

# Appendix for Improved Analysis of Penalty-Based Methods for Bilevel Optimization with Coupled Constraints

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## I. PRELIMINARY KNOWLEDGE

**Definition 1** (Lipschitz Continuity and Smoothness). *Let  $h : \mathcal{Q} \rightarrow \mathbb{R}$ . We say  $h(q)$  is  $l_{h,0}$ -Lipschitz on  $\mathcal{S} \subseteq \mathcal{Q}$  if*

$$\|h(q_1) - h(q_2)\| \leq l_{h,1}\|q_1 - q_2\|, \quad \forall q_1, q_2 \in \mathcal{S}. \quad (1)$$

*If  $h(q)$  is differentiable on  $\mathcal{S}$ , we say  $h(q)$  is  $l_{h,1}$ -smooth on  $\mathcal{S}$  if  $\nabla h(q)$  is  $l_{h,1}$ -Lipschitz on  $\mathcal{S}$ .*

**Definition 2** (Proximal Gradient). *Let  $h : \mathcal{Q} \rightarrow \mathbb{R}$  be differentiable on  $\mathcal{S} \subseteq \mathcal{Q}$ , and  $\eta > 0$  be some small scalar. We say the proximal gradient of  $h(q)$  on  $\mathcal{S}$  is*

$$G_{h,\mathcal{S}}(q) = \frac{1}{\eta} \left( q - \text{Proj}_{\mathcal{S}}(q - \eta \nabla h(q)) \right), \quad \forall q \in \mathcal{S}. \quad (2)$$

**Definition 3** (Proximal PL). *Let  $h : \mathcal{Q} \rightarrow \mathbb{R}$  be differentiable on  $\mathcal{S} \subseteq \mathcal{Q}$ . We say  $h(q)$  satisfies proximal  $\mu_h$ -Polyak-Łojasiewicz (PL) condition on  $\mathcal{S}$  if*

$$h(q) - \min_{q \in \mathcal{S}} h(q) \leq \frac{1}{2\mu_h} G_{h,\mathcal{S}}^2(q), \quad \forall q \in \mathcal{S}. \quad (3)$$

**Lemma 1** (Lipschitz-Continuity of  $S_g^*(x)$  [6, Lemma 6]). *Suppose  $\mathcal{Y}$  is closed and convex,  $g(x, y)$  satisfies PL condition in  $y \in \mathcal{Y}$ , and  $\nabla_y g(x, y)$  is Lipschitz in  $x$ . Then there exist a constant  $L_y^g \geq 0$  such that for any  $x_1, x_2 \in \mathcal{X}$  and  $y_1 \in S_g^*(x_1) = \arg \min_{y \in \mathcal{Y}} g(x_1, y)$ , there exists  $y_2 \in S_g^*(x_2) = \arg \min_{y \in \mathcal{Y}} g(x_2, y)$  such that*

$$\|y_1 - y_2\| \leq L_y^g \|x_1 - x_2\|. \quad (4)$$

**Lemma 2** (Lemma 3.1 in [2]). *Suppose  $\mathcal{Q} \subseteq \mathbb{R}^{d_q}$  is convex, closed, and nonempty. For any  $q_1 \in \mathbb{R}^{d_q}$  and any  $q_2 \in \mathcal{Q}$ , it follows that*

$$\langle \text{Proj}_{\mathcal{Q}}(q_1) - q_2, \text{Proj}_{\mathcal{Q}}(q_1) - q_1 \rangle \leq 0. \quad (5)$$

*In this way, take  $q_1 = q_3 - \eta g$  for any  $q_3 \in \mathcal{Q}$ , and denote  $q_3^{\eta,g} = \text{Proj}_{\mathcal{Q}}(q_3 - \eta g)$  as a projected gradient update in direction  $g$  with stepsize  $\eta$ , we have,*

$$\langle g, q_3^{\eta,g} - q_2 \rangle \leq -\frac{1}{\eta} \langle q_3^{\eta,g} - q_2, q_3^{\eta,g} - q_3 \rangle, \quad \forall q_2, q_3 \in \mathcal{Q}. \quad (6)$$

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## II. IMPROVED ANALYSIS UNDER SMALLER SMOOTHNESS CONSTANT

### A. Proof of Lemma 3

Before proceed to the proof of Lemma 3, we present the following useful lemma.

**Lemma 3.** *Denote  $v(x) = \min_{y \in \mathcal{Y}} g(x, y)$ ,  $S_g^*(x) = \arg \min_{y \in \mathcal{Y}} g(x, y)$ . Suppose  $\mathcal{Y}$  is closed and convex,  $g(x, y)$  is  $l_{g,1}$ -smooth, and there exists constant  $L_y^g$  such that for arbitrary  $x_1, x_2 \in \mathcal{X}$ ,  $d_{S_g^*(x_2)}(y_1) \leq L_y^g \|x_1 - x_2\|$  for any  $y_1 \in S_g^*(x_1)$ . Then for  $v(x) = \min_{y \in \mathcal{Y}} g(x, y)$ , there is*

$$\nabla v(x) = \nabla_x g(x, y_g^*(x)), \quad \forall y_g^*(x) \in S_g^*(x). \quad (7)$$

*Moreover, fix any  $y_g^*(x) \in S_g^*(x)$ , and for arbitrary  $d \in \mathbb{R}^{d_x}$ , denote  $y_{g,r}$  as some element in  $S_g^*(x + rd)$ . There is*

$$\langle \nabla_y g(x, y_g^*(x)), \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \rangle = 0. \quad (8)$$

*Proof.* The gradient of value function

$$\nabla v(x) = \nabla_x g(x, y_g^*(x)), \quad \forall y_g^*(x) \in S_g^*(x) \quad (9)$$

is an established outcome, see e.g. [6, Proposition 7]. In this way, denoting  $y_{g,r} \in S_g^*(x + rd)$ , the directional derivative  $v(x)$  in unit direction  $d \in \mathbb{R}^{d_x}$  is

$$D_d(v(x)) \stackrel{(a)}{=} \langle \nabla v(x), d \rangle = \langle \nabla_x g(x, y_{g,0}), d \rangle \quad (10)$$

$$\stackrel{(b)}{=} \lim_{r \downarrow 0} \frac{1}{r} (g(x + rd, y_{g,r}) - g(x, y_{g,0})) \quad (11)$$

$$\stackrel{(c)}{=} \langle \nabla_x g(x, y_{g,0}), d \rangle \quad (12)$$

$$+ \langle \nabla_y g(x, y_{g,0}), \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \rangle \quad (13)$$

where (a) follows the  $\nabla v(x) = \nabla_x g(x, y_{g,0})$ ; (b) is the definition of directional derivative; and (c) applies Taylor expansion. In this way, we can conclude

$$\langle \nabla_y g(x, y_{g,0}), \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \rangle = 0. \quad (14)$$

□

With Lemma 3 prepared, we are ready to explore some features of the directional derivative of  $y_g^*(x)$  and show the first part of Lemma 3.

**Lemma 4.** Suppose all conditions in Lemma 3 hold. For any unit direction  $d \in \mathbb{R}^{d_x}$ , there exists an index set  $\mathcal{I} \subseteq [d_y]$  such that the directional derivative of  $y_g^*(x)$ ,  $D_d(y_g^*(x))$  satisfies

$$\left[ \lim_{r \downarrow 0} \frac{y_g^*(x+rd) - y_g^*(x)}{r} \right]_{[d_y] \setminus \mathcal{I}} = 0, \quad \text{and} \quad (15)$$

$$\left[ \lim_{r \downarrow 0} \frac{y_g^*(x+rd) - y_g^*(x)}{r} \right]_{\mathcal{I}} = C(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B(x)_{[\cdot, \mathcal{I}]}^\top d, \quad (16)$$

and the second-order directional derivative of  $v(x)$  is

$$D_{dd}^2(v(x)) = \left( A(x) - B(x) \begin{bmatrix} C(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B(x)_{[\cdot, \mathcal{I}]}^\top \\ 0 \end{bmatrix} \right) d, \quad (17)$$

where

$$\begin{aligned} A(x) &= \nabla_{xx} g(x, y_g^*(x)), \\ B(x) &= \nabla_{xy} g(x, y_g^*(x)), \\ C(x) &= \nabla_{yy} g(x, y_g^*(x)). \end{aligned}$$

**Remark 1.** This means the non-zero part of  $D_d(y_g^*(x))$ , indexed by  $\mathcal{I}$ , is determined by the submatrices of  $\nabla_{yy} g(x, y_g^*(x))$  and  $\nabla_{xy} g(x, y_g^*(x))$  also indexed by  $\mathcal{I}$ .

*Proof.* According to Lemma 2,

$$\nabla v(x) = \nabla_x g(x, y_g^*(x)), \quad \forall y_g^*(x) \in S_g^*(x). \quad (18)$$

Fix any  $x \in \mathcal{X}$ . For arbitrary  $d \in \mathbb{R}^{d_x}$ , denote  $y_{g,r} = \arg \min_{y \in \mathcal{Y}(x)} g(x+rd, y)$  for some scalar  $r \geq 0$ . Here,  $y_{g,0} = y_g^*(x)$ . According to Lemma 3, there is

$$\begin{aligned} 0 &= \lim_{r, r' \downarrow 0} \frac{1}{rr'} \langle \nabla_y g(x+rd, y_{g,r}) - \nabla_y g(x, y_{g,0}), \\ &\quad y_{g,r'} - y_{g,0} \rangle \\ &= \lim_{r \downarrow 0} \langle \langle \nabla_{xy} g(x, y_{g,0}), d \rangle + \langle \nabla_{yy} g(x, y_{g,0}), \frac{y_{g,r} - y_{g,0}}{r} \rangle \\ &\quad + \mathcal{O}(\|rd\|^2), \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_{g,0}}{r'} \rangle \\ &= \langle B(x)^\top d + C(x) \left( \lim_{r \downarrow 0} \frac{y_{g,r} - y_{g,0}}{r} \right), \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_{g,0}}{r'} \rangle. \end{aligned} \quad (19)$$

where the second equality is by Taylor's expansion, and the fact that  $\|y_{g,0} - y_{g,r}\| \leq L_y^g \|x - (x+rd)\|$  for some constant  $L_y^g > 0$  according to [6, Lemma 5], and the third is from rearranging.

For simplicity, denote the directional derivative of  $y_g^*(x)$  as

$$dy = D_d(y_g^*(x)) = \lim_{r \downarrow 0} \frac{y_{g,r} - y_{g,0}}{r}. \quad (20)$$

In this way, (19) can be written as

$$0 = dy^\top C(x) dy + dy^\top B(x)^\top d. \quad (21)$$

Denote  $\mathcal{I} = \{i : dy_i \neq 0\} \subseteq [d_y]$  as the collection of indices of non-zero elements in  $dy$ . Without the loss of generality, take  $dy = [dy'; 0]^\top$  where  $dy' = dy_{\mathcal{I}}$  is the stack of non-zero

elements in  $dy$ . In this way, writing  $A$  and  $B$  in block matrix form, (21) is equivalent to

$$\begin{aligned} 0 &= [dy' \quad 0] \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{bmatrix} dy' \\ 0 \end{bmatrix} + [dy' \quad 0] \begin{bmatrix} B_1^\top d \\ B_2^\top d \end{bmatrix} \\ &= dy'^\top C_{11} dy' + dy'^\top B_1^\top d. \end{aligned} \quad (22)$$

where  $C_{11} = C(x)_{[\mathcal{I}, \mathcal{I}]}$ ,  $B_1 = B(x)_{[\cdot, \mathcal{I}]}$ .

As  $g$  is strongly convex in  $y$ , its hessian with respect to  $y$ ,  $C(x)$  is positive definite. Therefore, any of its principal sub-matrix  $C_{11}$  is positive definite and full rank. In this way, Solving (22) therefore gives

$$dy' = C_{11}^{-1} B_1^\top d. \quad (23)$$

This proves (61).

As  $v(x)$  is differentiable, the first order directional derivative for  $v(x)$  is

$$D_d(v(x)) = \nabla v(x)^\top d = \nabla_x g(x, y_g^*(x))^\top d \quad (24)$$

In this way, the second order directional derivative for  $v(x)$  is

$$\begin{aligned} D_{dd}^2(v(x)) &= \lim_{r \downarrow 0} \frac{1}{r} \left( \nabla D_d(v(x+rd)) - \nabla D_d(v(x)) \right) \\ &= \lim_{r \downarrow 0} \frac{1}{r} d^\top \left( \nabla_x g(x+rd, y_{g,r}) - \nabla_x g(x, y_{g,0}) \right) \\ &= d^\top \nabla_{xx} g(x, y_{g,0}) d + d^\top \nabla_{xy} g(x, y_{g,0}) \lim_{r \downarrow 0} \frac{1}{r} (y_{g,r} - y_{g,0}) \\ &= d^\top A(x) d - d^\top B(x) \begin{bmatrix} dy' \\ 0 \end{bmatrix} \\ &= d^\top A(x) d - d^\top B(x) \begin{bmatrix} C(x)_{11}^{-1} B(x)_1^\top d \\ 0 \end{bmatrix} \\ &= d^\top \left( A(x) - B(x) \begin{bmatrix} C(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B(x)_{[\cdot, \mathcal{I}]}^\top \\ 0 \end{bmatrix} \right) d \end{aligned} \quad (25)$$

where the first equality is the definition of second-order directional derivative; the second is by plugging the first-order directional derivative; the third follows Taylor's expansion; and the following is by plugging  $\lim_{r \downarrow 0} \frac{1}{r} (y_{g,r} - y_{g,0})$ . This completes the proof.  $\square$

In this way, we finished proving the first part of Lemma 3. For the second part, we look into the relation between  $\mathcal{I}$ , the non-zero index of  $D_d(y_g^*(x))$ , and  $\mathcal{I}_\gamma$ , the non-zero index of the counterpart  $D_d(y_\gamma^*(x))$ .

**Lemma 5.** Suppose  $\lim_{\gamma \rightarrow \infty} y_\gamma^*(x) = y_g^*(x)$  for all  $x \in \mathcal{X}$ . Fix any unit direction  $d \in \mathbb{R}^{d_x}$ , denote  $\mathcal{I} \subseteq [d_y]$  as the index set for non-zero elements in  $D_d(y_g^*(x)) = \lim_{r \downarrow 0} \frac{y_g^*(x+rd) - y_g^*(x)}{r}$ , and  $\mathcal{I}_\gamma \subseteq [d_y]$  as the index set for non-zero elements in  $D_d(y_\gamma^*(x)) = \lim_{r \downarrow 0} \frac{y_\gamma^*(x+rd) - y_\gamma^*(x)}{r}$ . Then, for any  $\delta > 0$ , there exists a finite  $\gamma^*$  such that for all  $\gamma > 0$ ,

- 1)  $\mathcal{I} \subseteq \mathcal{I}_\gamma$ , and
- 2)  $[D_d(y_\gamma^*(x))]_i < \delta$  for all  $i \in \mathcal{I}_\gamma \setminus \mathcal{I}$ .

*Proof.* Similarly denote  $y_{\gamma,r} = \arg \min_{y \in \mathcal{Y}(x)} \gamma^{-1} f(x, y) + g(x, y)$  for scalar  $r \geq 0$ , the directional derivative of  $y_\gamma^*(x)$  as

$$dy_\gamma = D_d(y_\gamma^*(x)) = \lim_{r \downarrow 0} \frac{y_{\gamma,r} - y_{\gamma,0}}{r}, \quad (26)$$

and  $dy'_\gamma = [dy_\gamma]_{\mathcal{I}_\gamma}$  where  $\mathcal{I}_\gamma = \{i : dy_{\gamma_i} \neq 0\} \subseteq [d_y]$  is the collection of indices of non-zero elements in  $dy_\gamma$ .

For any  $i \in \mathcal{I}$ ,  $dy_i \neq 0$ . i.e.

$$\lim_{r \downarrow 0} \left| \frac{[y_{g,r}]_i - [y_{g,0}]_i}{r} \right| = |dy_i| > 0 \quad (27)$$

Moreover, according to Lemma 1,  $y_{\gamma,r} \rightarrow y_g$  for  $\gamma \rightarrow \infty$ . Thus, for any  $r > 0$ ,

$$\lim_{\gamma \rightarrow \infty} \frac{y_{\gamma,r} - y_{\gamma,0}}{r} = \frac{y_{g,r} - y_{g,0}}{r}. \quad (28)$$

i.e. for any  $\delta > 0$ , there exist  $\gamma^* > 0$  such that for all  $\gamma > \gamma^*$ ,

$$\left| \frac{[y_{\gamma,r}]_i - [y_{\gamma,0}]_i}{r} - \frac{[y_{g,r}]_i - [y_{g,0}]_i}{r} \right| < \delta \quad (29)$$

Fix  $\delta = \min_{i \in \mathcal{I}} |dy_i|/2$ , following triangle inequality, there is

$$\begin{aligned} & \lim_{r \downarrow 0} \left| \frac{[y_{\gamma,r}]_i - [y_{\gamma,0}]_i}{r} \right| \\ & \geq \lim_{r \downarrow 0} \left| \frac{[y_{g,r}]_i - [y_{g,0}]_i}{r} \right| \\ & \quad - \lim_{r \downarrow 0} \left| \frac{[y_{g,r}]_i - [y_{g,0}]_i}{r} - \frac{[y_{\gamma,r}]_i - [y_{\gamma,0}]_i}{r} \right| \\ & \geq |dy_i| - \min_{i \in \mathcal{I}} |dy_i|/2 > 0. \end{aligned} \quad (30)$$

i.e.  $\frac{[y_{\gamma,r}]_i - [y_{\gamma,0}]_i}{r} \neq 0$ . So  $\mathcal{I} \subseteq \mathcal{I}_\gamma$  for all  $\gamma > \gamma_1^*$ . This completes the first part of the lemma.

For the second part,  $i \in [d_y] \setminus \mathcal{I}$ , similarly use triangle inequality, there is

$$\begin{aligned} & \lim_{r \downarrow 0} \left| \frac{[y_{\gamma,r}]_i - [y_{\gamma,0}]_i}{r} \right| \\ & \leq \lim_{r \downarrow 0} \left| \frac{[y_{g,r}]_i - [y_{g,0}]_i}{r} \right| \\ & \quad + \lim_{r \downarrow 0} \left| \frac{[y_{g,r}]_i - [y_{g,0}]_i}{r} - \frac{[y_{\gamma,r}]_i - [y_{\gamma,0}]_i}{r} \right| \\ & < 0 + \delta = \delta. \end{aligned} \quad (31)$$

for all  $\gamma > \gamma^*$ . In this way,  $dy_{\gamma_i} < \delta$  for all  $i \in \mathcal{I}_\gamma \setminus \mathcal{I}$ .  $\square$

Now we are ready to prove the second part of Lemma 3.

**Lemma 6.** Suppose all conditions in Lemma 4 hold. Fix any unit direction  $d \in \mathbb{R}^{d_x}$ , denote  $\mathcal{I} \subseteq [d_y]$  as the index set for non-zero elements in  $D_d(y_g^*(x))$ . For any  $\delta > 0$ , there exists a finite  $\gamma^* > 0$  such that the second-order directional derivative of  $v_\gamma(x)$  is

$$\begin{aligned} & D_{dd}^2(v_\gamma(x)) \\ & = \left( A_\gamma(x) - B_\gamma(x) \begin{bmatrix} C_\gamma(x)^{-1}_{[\mathcal{I}, \mathcal{I}]} B_\gamma(x)_{[:, \mathcal{I}]}^\top \\ 0 \end{bmatrix} \right) d + \mathcal{O}(\delta) \end{aligned} \quad (32)$$

where

$$\begin{aligned} A_\gamma(x) &= \nabla_{xx} \gamma^{-1} f(x, y_\gamma(x)) + g(x, y_\gamma^*(x)), \\ B_\gamma(x) &= \nabla_{xy} \gamma^{-1} f(x, y_\gamma(x)) + g(x, y_\gamma^*(x)), \\ C_\gamma(x) &= \nabla_{yy} \gamma^{-1} f(x, y_\gamma(x)) + g(x, y_\gamma^*(x)). \end{aligned}$$

*Proof.* Denote  $y_{\gamma,r} = \arg \min_{y \in \mathcal{Y}(x)} \gamma^{-1} f(x, y) + g(x, y)$  for scalar  $r \geq 0$ , the directional derivative of  $y_\gamma^*(x)$  as

$$dy_\gamma = D_d(y_\gamma^*(x)) = \lim_{r \downarrow 0} \frac{y_{\gamma,r} - y_{\gamma,0}}{r}, \quad (33)$$

and  $dy'_\gamma = [dy_\gamma]_{\mathcal{I}_\gamma}$  where  $\mathcal{I}_\gamma = \{i : dy_{\gamma_i} \neq 0\} \subseteq [d_y]$  is the collection of indices of non-zero elements in  $dy_\gamma$ .

Without loss of generality, partition  $dy'_\gamma = [[dy_\gamma]_{\mathcal{I}_1}, [dy_\gamma]_{\mathcal{I}_2}]$  where  $\mathcal{I}_1 = \mathcal{I}$  and  $\mathcal{I}_2 = \mathcal{I}_\gamma \setminus \mathcal{I}$  as  $\mathcal{I} \subseteq \mathcal{I}_\gamma$  according to Lemma 5. Following Lemma 4, there is

$$\begin{aligned} dy'_\gamma &= C_\gamma(x)^{-1}_{[\mathcal{I}_\gamma, \mathcal{I}_\gamma]} B_\gamma(x)_{[:, \mathcal{I}_\gamma]}^\top d \\ &= \begin{bmatrix} C_\gamma(x)_{[\mathcal{I}_1, \mathcal{I}_1]} & C_\gamma(x)_{[\mathcal{I}_1, \mathcal{I}_2]} \\ C_\gamma(x)_{[\mathcal{I}_2, \mathcal{I}_1]} & C_\gamma(x)_{[\mathcal{I}_2, \mathcal{I}_2]} \end{bmatrix}^{-1} \begin{bmatrix} B_\gamma(x)_{[:, \mathcal{I}_1]}^\top \\ B_\gamma(x)_{[:, \mathcal{I}_2]}^\top \end{bmatrix} d. \end{aligned}$$

Denote  $C_{11} = C_\gamma(x)_{[\mathcal{I}_1, \mathcal{I}_1]}$ ,  $C_{12} = C_\gamma(x)_{[\mathcal{I}_1, \mathcal{I}_2]}$ ,  $C_{21} C_\gamma(x)_{[\mathcal{I}_2, \mathcal{I}_1]}$ , and  $C_{22} C_\gamma(x)_{[\mathcal{I}_2, \mathcal{I}_2]}$ , and  $S$  is the Schur complement of  $C_{11}$  in  $C$ , given by  $S = C_{22} - C_{21} C_{11}^{-1} C_{12}$ . There is

$$\begin{aligned} \begin{bmatrix} dy_{\mathcal{I}_1} \\ dy_{\mathcal{I}_2} \end{bmatrix} &= \begin{bmatrix} C_{11}^{-1} + C_{11}^{-1} C_{12} S^{-1} C_{21} C_{11}^{-1} & -C_{11}^{-1} C_{12} S^{-1} \\ -S^{-1} C_{21} C_{11}^{-1} & S^{-1} \end{bmatrix} \\ &\quad \times \begin{bmatrix} B_\gamma(x)_{[:, \mathcal{I}_1]}^\top \\ B_\gamma(x)_{[:, \mathcal{I}_2]}^\top \end{bmatrix} d. \end{aligned}$$

In this way, there is

$$\begin{aligned} dy_{\mathcal{I}_2} &= -S^{-1} C_{21} C_{11}^{-1} B_\gamma(x)_{[:, \mathcal{I}_1]}^\top d + S^{-1} B_\gamma(x)_{[:, \mathcal{I}_2]}^\top d, \\ \text{and } dy_{\mathcal{I}_1} &= C_{11}^{-1} B_\gamma(x)_{[:, \mathcal{I}_1]}^\top d - C_{11}^{-1} C_{12} dy_{\mathcal{I}_2} \end{aligned} \quad (34)$$

From Lemma 5, we know  $v_{\mathcal{I}_2} = \mathcal{O}(\delta)$  for all  $\gamma > \gamma^*$ . Additionally, as  $C_\gamma(x)$  is the hessian of a strongly convex function, its principle submatrix  $C_{11}$ , is also of full rank with its smallest eigenvalue  $\lambda_-(C_{11}) \geq \mu_g$  [3, Lemma F.6] and thus  $\|C_{11}^{-1}\| \leq \frac{1}{\mu}$ . Moreover, as  $C_\gamma(x)$  is also the hessian of a smooth function, so  $\|C_\gamma(x)\|$  is bounded so as its submatrix  $\|C_{12}\|$ . In this way, we know  $\|C_{11}^{-1} C_{12} dy_{\mathcal{I}_2}\| = \mathcal{O}(\delta)$  and we can conclude that

$$dy_{\mathcal{I}_1} = C_{11}^{-1} B_\gamma(x)_{[:, \mathcal{I}_1]}^\top d + \mathcal{O}(\delta). \quad (35)$$

In this way, we can similarly complete the proof as in (25).  $\square$

In this way, Lemma 3 follows directly from Lemma 4 and Lemma 12.

## B. Proof of Theorem 1

Fix arbitrary  $x \in \mathcal{X}$ . For notation simplicity, we follow a similar notation rule as in Lemma 3, where

$$\begin{aligned} A &= \nabla_{xx} g(x, y_g^*(x)), \\ B &= \nabla_{xy} g(x, y_g^*(x)), \\ C &= \nabla_{yy} g(x, y_g^*(x)), \\ E_A &= A - \nabla_{xx} \gamma^{-1} f(x, y_\gamma(x)) + g(x, y_\gamma^*(x)), \\ E_B &= B - \nabla_{xy} \gamma^{-1} f(x, y_\gamma(x)) + g(x, y_\gamma^*(x)), \\ E_C &= C - \nabla_{yy} \gamma^{-1} f(x, y_\gamma(x)) + g(x, y_\gamma^*(x)). \end{aligned}$$

Here,  $\|A\|, \|B\|, \|C\| \leq l_{g,1}$  by the  $l_{g,1}$ -Lipschitzness of  $\nabla g$ . Moreover,

$$\begin{aligned} \|E_A\| &= \|\gamma^{-1} \nabla_{xx} f(x, y_\gamma^*(x)) \\ &\quad + \nabla_{xx} g(x, y_\gamma^*(x)) - \nabla_{xx} g(x, y_g^*(x))\| \\ &\leq \gamma^{-1} \|\nabla_{xx} f(x, y_\gamma^*(x))\| \\ &\quad + \|\nabla_{xx} g(x, y_\gamma^*(x)) - \nabla_{xx} g(x, y_g^*(x))\| \\ &\leq \gamma^{-1} l_{f,1} + l_{g,2} \|y_\gamma^*(x) - y_g^*(x)\| \\ &\leq \frac{l_{f,1}}{\gamma} + l_{g,2} \frac{l_{f,0}}{\mu_g \gamma}. \end{aligned} \quad (36)$$

The first inequality applies triangle inequality; the second uses the  $l_{f,1}$ -smoothness of  $f$  and the  $l_{g,2}$ -Lipschitz of  $\nabla^2 g$ ; and the last follows Lemma 1. Following similar analysis,

$$\begin{aligned} \|E_B\| &= \|\gamma^{-1} \nabla_{xy} f(x, y_\gamma^*(x)) + \nabla_{xy} g(x, y_\gamma^*(x)) \\ &\quad - \nabla_{xy} g(x, y_g^*(x))\| \\ &\leq \frac{l_{f,1}}{\gamma} + l_{g,2} \frac{l_{f,0}}{\mu_g \gamma}, \end{aligned} \quad (37)$$

$$\begin{aligned} \text{and } \|E_C\| &= \|\gamma^{-1} \nabla_{yy} f(x, y_\gamma^*(x)) + \nabla_{yy} g(x, y_\gamma^*(x)) \\ &\quad - \nabla_{yy} g(x, y_g^*(x))\| \\ &\leq \frac{l_{f,1}}{\gamma} + l_{g,2} \frac{l_{f,0}}{\mu_g \gamma}. \end{aligned} \quad (38)$$

Additionally, the  $\mu_g$ -Strongly convexity condition guarantees the smallest eigenvalue of  $C$ ,  $\lambda_{\min}^+(C) \geq \mu_g$  and similarly  $\lambda_{\min}^+(C + E_C) \geq \mu_g$  for  $\gamma \geq \frac{l_{g,1}}{l_{f,1}}$ , according to [3, Lemma F.6]. The same holds for the principle submatrices  $C_{[I,I]}$  and  $(C + E_C)_{[I,I]}$  as well. In this way, following [8], we have

$$\|E_{C^{-1}}\| = \|C_{[I,I]}^{-1} - (C + E_C)_{[I,I]}^{-1}\| \leq \frac{1 + \sqrt{5}}{2\mu_g} \|E_C\|.$$

As the penalty function  $F_\gamma(x) = \gamma(v^h(x, y) - v(x))$ , for any unit directional  $d$ , its second order directional derivative is

$$D_{dd}^2(F_\gamma(x)) = \gamma \left( D_{dd}^2(v_\gamma(x)) - D_{dd}^2(v(x)) \right) \quad (39)$$

where

$$\begin{aligned} D_{dd}^2(v(x)) &= d^\top \left( A - B \begin{bmatrix} C_{[I,I]}^{-1} B_{[:,I]}^\top \\ 0 \end{bmatrix} \right) d, \quad \text{and} \\ D_{dd}^2(v_\gamma(x)) &= d^\top (A + E_A) d + \mathcal{O}(\delta) \\ &\quad - d^\top (B + E_B) \begin{bmatrix} (C + E_C)_{[I,I]}^{-1} (B + E_B)_{[:,I]}^\top \\ 0 \end{bmatrix} d. \end{aligned} \quad (40)$$

In this way,

$$\begin{aligned} \|D_{dd}^2(F_\gamma(x))\| &= \mathcal{O}(\delta) + \gamma \|D_{dd}^2(v_\gamma(x)) - D_{dd}^2(v(x))\| \\ &\leq \gamma \|E_A\| + \gamma \left( l_{g,1}^2 \|E_{C^{-1}}\| + 2 \frac{l_{g,1}}{\mu_g} \|E_B\| \right. \\ &\quad \left. + (2l_{g,1} + \frac{1}{\mu_g}) \|E_B\| \|E_{C^{-1}}\| + \|E_B\|^2 \|E_{C^{-1}}\| \right) \\ &\leq \gamma \left( 1 + l_{g,1}^2 \frac{1 + \sqrt{5}}{2\mu_g} + 2 \frac{l_{g,1}}{\mu_g} \right) \left( \gamma^{-1} l_{f,1} + l_{g,2} \|y_\gamma^*(x) - y_g^*(x)\| \right) \\ &\quad + \gamma \left( 2l_{g,1} + \mu_g^{-1} \right) \frac{1 + \sqrt{5}}{2\mu_g} \left( \gamma^{-1} l_{f,1} + l_{g,2} \|y_\gamma^*(x) - y_g^*(x)\| \right)^2 \\ &\quad + \gamma \frac{1 + \sqrt{5}}{2\mu_g} \left( \gamma^{-1} l_{f,1} + l_{g,2} \|y_\gamma^*(x) - y_g^*(x)\| \right)^3 + \mathcal{O}(\delta) \\ &\leq C_1 C_0 + \frac{1}{\gamma} C_2 C_0^2 + \frac{1}{\gamma^2} C_3 C_0^3 + \mathcal{O}(\delta), \end{aligned}$$

$$\text{where } \begin{cases} C_0 = l_{f,1} + l_{g,2} l_{f,0} \mu_g^{-1} \\ C_1 = 1 + l_{g,1}^2 \frac{1 + \sqrt{5}}{2\mu_g} + 2 \frac{l_{g,1}}{\mu_g} \\ C_2 = \left( 2l_{g,1} + \mu_g^{-1} \right) \frac{1 + \sqrt{5}}{2\mu_g} \\ C_3 = \frac{1 + \sqrt{5}}{2\mu_g} \end{cases}$$

Here, the first inequality is from triangle inequality, Cauchy-Schwartz inequality and  $\|B\| \leq l_{g,1}$ ,  $\|C_\dagger\| \leq \frac{1}{\mu_g}$ ; the second is by the upper bounds of  $\|E_A\|$ ,  $\|E_B\|$ ,  $\|E_C\|$ , and  $\|E_{C^{-1}}\|$ , and the last is by the upper bound for  $\|y_\gamma^*(x) - y_g^*(x)\|$  in Lemma 1.

### C. Proof of Proposition 2

According to [5], to achieve

$$\|y_t - y_g^*(x_t)\|^2, \|y_t - y_\gamma^*(x_t)\|^2 < \epsilon^2, \quad (41)$$

we can apply PGD on

$$\min_{y \in \{y \in \mathcal{Y} : c(y) \leq 0\}} g(x, y), \quad \text{and} \quad (42)$$

$$\min_{y \in \{y \in \mathcal{Y} : c(y) \leq 0\}} \gamma^{-1} f(x, y) + g(x, y) \quad (43)$$

with algorithm complexity  $\mathcal{O}(\ln(\epsilon^{-1}))$ . In this way, the update bias

$$\begin{aligned} \|b(x_t)\|^2 &= \|\nabla F_\gamma(x_t) - g_t\|^2 \\ &\leq \gamma \|\gamma^{-1} \nabla_x f(x_t, y_\gamma^*(x_t)) + \nabla_x g(x_t, y_\gamma^*(x_t)) - \nabla_x g(x_t, y_g^*(x_t)) \\ &\quad - (\gamma^{-1} \nabla_x f(x_t, y_t^\gamma) + \nabla_x g(x_t, y_t^\gamma) - \nabla_x g(x_t, y_t^g))\|^2 \\ &\leq 2 \|\nabla_x f(x_t, y_\gamma^*(x_t)) + \gamma \nabla_x g(x_t, y_\gamma^*(x_t)) \\ &\quad - (\nabla_x f(x_t, y_t^\gamma) + \gamma \nabla_x g(x_t, y_t^\gamma))\|^2 \\ &\quad + 2 \|\gamma \nabla_x g(x_t, y_\gamma^*(x_t)) - \gamma \nabla_x g(x_t, y_t^g)\|^2 \\ &\leq 2(l_{f,1} + \gamma l_{g,1})^2 \|y_\gamma^*(x_t) - y_t^\gamma\|^2 + 2\gamma^2 l_{g,1}^2 \|y_g^*(x_t) - y_t^g\|^2 \\ &\leq \mathcal{O}(\gamma^2 \epsilon^2) = \mathcal{O}(\epsilon). \end{aligned} \quad (44)$$

where the second inequality is by Young's inequality; the third is from the smoothness of  $f$  and  $g$ ; and the last is from (41) and  $\gamma = \mathcal{O}(\epsilon^{-0.5})$ .

According to smoothness of  $F_\gamma(x)$ , there is

$$\begin{aligned} F_\gamma(x_{t+1}) &\leq F_\gamma(x_t) + \langle \nabla F_\gamma(x_t), x_{t+1} - x_t \rangle + \frac{l_{F,1}}{2} \|x_{t+1} - x_t\|^2 \\ &\leq F_\gamma(x_t) + \langle g_t, x_{t+1} - x_t \rangle + \frac{1}{2\eta} \|x_{t+1} - x_t\|^2 \\ &\quad + \langle b(x_t), x_{t+1} - x_t \rangle, \end{aligned} \quad (45)$$

where the second inequality is by  $\eta \leq \frac{1}{l_{F,1}}$ . The projection guarantees that  $x_{t+1}$  and  $x_t$  are in  $\mathcal{X}$ . In this way, Following lemma 2, we know that

$$\langle g_t, x_{t+1} - x_t \rangle \leq -\frac{1}{\eta} \|x_{t+1} - x_t\|^2.$$

Plugging this back to (45),

$$\begin{aligned} F_\gamma(x_{t+1}) &\leq F_\gamma(x_t) - \frac{1}{2\eta} \|x_{t+1} - x_t\|^2 + \langle b(x_t), x_{t+1} - x_t \rangle \\ &\leq F_\gamma(x_t) - \frac{1}{2\eta} \|x_{t+1} - x_t\|^2 + \eta \|b(x_t)\|^2 \\ &\quad + \frac{1}{4\eta} \|x_{t+1} - x_t\|^2 \\ &= F_\gamma(x_t) - \frac{1}{4\eta} \|x_{t+1} - x_t\|^2 + \eta \|b(x_t)\|^2, \end{aligned}$$

where the second inequality is from Young's inequality. Telescoping therefore gives

$$\begin{aligned} &\frac{1}{T} \sum_{t=0}^{T-1} \left\| \frac{x_t - \text{Proj}_{\mathcal{X}}(x_t - \eta g_t)}{\eta} \right\|^2 \\ &\leq \frac{4}{\eta T} (F_\gamma(x_0) - F_\gamma(x_t)) + \frac{4}{T} \sum_{t=0}^{T-1} \|b(x_t)\|^2. \end{aligned} \quad (46)$$

In this way

$$\begin{aligned} &\frac{1}{T} \sum_{t=0}^{T-1} \|G_\eta(x_t)\|^2 \\ &= \frac{1}{T} \sum_{t=0}^{T-1} \left\| \frac{x_t - \text{Proj}_{\mathcal{X}}(x_t - \eta \nabla F_\gamma(x_t))}{\eta} \right\|^2 \\ &= \frac{1}{T} \sum_{t=0}^{T-1} \left\| \frac{x_t - \text{Proj}_{\mathcal{X}}(x_t - \eta g_t)}{\eta} \right\|^2 + \frac{1}{T} \sum_{t=0}^{T-1} \|b(x_t)\|^2 \\ &\leq \frac{4}{\eta T} (F_\gamma(x_0) - F_\gamma(x_t)) + \frac{5}{T} \sum_{t=0}^{T-1} \|b(x_t)\|^2 \end{aligned} \quad (47)$$

$$= \mathcal{O}(\eta^{-1} T^{-1} + \epsilon) \quad (48)$$

As  $\eta = \mathcal{O}(1)$ , to achieve  $\frac{1}{T} \sum_{t=0}^{T-1} \|G_\eta(x_t)\|^2 \leq \epsilon$ , we require complexity

$$T = \mathcal{O}(\epsilon^{-1}). \quad (49)$$

In this way, counting in the inner  $\mathcal{O}(\ln(\epsilon^{-1}))$  complexity, the total algorithm complexity is

$$\mathcal{O}(\epsilon^{-1} \ln(\epsilon^{-1})) = \tilde{\mathcal{O}}(\epsilon^{-1}). \quad (50)$$

### III. EXTENSION TO COUPLED CONSTRAINT SETTING

#### A. Extension to Coupled Constraint setting

**Lemma 7** (Generalized Lemma 3). *Consider  $\mathcal{Y}(x) = \{y \in \mathcal{Y} : c(x, y) \leq 0\}$ . Suppose Assumption 1, 2, 3, 4, and 5 hold. For any unit direction  $d \in \mathbb{R}^{d_x}$ , there exists an index set  $\mathcal{I} \subseteq [d_y]$  such that the second-order directional derivative of  $v(x)$ ,*

$$\begin{aligned} &D_{dd}^2(v(x)) \\ &= d^\top B'(x)_{[:,\mathcal{I}]} C'(x)_{[\mathcal{I},\mathcal{I}]}^{-1} C(x)_{[\mathcal{I},\mathcal{I}]} C'(x)_{[\mathcal{I},\mathcal{I}]}^{-1} B'(x)_{[:,\mathcal{I}]}^\top d \\ &\quad + d^\top \nabla_{xx} A(x) d \\ &\quad - d^\top B'(x)_{[:,\mathcal{I}]} C'(x)_{[\mathcal{I},\mathcal{I}]}^{-1} B(x)_{[\mathcal{I},:] } d \\ &\quad - d^\top B(x)_{[:,\mathcal{I}]} C'(x)_{[\mathcal{I},\mathcal{I}]}^{-1} B'(x)_{[:,\mathcal{I}]}^\top d. \end{aligned} \quad (51)$$

where  $A(x)$ ,  $B(x)$ , and  $C(x)$  are defined in (12), and

$$\begin{aligned} B'(x) &= \nabla_{xy} L_g(x, y_g^*(x), \lambda_g^*(x)), \\ C'(x) &= \nabla_{yy} L_g(x, y_g^*(x), \lambda_g^*(x)). \end{aligned}$$

Moreover, for any  $\delta > 0$ , there exists a finite  $\gamma^*$  such that

$$\begin{aligned} &D_{dd}^2(v_\gamma(x)) \\ &= d^\top B'_\gamma(x)_{[:,\mathcal{I}]} C'_\gamma(x)_{[\mathcal{I},\mathcal{I}]}^{-1} C_\gamma(x)_{[\mathcal{I},\mathcal{I}]} C'_\gamma(x)_{[\mathcal{I},\mathcal{I}]}^{-1} B'_\gamma(x)_{[:,\mathcal{I}]}^\top d \\ &\quad + d^\top \nabla_{xx} A_\gamma(x) d \\ &\quad - d^\top B'_\gamma(x)_{[:,\mathcal{I}]} C'_\gamma(x)_{[\mathcal{I},\mathcal{I}]}^{-1} B_\gamma(x)_{[\mathcal{I},:] } d \\ &\quad - d^\top B(x)_{[:,\mathcal{I}]} C'_\gamma(x)_{[\mathcal{I},\mathcal{I}]}^{-1} B'_\gamma(x)_{[:,\mathcal{I}]}^\top d. \end{aligned} \quad (52)$$

for all  $\gamma > \gamma^*$ , for the same  $\mathcal{I}$ , where

$$\begin{aligned} B'_\gamma(x) &= \nabla_{xy} L_\gamma(x, y_\gamma^*(x), \lambda_\gamma^*(x)), \\ C'_\gamma(x) &= \nabla_{yy} L_\gamma(x, y_\gamma^*(x), \lambda_\gamma^*(x)). \end{aligned}$$

Before we proceed to the proof of Lemma 7, we present the following as an extension to Lemma 3 for BLO with coupled constraint setting.

**Lemma 8.** *Suppose  $\mathcal{Y} \subseteq \mathbb{R}^{d_y}$  is a closed and convex set with smooth boundary,  $\nabla_y g(x, y)$  is continuous in  $y$ , and Lipschitz in  $x$ , and  $g(x, y)$  satisfies  $\mu_g$ -Proximal PL in  $y$  on  $\mathcal{Y}$  and on a disturbed domain  $\mathcal{Y}_\delta$  such that (i)  $\mathcal{Y} \subset \mathcal{Y}_\delta$ , and (ii)  $d_{\mathcal{Y}}(y) = \delta$  for any  $y \in \text{bd}(\mathcal{Y}_\delta)$ . Fix any  $y_g^*(x) \in S_g^*(x)$ , and for arbitrary unit direction  $d \in \mathbb{R}^{d_x}$ , denote  $y_{g,r}$  as some element in  $S_g^*(x + rd)$ . Then,*

$$\langle \nabla_y g(x, y_g^*(x)), \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \rangle = 0 \quad (53)$$

*Proof.* When  $\nabla_y g(x, y_g^*(x)) = 0$ , the equality automatically hold. We consider in the following the case  $\nabla_y g(x, y_g^*(x)) \neq 0$ .

When  $\nabla_y g(x, y_g^*(x)) \neq 0$ ,  $y_g$  is on the boundary of  $\mathcal{Y}$ , i.e.  $y_g^*(x) \in \text{bd}(\mathcal{Y})$ , as the (local) optimum of a differentiable function happens either at stationary point or at extreme (i.e. boundary).

Additionally,  $\{y^* \in \mathbb{R}^{d_y} : \nabla_y g(x, y^*) = 0\}$  is a closed set, as  $\{0\}$  is closed and the closeness is preserved by continuous image mapping,  $\nabla_y g(x, \cdot)$ . In this way, there exists  $\delta_0 > 0$  such that  $\|y_g^*(x) - y^*\| \geq \delta_0$  for any  $y^* \in \{y^* \notin \mathcal{Y} : \nabla_y g(x, y^*) = 0\} \subseteq \{y^* \in \mathbb{R}^{d_y} : \nabla_y g(x, y^*) = 0\}$ .

Denote some  $y_g^\delta \in \min_{y \in \mathcal{Y}_\delta} g(x, y)$ . According to [1, Theorem 2.87],  $\|y_g^\delta - y_g^*(x)\| = \mathcal{O}(\delta)$ . In this way, there exists some  $\delta_1 > 0$  of the order  $\delta_0$  such that for all  $0 < \delta < \delta_1$ ,  $\nabla_y g(x, y_g^\delta) \neq 0$ , indicating that  $y_g^\delta$  is on the boundary of  $\mathcal{Y}_\delta$ , i.e.  $y_g^\delta \in \text{bd}(\mathcal{Y}_\delta)$ .

Moreover, under the condition that Proximal PL condition for  $g(x, y)$  also holds for  $y \in \mathcal{Y}_\delta$ , there exist  $y_{g,r}^\delta \in \arg \min_{y \in \mathcal{Y}_\delta} g(x + rd, y)$  such that  $\|y_g^\delta - y_{g,r}^\delta\| \leq L_y^g r$  according to Lemma 1. In this way, there exists some  $r_0 > 0$  such that for all  $0 < r < r_0$ ,  $\|y_g^\delta - y_{g,r}^\delta\| < \delta$ , i.e.  $y_{g,r}^\delta \in \mathcal{Y}_\delta \setminus \mathcal{Y}$  as  $y_g^\delta$  is on the boundary of  $\mathcal{Y}_\delta$ , which is in  $\delta$  distance to  $\mathcal{Y}$ . This directly implies  $\nabla_y g(x, y_{g,r}^\delta) \neq 0$  as otherwise  $y_{g,r}^\delta = y_{g,r} \in \mathcal{Y}$ . This gives  $y_{g,r} \in \text{bd}(\mathcal{Y})$ , for all  $0 < r < r_0$ .

In this way, as  $y_g, y_{g,r}$  are both on  $\text{bd}(\mathcal{Y})$  and  $y_{g,r}$  approaches to  $y_g$ , we know the limiting direction of  $y_g$  to  $y_{g,r}$  is in the tangent cone of  $\mathcal{Y}$  on boundary point  $y_g$ :

$$\lim_{\|y_{g,r} - y_g^*(x)\| \downarrow 0} \frac{y_{g,r} - y_g}{\|y_{g,r} - y_g^*(x)\|} \in T_{\mathcal{Y}}(y_g^*(x)). \quad (54)$$

Moreover, as  $\|y_{g,r} - y_g^*(x)\| \leq L_y^g r$ , so  $\lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r}$  either equals 0, which directly leads to the equality proved, or

$$\lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \in T_{\mathcal{Y}}(y_g^*(x)). \quad (55)$$

In this way, as  $\mathcal{Y}$  is smooth on the boundary,  $\nabla_y g(x, y_g^*(x)) \perp T_{\mathcal{Y}}(y_g^*(x))$  and we can conclude the lemma.  $\square$

**Lemma 9.** Suppose  $\mathcal{Y}$  is smooth on its boundary,  $\|\lambda_g^*(x)\| < B_\lambda$  for all  $x \in \mathcal{X}$ , and Assumption 2, 3 hold. Fix any  $x \in \mathcal{X}$ , denote  $y_g^*(x) = \arg \min_{y \in \mathcal{Y}} g^\lambda(x, y)$ , and for arbitrary unit direction  $d \in \mathbb{R}^{d_x}$ , denote  $y_{g,r} = \arg \min_{y \in \mathcal{Y}} g^\lambda(x + rd, y)$ . For  $\lambda_g^*(x) = \arg \max_{\lambda \in \mathbb{R}^{d_x}} (\min_{y \in \mathcal{Y}} g(x, y) + \langle \lambda, c(x, y) \rangle)$  being the unique Lagrangian multiplier [7], then,

$$\left\langle \nabla_y g(x, y_g^*(x)) + \langle \lambda_g, \nabla_x c(x, y_g^*(x)) \rangle, \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \right\rangle = 0 \quad (56)$$

*Proof.* The proof follows directly from Lemma 8. Denote  $g^\lambda(x, y) = g(x, y) + \langle \lambda_g^*(x), c(x, y) \rangle$ . Here we can easily conclude that  $g^\lambda(x, y)$  is proximal-PL in  $y \in \mathcal{Y}$  and any disturbed domain  $\mathcal{Y}_\delta$  defined in Lemma 8, as  $g(x, y)$  is strongly convex in  $y$  and  $c(x, y)$  is convex in  $y$ , according to [5]. Moreover, as  $\nabla_y g^\lambda(x, y) = \nabla_y g(x, y) + \langle \lambda_g^*(x), \nabla_y c(x, y) \rangle$ , and as assuming  $\|\lambda_g^*(x)\| < B_\lambda$  for all  $x \in \mathcal{X}$ , there is, for any  $x_1, x_2 \in \mathcal{X}$ ,

$$\begin{aligned} & \|\nabla_y g^\lambda(x_1, y) - \nabla_y g^\lambda(x_2, y)\| \\ & \leq (l_{g,1} + l_{c,1} \|\lambda_g^*(x)\|) \|x_1 - x_2\| \\ & \leq (l_{g,1} + l_{c,1} B_\lambda) \|x_1 - x_2\|. \end{aligned}$$

i.e.  $\nabla_y g^\lambda(x, y)$  is Lipschitz in  $x$ . So all conditions in Lemma 8 are checked and therefore proved.  $\square$

**Lemma 10.** Under all assumptions and notations in Lemma 9, and suppose  $g(x, y)$ ,  $c(x, y)$  is locally Lipschitz at  $(x, y_g^*(x))$ , there is

$$\left\langle \lim_{r \downarrow 0} \frac{\lambda_g^*(x + rd) - \lambda_g^*(x)}{r}, c(x, y_g^*(x)) \right\rangle = 0. \quad (57)$$

*Proof.* The directional derivative of  $v(x)$  in unit direction  $d \in \mathbb{R}^{d_x}$  is

$$\begin{aligned} D_d(v) &= \lim_{r \downarrow 0} \frac{1}{r} (c(x + rd, y_{g,r}) + \langle \lambda_g^*(x + rd), c(x + rd, y_{g,r}) \rangle \\ &\quad - c(x + rd, y_{g,r}) + \langle \lambda_g^*(x + rd), c(x + rd, y_{g,r}) \rangle) \\ &= \lim_{r \downarrow 0} \frac{1}{r} (c(x + rd, y_{g,r}) + \langle \lambda_g^*(x), c(x + rd, y_{g,r}) \rangle \\ &\quad + \langle \lambda_g^*(x + rd) - \lambda_g^*(x), c(x + rd, y_{g,r}) \rangle \\ &\quad - c(x + rd, y_{g,r}) + \langle \lambda_g^*(x + rd), c(x + rd, y_{g,r}) \rangle) \\ &= \langle \nabla_x g(x, y_g^*(x)) + \langle \lambda_g^*(x), \nabla_x c(x, y_g^*(x)) \rangle, d \rangle \\ &\quad + \langle \nabla_y g(x, y_g^*(x)) + \langle \lambda_g^*(x), \nabla_y c(x, y_g^*(x)) \rangle, \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \rangle \\ &\quad + \langle \lim_{r \downarrow 0} \frac{\lambda_g^*(x + rd) - \lambda_g^*(x)}{r}, c(x, y_g^*(x)) \rangle \end{aligned}$$

where the last equality is by Taylor expansion and  $y_g$  being Lipschitz according to Lemma 1. By Lemma 9, there is  $\langle \nabla_y g(x, y_g^*(x)) + \langle \lambda_g^*(x), \nabla_y c(x, y_g^*(x)) \rangle, \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \rangle = 0$ . Moreover, according to [4, Lemma 2], when  $g(x, y)$ ,  $c(x, y)$  is locally Lipschitz at  $(x, y_g^*(x))$ , there is

$$\nabla v(x) = \nabla_x c(x, y) + \langle \lambda_g^*(x), c(x, y) \rangle. \quad (58)$$

Therefore, we know

$$\left\langle \lim_{r \downarrow 0} \frac{\lambda_g^*(x + rd) - \lambda_g^*(x)}{r}, c(x, y_g^*(x)) \right\rangle = 0. \quad (59)$$

$\square$

In this way, we can similarly show a generalized version of Lemma 4.

**Lemma 11.** Suppose all conditions in Lemma 7 hold. For any unit direction  $d \in \mathbb{R}^{d_x}$ , there exists an index set  $\mathcal{I} \subseteq [d_y]$  such that the directional derivative of  $y_g^*(x)$ ,  $D_d(y_g^*(x))$  satisfies

$$\left[ \lim_{r \downarrow 0} \frac{y_g^*(x + rd) - y_g^*(x)}{r} \right]_{[d_y] \setminus \mathcal{I}} = 0, \quad \text{and} \quad (60)$$

$$\left[ \lim_{r \downarrow 0} \frac{y_g^*(x + rd) - y_g^*(x)}{r} \right]_{\mathcal{I}} = C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[\cdot, \mathcal{I}]}^\top d, \quad (61)$$

and the 2nd-order directional derivative of  $v(x)$  in direction  $d$  is

$$\begin{aligned} & D_{dd}^2(v(x)) \\ &= d^\top B'(x)_{[\cdot, \mathcal{I}]} C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} C'(x)_{[\mathcal{I}, \mathcal{I}]} C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[\cdot, \mathcal{I}]}^\top d \\ &\quad + d^\top \nabla_{xx} A(x) d \\ &\quad - d^\top B'(x)_{[\cdot, \mathcal{I}]} C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B(x)_{[\mathcal{I}, \cdot]} d \\ &\quad - d^\top B(x)_{[\cdot, \mathcal{I}]} C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[\cdot, \mathcal{I}]}^\top d. \end{aligned} \quad (62)$$

where  $A(x)$ ,  $B(x)$ , and  $C(x)$  are defined in (12), and

$$\begin{aligned} B'(x) &= \nabla_{xy} L_g(x, y_g^*(x), \lambda_g^*(x)), \\ C'(x) &= \nabla_{yy} L_g(x, y_g^*(x), \lambda_g^*(x)). \end{aligned}$$

*Proof.* Fix arbitrary unit direction  $d$ , denote  $y_{g,r}$  as solution to  $\min_{y \in \mathcal{Y}(x)} g(x + rd + \frac{1}{2}r'^2d)$ . According to [1], the second order directional derivative of  $v(x)$  in direction unit direction  $d$  is

$$\begin{aligned} & D_{dd}^2(v(x)) \\ &= \lim_{r, r' \downarrow 0} \frac{1}{\frac{1}{2}rr'} \left( g(x + rd + \frac{1}{2}r^2d, y_{g,r}) - g(x, y_g^*(x)) \right. \\ &\quad \left. - \langle \nabla v(x), rd \rangle \right) \\ &\stackrel{(a)}{=} \lim_{r, r' \downarrow 0} \frac{1}{\frac{1}{2}rr'} \left( \langle \nabla_x g(x, y_g^*(x)), rd \rangle \right. \\ &\quad + \langle \nabla_y g(x, y_g^*(x)), y_{g,r} - y_g^*(x) \rangle \\ &\quad + \frac{1}{2} (y_{g,r} - y_g^*(x))^\top \nabla_{yy} g(x, y_g^*(x)) (y_{g,r} - y_g^*(x)) \\ &\quad + \frac{rr'}{2} d^\top \nabla_{xx} g(x, y_g^*(x)) d \\ &\quad + \frac{r'}{2} d^\top \nabla_{xy} g(x, y_g^*(x)) (y_{g,r} - y_g^*(x)) \\ &\quad + \frac{r}{2} (y_{g,r} - y_g^*(x))^\top \nabla_{yx} g(x, y_g^*(x)) d \\ &\quad \left. - \langle \nabla_x g(x, y_g^*(x)) + \lambda_g^\top \nabla_x c(x, y_g^*(x)), rd \rangle \right) \\ &\stackrel{(b)}{=} \left( \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r'} \right)^\top \nabla_{yy} g(x, y_g^*(x)) \left( \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \right) \\ &\quad + d^\top \nabla_{xx} g(x, y_g^*(x)) d \\ &\quad + \left( \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r} \right)^\top \nabla_{xy} g(x, y_g^*(x)) d \\ &\quad + d^\top \nabla_{yx} g(x, y_g^*(x)) \left( \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \right). \end{aligned} \quad (63)$$

where the (a) is by 2nd order of Taylor expansion; (b) is from  $\langle \nabla_x g(x, y_g^*(x)), rd \rangle + \langle \nabla_y g(x, y_g^*(x)), y_{g,r} - y_g^*(x) \rangle = \langle \nabla_x g(x, y_g^*(x)) + \lambda_g^\top \nabla_x c(x, y_g^*(x)), rd \rangle$  and they are two equivalent expression of the directional  $\nabla v(x)$ . Notice that the directional hessian relies on  $\lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r}$ , we investigate it in the following.

Following Lemma 9 and 10, we have

$$\begin{aligned} & \langle \nabla_y g(x, y_g^*(x)) + \lambda_g^\top \nabla_y c(x, y_g^*(x)), \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \rangle = 0, \\ & \text{and } \langle c(x, y_g^*(x)), \lim_{r \downarrow 0} \frac{\lambda_{g,r} - \lambda_g}{r} \rangle = 0, \end{aligned} \quad (64)$$

In this way, denote  $y_{g,r}$  as the optimal solution for  $\min_{y \in \mathcal{Y}(x)} g(x + rd, y)$  and  $\lambda_{g,r}$  as the corresponding La-

grangian multiplier, we have

$$\begin{aligned} 0 &= \lim_{r \downarrow 0} \frac{1}{r} \langle \nabla_y g(x + rd, y_{g,r}) + \lambda_{g,r}^\top \nabla_y c(x + rd, y_{g,r}) \\ &\quad - (\nabla_y g(x, y_g^*(x)) + \lambda_g^\top \nabla_y c(x, y_g^*(x))), \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r'} \rangle \\ &= \lim_{r \downarrow 0} \frac{1}{r} \langle \nabla_y g(x + rd, y_{g,r}) + \lambda_g^\top \nabla_y c(x + rd, y_{g,r}) \\ &\quad - (\nabla_y g(x, y_g^*(x)) + \lambda_g^\top \nabla_y c(x, y_g^*(x))), \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r'} \rangle \\ &\quad + \lim_{r \downarrow 0} \frac{1}{r} \langle (\lambda_{g,r} - \lambda_g)^\top \nabla_y c(x + rd, y_{g,r}), \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r'} \rangle \\ &\stackrel{(a)}{=} \lim_{r \downarrow 0} \frac{1}{r} \langle \nabla_y g(x + rd, y_{g,r}) + \lambda_g^\top \nabla_y c(x + rd, y_{g,r}) \\ &\quad - (\nabla_y g(x, y_g^*(x)) + \lambda_g^\top \nabla_y c(x, y_g^*(x))), \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r'} \rangle \\ &\quad + \lim_{r' \downarrow 0} \frac{1}{r'} \left( \lim_{r \downarrow 0} \frac{\lambda_{g,r} - \lambda_g}{r} \right)^\top (c(x + rd, y_{g,r'}) \\ &\quad - c(x + rd, y_g)) \\ &\stackrel{(b)}{=} \lim_{r \downarrow 0} \langle \nabla_y g(x + rd, y_{g,r}) + \lambda_g^\top \nabla_y c(x + rd, y_{g,r}) \\ &\quad - (\nabla_y g(x, y_g^*(x)) + \lambda_g^\top \nabla_y c(x, y_g^*(x))), \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r'} \rangle \\ &\stackrel{(c)}{=} \left\langle (\nabla_{yx} g(x, y_g^*(x)) + \lambda_g^\top \nabla_{yx} c(x, y_g^*(x))) d \right. \\ &\quad \left. + (\nabla_{yy} g(x, y_g^*(x)) + \lambda_g^\top \nabla_{yy} c(x, y_g^*(x))) \left( \lim_{r' \downarrow 0} \frac{y_{g,r} - y_g}{r} \right), \right. \\ &\quad \left. \lim_{r' \downarrow 0} \frac{y_{g,r'} - y_g}{r'} \right\rangle. \end{aligned}$$

where (a) uses Taylor expansion; (b) is by choosing  $r' = r$  and calling (64); and (c) follows Taylor expansion as well.

In this way, denote  $\mathcal{I}$  as the index set for non-zero elements in  $\lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r}$ , we have

$$\begin{aligned} 0 &= \nabla_{xy} L_g(x, y_g^*(x), \lambda_g^*(x))_{[\cdot, \mathcal{I}]}^\top d \\ &\quad + \nabla_{yy} L_g(x, y_g^*(x), \lambda_g^*(x))_{[\mathcal{I}, \mathcal{I}]} \left[ \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \right]_{\mathcal{I}} \end{aligned} \quad (65)$$

where  $L_g(x, y, \lambda)$  is defined in (16). In this way, following a similar analysis as the one for Lemma 4, there is

$$\begin{aligned} & \left[ \lim_{r \downarrow 0} \frac{y_{g,r} - y_g}{r} \right]_{\mathcal{I}} \\ &= - \nabla_{yy} L(x, y_g; \lambda_g)_{[\mathcal{I}, \mathcal{I}]}^{-1} \nabla_{xy} L(x, y_g; \lambda_g)_{[\cdot, \mathcal{I}]}^\top d \\ &= - C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[\cdot, \mathcal{I}]}^\top d \end{aligned} \quad (66)$$

This proves the first part of the Lemma.

In this way, plugging the result back in (63), we have

$$\begin{aligned}
& D_{dd}^2(v(x)) \\
&= \left( C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[:, \mathcal{I}]}^\top d \right)^\top \\
& C(x)_{[\mathcal{I}, \mathcal{I}]} \left( C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[:, \mathcal{I}]}^\top d \right) \\
&+ d^\top \nabla_{xx} g(x, y_g^*(x)) d \\
&+ \left( -C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[:, \mathcal{I}]}^\top d \right)^\top B(x)_{[\mathcal{I}, :]} d \\
&+ d^\top B(x)_{[:, \mathcal{I}]} \left( -C'(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'(x)_{[:, \mathcal{I}]}^\top d \right). \quad (67)
\end{aligned}$$

Therefore, rearranging completes the proof.  $\square$

Moreover, Lemma 5 is also applicable to this coupled constraint setting  $\mathcal{Y}(x) = \{y \in \mathcal{Y} : c(x, y) \leq 0\}$ . In this way, the generalized version of Lemma 12 can directly be concluded with the same analysis as the one for Lemma 12. We omit the proof here as the analysis follows the same technique.

**Lemma 12.** *Suppose all conditions in Lemma 7 hold. Fix any unit direction  $d \in \mathbb{R}^{d_x}$ , denote  $\mathcal{I} \subseteq [d_y]$  as the index set for non-zero elements in  $D_d(y_g^*(x))$ . For any  $\delta > 0$ , there exists a finite  $\gamma^* > 0$  such that the second-order directional derivative of  $v_\gamma(x)$  is*

$$\begin{aligned}
& D_{dd}^2(v_\gamma(x)) \\
&= d^\top B'_\gamma(x)_{[:, \mathcal{I}]} C'_\gamma(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} C_\gamma(x)_{[\mathcal{I}, \mathcal{I}]} C'_\gamma(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'_\gamma(x)_{[:, \mathcal{I}]}^\top d \\
&+ d^\top \nabla_{xx} A_\gamma(x) d \\
&- d^\top B'_\gamma(x)_{[:, \mathcal{I}]} C'_\gamma(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B_\gamma(x)_{[\mathcal{I}, :]} d \\
&- d^\top B(x)_{[:, \mathcal{I}]} C'_\gamma(x)_{[\mathcal{I}, \mathcal{I}]}^{-1} B'_\gamma(x)_{[:, \mathcal{I}]}^\top d. \quad (68)
\end{aligned}$$

where  $A(x)$ ,  $B(x)$ , and  $C(x)$  are defined in (12), and

$$\begin{aligned}
B'_\gamma(x) &= \nabla_{xy} L_\gamma(x, y_\gamma^*(x), \lambda_g^*(x)), \\
C'_\gamma(x) &= \nabla_{yy} L_\gamma(x, y_\gamma^*(x), \lambda_g^*(x)).
\end{aligned}$$

In this way, we can show Theorem 1 easily following a similar analysis as for Theorem 3 in Appendix II-B.

*Proof of Theorem 3.* As  $\nabla^2 L$ ,  $\nabla^2 L^\gamma$ ,  $\nabla^2 g$ ,  $\nabla^2 f$  are all Lipschitz in  $y$ , we have  $\|\nabla^2 v(x) - \nabla^2 v^\gamma(x)\| = \mathcal{O}(\gamma^{-1})$  following similar analysis as in Appendix II-B. In this way,

$$\|D_{dd}^2(F_\gamma(x))\| = \gamma \|D_{dd}^2(v_\gamma(x)) - D_{dd}^2(v(x))\| = \mathcal{O}(1).$$

So we can conclude that  $\nabla F_\gamma(x)$  is  $\mathcal{O}(1)$ -smooth.  $\square$

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