*

$$\mathcal{J}_f^C(\mathbf{x}) := \mathrm{conv}\{\lim \mathcal{J}_f(\mathbf{x}_i) : \mathbf{x}_i \to \mathbf{x},\, \mathbf{x}_i \notin \Omega_f\}.$$

In order to estimate the Lipschitz constant $L_{F,\mathcal{S}}^q$, we need the following lemma:

Lemma 3 *Let $F : \mathbb{R}^{p_0} \to \mathbb{R}^K, \mathbf{x} \mapsto \mathbf{C}\mathbf{z}(\mathbf{x})$ be the fully-connected monDEQ. Its Lipschitz constant is upper bounded by the supremum of the operator norm of its generalized Jacobian, i.e., define*

$$\bar{L}_{F,\mathcal{S}}^q := \sup_{\mathbf{t},\mathbf{x}\in\mathbb{R}^{p_0},\mathbf{v},\mathbf{w}\in\mathbb{R}^K,\mathbf{J}\in\mathcal{J}_{\mathbf{z}}^C(\mathbf{x})} \{\mathbf{t}^T\mathbf{J}^T\mathbf{C}^T\mathbf{v} : \|\mathbf{t}\|_q \le 1,\, \mathbf{w}^T\mathbf{v} \le 1,\, \|\mathbf{w}\|_q \le 1,\, \mathbf{x} \in \mathcal{S}\}\,, \tag{6}$$

then $L_{F,\mathcal{S}}^q \le \bar{L}_{F,\mathcal{S}}^q$.

Proof : Since $\mathbf{z}(\mathbf{x}) = \mathrm{ReLU}(\mathbf{W}\mathbf{z}(\mathbf{x}) + \mathbf{U}\mathbf{x} + \mathbf{u})$ by definition of monDEQ, $\mathbf{z}(\mathbf{x})$ is Lipschitz according to [34, Theorem 1]. Furthermore, $\mathbf{z}(\mathbf{x})$ is semialgebraic by the semialgebraicity of ReLU in (1). Therefore, the Clarke Jacobian of $\mathbf{z}$ is conservative. Indeed by [10, Proposition 2.6.2], the Clarke Jacobian is included in the product of subgradients of its coordinates which is a conservative field by [7, Lemma 3, Theorems 2 and 3]. Since $F = \mathbf{C} \circ \mathbf{z}$, the mapping $\mathbf{C}\mathcal{J}_{\mathbf{z}}^C : \mathbf{x} \rightrightarrows \mathbf{C}\mathbf{J}$, where $\mathbf{J} \in \mathcal{J}_{\mathbf{z}}^C$, is conservative for F by [7, Lemma 5]. So it satisfies an integration formula along segments. Let $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{E}$, and let $\gamma : [0,1] \to \mathbb{R}^{p_0}$ be a parametrization of the segment defined by $\gamma(t) = \mathbf{x}_1 + t(\mathbf{x}_2 - \mathbf{x}_1)$ (which is absolutely continuous). For almost all $t \in [0,1]$, we have $\frac{\mathrm{d}}{\mathrm{d}t}F(\gamma(t)) = \mathbf{C}\mathbf{J}\gamma'(t) = \mathbf{C}\mathbf{J}(\mathbf{x}_2 - \mathbf{x}_1)$ for all $\mathbf{J} \in \mathcal{J}_{\mathbf{z}}^C(\gamma(t))$.

Let $M = \sup_{\mathbf{x}\in\mathcal{S},\mathbf{J}\in\mathcal{J}_{\mathbf{z}}^C(\mathbf{x})} |||\mathbf{C}\mathbf{J}|||_q$ be the supremum of the operator norm $|||\mathbf{C}\mathbf{J}|||_q$ for all $\mathbf{J} \in \mathcal{J}_{\mathbf{z}}^C(\mathbf{x})$ and all $\mathbf{x} \in \mathcal{S}$. We prove that $M < +\infty$. Indeed, $\mathbf{z}(\mathbf{x})$ is Lipschitz, hence there exists $N > 0$ such that $|||\mathbf{J}|||_q < N$ for all $\mathbf{J} \in \mathcal{J}_{\mathbf{z}}^C(\mathbf{x})$ and all $\mathbf{x} \in \mathcal{S}$. The value M is thus upper bounded by $|||\mathbf{C}|||_q N$.

Therefore, for almost all $t \in [0,1]$, $\|\frac{\mathrm{d}}{\mathrm{d}t}F(\gamma(t))\|_q \le M\|\mathbf{x}_2 - \mathbf{x}_1\|_q$, and by integration,

$$\|F(\mathbf{x}_2) - F(\mathbf{x}_1)\|_q = \left\| \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} F(\gamma(t))\mathrm{d}t \right\|_q \le \int_0^1 \left\| \frac{\mathrm{d}}{\mathrm{d}t} F(\gamma(t)) \right\|_q \mathrm{d}t \le M\|\mathbf{x}_2 - \mathbf{x}_1\|_q\,, \tag{7}$$

which proves that $L_{F,\mathcal{S}}^q \le M$. Let us show that $M = \bar{L}_{F,\mathcal{S}}^q$. Fix $\mathbf{x} \in \mathbb{R}^{p_0}$ and $\mathbf{J} \in \mathcal{J}_{\mathbf{z}}^C(\mathbf{x})$. By the definition of operator norm,

$$\begin{aligned} |||\mathbf{C}\mathbf{J}|||_q &= |||(\mathbf{C}\mathbf{J})^T|||_q^* = \max_{\mathbf{v}\in\mathbb{R}^K} \{\|\mathbf{J}^T\mathbf{C}^T\mathbf{v}\|_q^* : \|\mathbf{v}\|_q^* \le 1\} \\ &= \max_{\mathbf{t}\in\mathbb{R}^{p_0},\mathbf{v}\in\mathbb{R}^K} \{\mathbf{t}^T\mathbf{J}^T\mathbf{C}^T\mathbf{v} : \|\mathbf{t}\|_q \le 1,\, \|\mathbf{v}\|_q^* \le 1\} \\ &= \max_{\mathbf{t}\in\mathbb{R}^{p_0},\mathbf{v},\mathbf{w}\in\mathbb{R}^K} \{\mathbf{t}^T\mathbf{J}^T\mathbf{C}^T\mathbf{v} : \|\mathbf{t}\|_q \le 1,\, \mathbf{w}^T\mathbf{v} \le 1,\, \|\mathbf{w}\|_q \le 1\}\,, \end{aligned} \tag{8}$$

where $\|\cdot\|_q^*$ denotes the dual norm of $\|\cdot\|_q$ defined by $\|\mathbf{v}\|_q^* := \sup_{\mathbf{w}\in\mathbb{R}^K}\{\mathbf{w}^T\mathbf{v} : \|\mathbf{w}\|_q \le 1\}$ for all $\mathbf{v} \in \mathbb{R}^K$, and the first equality is due to the fact that the operator norm of matrix $\mathbf{C}\mathbf{J}$ induced by norm $\|\cdot\|_q$ is equal to the operator norm of its transpose $(\mathbf{C}\mathbf{J})^T$ induced by the dual norm $\|\cdot\|_q^*$.

Indeed, by definition of operator norm and dual norm, we have

$$\begin{aligned}\|\mathbf{CJ}\|_q &= \sup_{\mathbf{x}\in\mathbb{R}^{p_0}} \{\|\mathbf{CJx}\|_q : \|\mathbf{x}\|_q \le 1\} = \sup_{\mathbf{x}\in\mathbb{R}^{p_0},\mathbf{y}\in\mathbb{R}^{p}} \{\mathbf{y}^T\mathbf{CJx} : \|\mathbf{x}\|_q \le 1, \|\mathbf{y}\|_q^* \le 1\} \\ &= \sup_{\mathbf{x}\in\mathbb{R}^{p_0},\mathbf{y}\in\mathbb{R}^{p}} \{\mathbf{x}^T(\mathbf{CJ})^T\mathbf{y} : \|\mathbf{x}\|_q \le 1, \|\mathbf{y}\|_q^* \le 1\} = \sup_{\mathbf{y}\in\mathbb{R}^{p}} \{\|(\mathbf{CJ})^T\mathbf{y}\|_q^* : \|\mathbf{y}\|_q^* \le 1\} \\ &= \left\|(\mathbf{CJ})^T\right\|_q^* .\end{aligned}$$

The quantity $\bar{L}^q_{F,\mathcal{S}}$ is just the maximization of Equation (8) for all $\mathbf{x}\in\mathbb{R}^{p_0}$ and all $\mathbf{J}\in\mathcal{J}^C_{\mathbf{z}}(\mathbf{x})$ and therefore equals M. $\square$

The function $\mathbf{z}$ is semialgebraic, and therefore, there exists a closed zero measure set $\Omega_{\mathbf{z}}$ such that $\mathbf{z}$ is continuously differentiable on the complement of $\Omega_{\mathbf{z}}$. For any $\mathbf{x}\notin\Omega_{\mathbf{z}}$, since $\mathbf{z}$ is C^1 at $\mathbf{x}$, we have $\mathcal{J}^C_{\mathbf{z}}(\mathbf{x}) = \{\mathcal{J}_{\mathbf{z}}(\mathbf{x})\}$ by definition of the Clarke Jacobian. Fix $\mathbf{x}\notin\Omega_{\mathbf{z}}$ arbitrary. According to the Corollary of Theorem 2.6.6, on page 75 of [10], we have

$$\begin{aligned}\mathcal{J}^C_{\mathbf{z}}(\mathbf{x}) &\subseteq \mathrm{conv}\{\mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}(\mathbf{x})+\mathbf{Ux}+\mathbf{u})\cdot\mathcal{J}^C_{\mathbf{Wz(x)+Ux+u}}(\mathbf{x})\} \\ &= \mathrm{conv}\{\mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}(\mathbf{x})+\mathbf{Ux}+\mathbf{u})\cdot(\mathbf{W}\cdot\mathcal{J}_{\mathbf{z}}(\mathbf{x})+\mathbf{U})\} \\ &= \mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}(\mathbf{x})+\mathbf{Ux}+\mathbf{u})\cdot(\mathbf{W}\cdot\mathcal{J}_{\mathbf{z}}(\mathbf{x})+\mathbf{U}),\end{aligned} \tag{9}$$

where the first inclusion is from the cited Corollary, the first equality is because $\mathbf{z}$ is C^1 at $\mathbf{x}$ so that the chain rule applies, and the last one is because the Clarke Jacobian is convex.

Fix any any $\bar{\mathbf{x}}\in\mathbb{R}^{p_0}$, then by definition $\mathcal{J}^C_{\mathbf{z}}(\bar{\mathbf{x}}) = \mathrm{conv}\{\lim \mathcal{J}_{\mathbf{z}}(\mathbf{x}_i) : \mathbf{x}_i\to\bar{\mathbf{x}}, i\to+\infty, \mathbf{x}_i\notin\Omega_{\mathbf{z}}\}$. Let $\{\mathbf{x}_i\}_{i\in\mathbb{N}}$ be a sequence not in $\Omega_{\mathbf{z}}$ converging to $\bar{\mathbf{x}}$, for each $\mathbf{x}_i\notin\Omega_{\mathbf{z}}$, we have by (9) that $\mathcal{J}_{\mathbf{z}}(\mathbf{x}_i)\in\mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}(\mathbf{x}_i)+\mathbf{Ux}_i+\mathbf{u})\cdot(\mathbf{W}\cdot\mathcal{J}_{\mathbf{z}}(\mathbf{x}_i)+\mathbf{U})$, i.e., there exists $\mathbf{Y}_i\in\mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}(\mathbf{x}_i)+\mathbf{Ux}_i+\mathbf{u})$ such that $\mathcal{J}_{\mathbf{z}}(\mathbf{x}_i) = \mathbf{Y}_i(\mathbf{W}\cdot\mathcal{J}_{\mathbf{z}}(\mathbf{x}_i)+\mathbf{U})$. By [10, proposition 2.6.2 (b)], $\mathcal{J}^C_{\mathrm{ReLU}}$ has closed graph. Therefore, by continuity of $\mathbf{z}$, up to a subsequence, $\mathbf{Y}_i\to\mathbf{Y}\in\mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}(\bar{\mathbf{x}})+\mathbf{U}\bar{\mathbf{x}}+\mathbf{u})$ for $i\to+\infty$, which means

$$\mathcal{J}^C_{\mathbf{z}}(\bar{\mathbf{x}}) \subseteq \{\mathbf{J}:\ \mathbf{Y}\in\mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}(\bar{\mathbf{x}})+\mathbf{U}\bar{\mathbf{x}}+\mathbf{u}),\ \mathbf{J}=\mathbf{Y}(\mathbf{WJ}+\mathbf{U})\}, \tag{10}$$

for all $\bar{\mathbf{x}}\in\mathbb{R}^{p_0}$. Let $\mathbf{Y}\in\mathcal{J}^C_{\mathrm{ReLU}}(\mathbf{Wz}+\mathbf{Ux}+\mathbf{u})$, since we have coordinate-wise applications of ReLU, we have that $\mathbf{Y}=\mathrm{diag}(\mathbf{s})$ with $\mathbf{s}\in\partial\mathrm{ReLU}(\mathbf{Wz}+\mathbf{Ux}+\mathbf{u})$. By equation (10), the right-hand side of equation (6) is upper bounded by

$$\begin{aligned}\max_{\mathbf{t},\mathbf{x}\in\mathbb{R}^{p_0},\mathbf{s},\mathbf{z}\in\mathbb{R}^{p},\mathbf{v},\mathbf{w}\in\mathbb{R}^{K},\mathbf{J}\in\mathbb{R}^{p\times p_0}} \{&\mathbf{t}^T\mathbf{J}^T\mathbf{C}^T\mathbf{v} : \|\mathbf{t}\|_q\le 1,\ \mathbf{w}^T\mathbf{v}\le 1,\ \|\mathbf{w}\|_q\le 1,\ \mathbf{x}\in\mathcal{S}, \\ &\mathbf{s}\in\partial\mathrm{ReLU}(\mathbf{Wz}+\mathbf{Ux}+\mathbf{u}),\ \mathbf{z}=\mathrm{ReLU}(\mathbf{Wz}+\mathbf{Ux}+\mathbf{u}), \\ &\mathbf{J}=\mathrm{diag}(\mathbf{s})\cdot(\mathbf{W}\cdot\mathbf{J}+\mathbf{U})\}.\end{aligned} \tag{LipMON-a}$$

Notice that in problem (LipMON-a), we have a matrix variable $\mathbf{J}$ of size $p\times p_0$, i.e., containing $p\times p_0$ many variables, which is too large for any SDP solvers. To reduce the size, we use the *vector-matrix product* trick introduced in [46] to reduce the size of the unknown variables. From equation $\mathbf{J}=\mathrm{diag}(\mathbf{s})\cdot(\mathbf{W}\cdot\mathbf{J}+\mathbf{U})$, we have $\mathbf{J}=(\mathbf{I}_p-\mathrm{diag}(\mathbf{s})\cdot\mathbf{W})^{-1}\cdot\mathrm{diag}(\mathbf{s})\cdot\mathbf{U}$. This inversion makes sense because of the strong monotonicity of $\mathbf{I}_p-\mathbf{W}$ and the fact that all entries of $\mathbf{s}$ lie in $[0,1]$ [46, Proposition 1]. Hence

$$\mathbf{v}^T\mathbf{CJ} = \mathbf{v}^T\mathbf{C}\cdot(\mathbf{I}_p-\mathrm{diag}(\mathbf{s})\cdot\mathbf{W})^{-1}\cdot\mathrm{diag}(\mathbf{s})\cdot\mathbf{U} = \mathbf{r}^T\cdot\mathrm{diag}(\mathbf{s})\cdot\mathbf{U}, \tag{11}$$

where $\mathbf{r}^T=\mathbf{v}^T\mathbf{C}\cdot(\mathbf{I}_p-\mathrm{diag}(\mathbf{s})\cdot\mathbf{W})^{-1}$, which means $\mathbf{r}-\mathbf{W}^T\cdot\mathrm{diag}(\mathbf{s})\cdot\mathbf{r}=\mathbf{C}^T\mathbf{v}$. Set $\mathbf{y}=\mathrm{diag}(\mathbf{s})\cdot\mathbf{r}$ and transpose both sides of equation (11), we have $\mathbf{J}^T\mathbf{C}^T\mathbf{v}=\mathbf{U}^T\mathbf{y}$ with $\mathbf{r}-\mathbf{W}^T\cdot\mathbf{y}=\mathbf{C}^T\mathbf{v}$. We can then rewrite the objective function of (LipMON-a) as $\mathbf{t}^T\mathbf{U}^T\mathbf{y}$, leading to the following equivalent problem

$$\begin{aligned}\max_{\mathbf{t},\mathbf{x}\in\mathbb{R}^{p_0},\mathbf{s},\mathbf{z},\mathbf{y},\mathbf{r}\in\mathbb{R}^{p},\mathbf{v},\mathbf{w}\in\mathbb{R}^{K}} \{&\mathbf{t}^T\mathbf{U}^T\mathbf{y} : \|\mathbf{t}\|_q\le 1,\ \mathbf{w}^T\mathbf{v}\le 1,\ \|\mathbf{w}\|_q\le 1,\ \mathbf{x}\in\mathcal{S}, \\ &\mathbf{s}\in\partial\mathrm{ReLU}(\mathbf{Wz}+\mathbf{Ux}+\mathbf{u}),\ \mathbf{z}=\mathrm{ReLU}(\mathbf{Wz}+\mathbf{Ux}+\mathbf{u}), \\ &\mathbf{r}-\mathbf{W}^T\mathbf{y}=\mathbf{C}^T\mathbf{v},\ \mathbf{y}=\mathrm{diag}(\mathbf{s})\cdot\mathbf{r}\}.\end{aligned} \tag{LipMON-b}$$

We have shown that (LipMON-b) is the right hand side of Equation (LipMON) in Lemma 1 and is an upper bound of the right hand side of Equation (6) in Lemma 3, i.e., $\bar{L}^q_{F,\mathcal{S}}\le\tilde{L}^q_{F,\mathcal{S}}$.

A.2 Redundant Constraints of the Lipschitz Model

In order to avoid possible numerical issues of problem (LipMON), and to improve the bounds, we add some redundant constraints to it. For variables $\mathbf{r}$ and $\mathbf{y}$. Note that $\mathbf{r} = (\mathbf{I}_p - \mathbf{W}^T \cdot \mathrm{diag}(\mathbf{s}))^{-1} \cdot \mathbf{C}^T\mathbf{v}$, hence $\|\mathbf{r}\|_2 \le \left|\!\left|\!\left|(\mathbf{I}_p - \mathbf{W}^T \cdot \mathrm{diag}(\mathbf{s}))^{-1}\right|\!\right|\!\right|_2 \cdot \left|\!\left|\!\left|\mathbf{C}^T\right|\!\right|\!\right|_2 \cdot \|\mathbf{v}\|_2$. The operator norm of a matrix induced by L_2 norm is its largest singular value. Hence the operator norm of $(\mathbf{I}_p - \mathbf{W}^T \cdot \mathrm{diag}(\mathbf{s}))^{-1}$ is the smallest singular value of matrix $\mathbf{I}_p - \mathbf{W}^T \cdot \mathrm{diag}(\mathbf{s})$, which is smaller or equal than 1 from the recent work [46]. In summary, we have $\|\mathbf{r}\|_2 \le |||\mathbf{C}|||_2 \cdot \|\mathbf{v}\|_2$ and $\|\mathbf{y}\|_2 \le |||\mathbf{C}|||_2 \cdot \|\mathbf{v}\|_2$. For Lipschitz Model w.r.t. L_2 norm, we have $\|\mathbf{v}\|_2 \le 1$; for Lipschitz Model w.r.t. L_∞ norm, we have $\|\mathbf{v}\|_\infty^* = \|\mathbf{v}\|_1 \le 1$, thus $\|\mathbf{v}\|_2 \le \|\mathbf{v}\|_1 \le 1$. Therefore, for both L_2 and L_∞ norm, we can bound the L_2 norm of variables $\mathbf{r}$ and $\mathbf{y}$ by $|||\mathbf{C}|||_2$. Moreover, we multiply the equality constraint $\mathbf{r} - \mathbf{W}^T \cdot \mathbf{y} = \mathbf{C}^T\mathbf{v}$ coordinate-wisely with variables $\mathbf{s}, \mathbf{z}, \mathbf{y}, \mathbf{r}$ to produce redundant constraints and improve the results. This strengthening technique is already included in the software Gloptipoly3 [20]. With all the discussion above, we now write the strengthened version of problem (LipMON-b) as follows:

$$
\begin{aligned}
\max_{\mathbf{t},\mathbf{x}\in\mathbb{R}^{p_0},\mathbf{s},\mathbf{z},\mathbf{y},\mathbf{r}\in\mathbb{R}^p,\mathbf{v},\mathbf{w}\in\mathbb{R}^K} & \{\mathbf{t}^T\mathbf{U}^T\mathbf{y} : \|\mathbf{t}\|_q \le 1,\ \mathbf{w}^T\mathbf{v} \le 1,\ \|\mathbf{w}\|_q \le 1,\ \mathbf{x} \in \mathcal{S}, \\
& \mathbf{s} \in \partial\mathrm{ReLU}(\mathbf{W}\mathbf{z} + \mathbf{U}\mathbf{x} + \mathbf{u}),\ \mathbf{z} = \mathrm{ReLU}(\mathbf{W}\mathbf{z} + \mathbf{U}\mathbf{x} + \mathbf{u}), \\
& \mathbf{r} - \mathbf{W}^T\mathbf{y} = \mathbf{C}^T\mathbf{v},\ \mathbf{y} = \mathrm{diag}(\mathbf{s}) \cdot \mathbf{r},\ \|\mathbf{y}\|_2 \le |||\mathbf{C}|||_2 \cdot \|\mathbf{v}\|_2,\ \|\mathbf{r}\|_2 \le |||\mathbf{C}|||_2 \cdot \|\mathbf{v}\|_2, \\
& \mathbf{s}(\mathbf{r} - \mathbf{W}^T\mathbf{y}) = \mathbf{s}(\mathbf{C}^T\mathbf{v}),\ \mathbf{z}(\mathbf{r} - \mathbf{W}^T\mathbf{y}) = \mathbf{z}(\mathbf{C}^T\mathbf{v}), \\
& \mathbf{y}(\mathbf{r} - \mathbf{W}^T\mathbf{y}) = \mathbf{y}(\mathbf{C}^T\mathbf{v}),\ \mathbf{r}(\mathbf{r} - \mathbf{W}^T\mathbf{y}) = \mathbf{r}(\mathbf{C}^T\mathbf{v})\}\,. \qquad \text{(LipMON-c)}
\end{aligned}
$$

A.3 Proof of Lemma 2

The SOS constraint in problem (EllipMON-SOS-d) can be written as

$$
\begin{aligned}
\sigma_0(\mathbf{x},\mathbf{z}) = -\big(&\|\mathbf{Q}(\mathbf{C}\mathbf{z} + \mathbf{c}) + \mathbf{b}\|_2^2 - 1 \qquad (=: f_1(\mathbf{x},\mathbf{z})) \\
&+ \sigma_1(\mathbf{x},\mathbf{z})^T g_q(\mathbf{x} - \mathbf{x}_0) \qquad (=: f_2(\mathbf{x},\mathbf{z})) \\
&+ \tau(\mathbf{x},\mathbf{z})^T(\mathbf{z}(\mathbf{z} - \mathbf{W}\mathbf{z} - \mathbf{U}\mathbf{x} - \mathbf{u})) \qquad (=: f_3(\mathbf{x},\mathbf{z})) \\
&+ \sigma_2(\mathbf{x},\mathbf{z})^T(\mathbf{z} - \mathbf{W}\mathbf{z} - \mathbf{U}\mathbf{x} - \mathbf{u}) \qquad (=: f_4(\mathbf{x},\mathbf{z})) \\
&+ \sigma_3(\mathbf{x},\mathbf{z})^T\mathbf{z}\big) \qquad (=: f_5(\mathbf{x},\mathbf{z})) \\
= -\big(&f_1(\mathbf{x},\mathbf{z}) + f_2(\mathbf{x},\mathbf{z}) + f_3(\mathbf{x},\mathbf{z}) + f_4(\mathbf{x},\mathbf{z}) + f_5(\mathbf{x},\mathbf{z})\big) =: -f(\mathbf{x},\mathbf{z})\,.
\end{aligned}
$$

For $d = 1$, denote by $\mathbf{M}_i$ the Gram matrix of polynomial $f_i(\mathbf{x},\mathbf{z})$ for $i = 1,\ldots,5$ and $\mathbf{M}$ the Gram matrix of polynomial $f(\mathbf{x},\mathbf{z})$, with basis $[\mathbf{x}^T, \mathbf{z}^T, 1]$. We have explicitly $\mathbf{M} = \sum_{i=1}^5 \mathbf{M}_i$, where $\mathbf{M}_i$

has the following form

$$\mathbf{M}_1 = \begin{bmatrix} \mathbf{0}_{p_0\times p_0} & \mathbf{0}_{p_0\times p} & \mathbf{0}_{p_0\times 1} \\ \mathbf{0}_{p\times p_0} & \mathbf{C}^T\mathbf{Q}^2\mathbf{C} & \mathbf{C}^T\mathbf{Q}^2\mathbf{c} + \mathbf{C}^T\mathbf{Q}\mathbf{b} \\ \mathbf{0}_{1\times p_0} & \mathbf{c}^T\mathbf{Q}^2\mathbf{C} + \mathbf{b}^T\mathbf{Q}\mathbf{C} & \mathbf{c}^T\mathbf{Q}^2\mathbf{c} + 2\mathbf{b}^T\mathbf{Q}\mathbf{c} + \mathbf{b}^T\mathbf{b} - 1 \end{bmatrix},$$

$$\mathbf{M}_2 = \begin{cases} \begin{bmatrix} -\mathrm{diag}(\sigma_1) & \mathbf{0}_{p_0\times p} & \mathrm{diag}(\sigma_1)\cdot\mathbf{x}_0 \\ \mathbf{0}_{p\times p_0} & \mathbf{0}_{p\times p} & \mathbf{0}_{p\times 1} \\ \mathbf{x}_0^T\cdot\mathrm{diag}(\sigma_1) & \mathbf{0}_{1\times p} & \sigma_1^T(\varepsilon^2 - \mathbf{x}_0^2) \end{bmatrix}, & \text{for } L_\infty\text{-norm}, \\ \sigma_1 \begin{bmatrix} -\mathbf{I}_{p_0} & \mathbf{0}_{p_0\times p} & \mathbf{x}_0 \\ \mathbf{0}_{p\times p_0} & \mathbf{0}_{p\times p} & \mathbf{0}_{p\times 1} \\ \mathbf{x}_0^T & \mathbf{0}_{1\times p} & \varepsilon^2 - \mathbf{x}_0^T\mathbf{x}_0 \end{bmatrix}, & \text{for } L_2\text{-norm}, \end{cases}$$

$$\mathbf{M}_3 = \begin{bmatrix} \mathbf{0}_{p_0\times p_0} & -\frac{1}{2}\mathbf{U}^T\mathrm{diag}(\tau) & \mathbf{0}_{p_0\times 1} \\ -\frac{1}{2}\mathrm{diag}(\tau)\mathbf{U} & \mathrm{diag}(\tau)(\mathbf{I}_p - \mathbf{W}) & -\frac{1}{2}\mathrm{diag}(\tau)\cdot\mathbf{u} \\ \mathbf{0}_{1\times p_0} & -\frac{1}{2}\mathbf{u}^T\cdot\mathrm{diag}(\tau) & 0 \end{bmatrix},$$

$$\mathbf{M}_4 = \begin{bmatrix} \mathbf{0}_{p_0\times p_0} & \mathbf{0}_{p_0\times p} & -\frac{1}{2}\mathbf{U}^T\sigma_3 \\ \mathbf{0}_{p\times p_0} & \mathbf{0}_{p\times p} & \frac{1}{2}(\mathbf{I}_p - \mathbf{W}^T)\sigma_3 \\ -\frac{1}{2}\sigma_3^T\mathbf{U} & \frac{1}{2}\sigma_3^T(\mathbf{I}_p - \mathbf{W}) & -\sigma_3^T\mathbf{u} \end{bmatrix},$$

$$\mathbf{M}_5 = \begin{bmatrix} \mathbf{0}_{p_0\times p_0} & \mathbf{0}_{p_0\times p} & \mathbf{0}_{p_0\times 1} \\ \mathbf{0}_{p\times p_0} & \mathbf{0}_{p\times p} & \frac{1}{2}\sigma_2 \\ \mathbf{0}_{1\times p_0} & \frac{1}{2}\sigma_2^T & 0 \end{bmatrix}.$$

Moreover, in order to improve the quality of the ellipsoid, we can also use the *slope restriction* condition of ReLU function as proposed in [22]: $(z_j - z_i)(\mathbf{W}_{j,:}\mathbf{z} + \mathbf{U}_{j,:}\mathbf{x} + u_j - \mathbf{W}_{i,:}\mathbf{z} - \mathbf{U}_{i,:}\mathbf{x} - u_i) - (z_j - z_i)^2 \geq 0$ for $i \neq j$. The Gram matrix of the SOS combination of these constraints with basis $[\mathbf{x}^T, \mathbf{z}^T, 1]$ has the form

$$\mathbf{M}_6 = \begin{bmatrix} \mathbf{U} & \mathbf{W} & \mathbf{u} \\ \mathbf{0}_{p\times p_0} & \mathbf{I}_p & \mathbf{0}_{p\times 1} \\ \mathbf{0}_{1\times p_0} & \mathbf{0}_{1\times p} & 1 \end{bmatrix}^T \begin{bmatrix} \mathbf{0}_{p_0\times p_0} & \mathbf{T} & \mathbf{0}_{p_0\times 1} \\ \mathbf{T} & -2\mathbf{T} & \mathbf{0}_{p\times 1} \\ \mathbf{0}_{1\times p_0} & \mathbf{0}_{1\times p} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{U} & \mathbf{W} & \mathbf{u} \\ \mathbf{0}_{p\times p_0} & \mathbf{I}_p & \mathbf{0}_{p\times 1} \\ \mathbf{0}_{1\times p_0} & \mathbf{0}_{1\times p} & 1 \end{bmatrix},$$

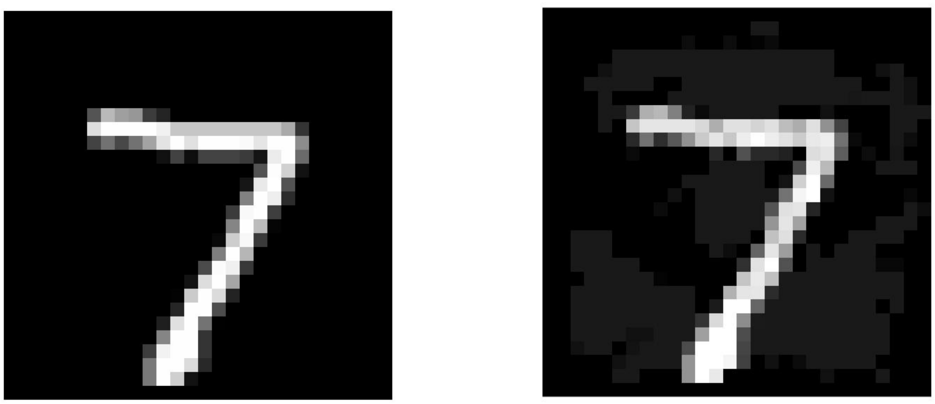
where $\mathbf{T} = \sum_{i=1}^{p-1}\sum_{j=i+1}^{p} \lambda_{ij}(\mathbf{e}_i - \mathbf{e}_j)(\mathbf{e}_i - \mathbf{e}_j)^T$ with $\lambda_{ij} \geq 0$ for all $i < j$, and $\{\mathbf{e}_i\}_{i=1}^p \subseteq \mathbb{R}^p$ is the canonical basis of $\mathbb{R}^p$. Since $\sigma_0(\mathbf{x}, \mathbf{z})$ is an SOS polynomial of degree at most 2, we conclude that $-\mathbf{M} \succeq 0$. According to Lemma 5 in [14], the constraint $-\mathbf{M} \succeq 0$ is equivalent to an SDP constraint using *Schur complements*, which finishes the proof of Lemma 2.

A.4 An Adversarial Example

A.5 Licenses of Used Assets

Table 4: Summary of the licenses of used assets

Software	License
Julia	MIT License
JuMP	Mozilla Public License
Matlab	Proprietary Software
CVX	CVX Standard License
Python	Python Software Foundation License
Pytorch	Berkeley Software Distribution
Mosek	Proprietary Software
Our code	CeCILL Free Software License



(a) Original example, classified as 7

(b) Adversarial example, classified as 3

Figure 2: An adversarial example of the first test MNIST input found by PGD algorithm for L_∞ norm with $\varepsilon = 0.1$.