Supplementary Material for "Closing the Gap: Tighter Analysis of Alternating Stochastic Gradient Methods for Bilevel Problems"

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A Proof for stochastic bilevel problem

A.1 Auxiliary Lemmas

Throughout the proof, we use $\mathcal{F}_{k,t} = \sigma\{y^0, x^0, \dots, y^k, x^k, y^{k,1}, \dots, y^{k,t}\}, \mathcal{F}'_k = \sigma\{y^0, x^0, \dots, y^{k+1}\},$ where $\sigma\{\cdot\}$ denotes the σ -algebra generated by the random variables.

We first present some results that will be used frequently in the proof.

Proposition 5 (Restatement of Proposition 1). *Under Assumptions 1–3, we have the gradients*

$$\nabla F(x) = \nabla_x f(x, y^*(x)) - \nabla_{xy}^2 g(x, y^*(x)) \left[\nabla_{yy}^2 g(x, y^*(x)) \right]^{-1} \nabla_y f(x, y^*(x)). \tag{32}$$

Proof. Define the Jacobian matrix

$$\nabla_x y(x) = \begin{bmatrix} \frac{\partial}{\partial x_1} y_1(x) & \cdots & \frac{\partial}{\partial x_d} y_1(x) \\ & \cdots & \\ \frac{\partial}{\partial x_1} y_{d'}(x) & \cdots & \frac{\partial}{\partial x_d} y_{d'}(x) \end{bmatrix}.$$

By the chain rule, it follows that

$$\nabla F(x) := \nabla_x f(x, y^*(x)) + \nabla_x y^*(x)^{\top} \nabla_y f(x, y^*(x)). \tag{33}$$

The minimizer $y^*(x)$ satisfies

$$\nabla_y g(x, y^*(x)) = 0, \quad \text{thus} \quad \nabla_x \left(\nabla_y g(x, y^*(x)) \right) = 0, \tag{34}$$

from which and the chain rule, it follows that

$$\nabla_{xy}^{2} g(x, y^{*}(x)) + \nabla_{x} y^{*}(x)^{\top} \nabla_{yy}^{2} g(x, y^{*}(x)) = 0.$$

By Assumption 2, $\nabla^2_{yy}g(x,y^*(x))$ is invertible, so from the last equation,

$$\nabla_x y^*(x)^{\top} := -\nabla_{xy}^2 g(x, y^*(x)) \left[\nabla_{yy}^2 g(x, y^*(x)) \right]^{-1}.$$
 (35)

Substituting (35) into (33) yields (6).

Lemma 4 ([16, Lemma 2.2]). Under Assumptions 1 and 2, we have

$$\|\overline{\nabla}_x f(x, y^*(x)) - \overline{\nabla}_x f(x, y)\| \le L_f \|y^*(x) - y\| \tag{36a}$$

$$\|\nabla F(x_1) - \nabla F(x_2)\| \le L_F \|x_1 - x_2\| \tag{36b}$$

$$||y^*(x_1) - y^*(x_2)|| \le L_y ||x_1 - x_2|| \tag{36c}$$

with the constants L_f, L_y, L_F given by

$$L_f := \ell_{f,1} + \frac{\ell_{g,1}\ell_{f,1}}{\mu_g} + \frac{\ell_{f,0}}{\mu_g} \left(\ell_{g,2} + \frac{\ell_{g,1}\ell_{g,2}}{\mu_g} \right) = \mathcal{O}(\kappa^2), \quad L_y := \frac{\ell_{g,1}}{\mu_g} = \mathcal{O}(\kappa)$$

$$L_F := \ell_{f,1} + \frac{\ell_{g,1}(\ell_{f,1} + L_f)}{\mu_g} + \frac{\ell_{f,0}}{\mu_g} \left(\ell_{g,2} + \frac{\ell_{g,1}\ell_{g,2}}{\mu_g} \right) = \mathcal{O}(\kappa^3),$$

where the other constants are defined in Assumptions 1-3.

Lemma 5 ([18, Lemma 11]). Recall the definition of h_f^k in (10). Define

$$\bar{h}_f^k := \mathbb{E}[h_f^k | \mathcal{F}_k'].$$

We have

$$\|\overline{\nabla}_x f(x^k, y^{k+1}) - \bar{h}_f^k\| \le \ell_{g,1} \ell_{f,1} \frac{1}{\mu_g} \left(1 - \frac{\mu_g}{\ell_{g,1}} \right)^N =: b_k$$

$$\mathbb{E}[\|h_f^k - \bar{h}_f^k\|^2] \le \sigma_f^2 + \frac{3}{\mu_g^2} \left[(\sigma_f^2 + \ell_{f,0}^2)(\sigma_{g,2}^2 + 2\ell_{g,1}^2) + \sigma_f^2 \ell_{g,1}^2 \right] =: \tilde{\sigma}_f^2 = \mathcal{O}(\kappa^2),$$

where κ is the condition number defined below Assumption 2.

A.2 Proof of Lemma 1

Using the Lipschitz property of ∇F in Lemma 4, we have

$$\mathbb{E}[F(x^{k+1})|\mathcal{F}'_{k}] \leq F(x^{k}) + \mathbb{E}[\langle \nabla F(x^{k}), x^{k+1} - x^{k} \rangle |\mathcal{F}'_{k}] + \frac{L_{F}}{2} \mathbb{E}[\|x^{k+1} - x^{k}\|^{2} |\mathcal{F}'_{k}] \\
= F(x^{k}) - \alpha_{k} \langle \nabla F(x^{k}), \bar{h}_{f}^{k} \rangle + \frac{L_{F}\alpha_{k}^{2}}{2} \mathbb{E}[\|h_{f}^{k}\|^{2} |\mathcal{F}'_{k}] \\
\stackrel{(a)}{=} F(x^{k}) - \frac{\alpha_{k}}{2} \|\nabla F(x^{k})\|^{2} - \frac{\alpha_{k}}{2} \|\bar{h}_{f}^{k}\|^{2} + \frac{\alpha_{k}}{2} \|\nabla F(x^{k}) - \bar{h}_{f}^{k}\|^{2} \\
+ \frac{L_{F}\alpha_{k}^{2}}{2} \|\bar{h}_{f}^{k}\|^{2} + \frac{L_{F}\alpha_{k}^{2}}{2} \mathbb{E}[\|h_{f}^{k} - \bar{h}_{f}^{k}\|^{2} |\mathcal{F}'_{k}] \\
\stackrel{(b)}{\leq} F(x^{k}) - \frac{\alpha_{k}}{2} \|\nabla F(x^{k})\|^{2} - \left(\frac{\alpha_{k}}{2} - \frac{L_{F}\alpha_{k}^{2}}{2}\right) \|\bar{h}_{f}^{k}\|^{2} \\
+ \frac{\alpha_{k}}{2} \|\nabla F(x^{k}) - \bar{h}_{f}^{k}\|^{2} + \frac{L_{F}\alpha_{k}^{2}}{2} \tilde{\sigma}_{f}^{2} \tag{37}$$

where (a) uses $2a^{T}b = ||a||^{2} + ||b||^{2} - ||a - b||^{2}$ twice and (b) uses Lemma 5.

We decompose the gradient bias term as follows

$$\|\nabla F(x^{k}) - \bar{h}_{f}^{k}\|^{2} = \|\overline{\nabla}f(x^{k}, y^{*}(x^{k})) - \overline{\nabla}f(x^{k}, y^{k+1}) + \overline{\nabla}f(x^{k}, y^{k+1}) - \bar{h}_{f}^{k}\|^{2}$$

$$\leq 2\|\overline{\nabla}f(x^{k}, y^{*}(x^{k})) - \overline{\nabla}f(x^{k}, y^{k+1})\|^{2} + 2\|\overline{\nabla}f(x^{k}, y^{k+1}) - \bar{h}_{f}^{k}\|^{2}$$

$$\stackrel{(a)}{\leq} 2L_{f}^{2}\|y^{k+1} - y^{*}(x^{k})\|^{2} + 2b_{k}^{2}$$
(38)

where (a) follows from Lemma 4 and Lemma 5. Plugging (38) into (37) completes the proof.

A.3 Proof of Lemma 2

Recalling the definition of $\nabla_x y^*(x)$ in (35), for any x_1, x_2 , we have

$$\begin{split} &\|\nabla_{x}y^{*}(x_{1}) - \nabla_{x}y^{*}(x_{2})\| \\ &= \|\nabla_{xy}^{2}g(x_{1}, y^{*}(x_{1}))[\nabla_{yy}^{2}g(x_{1}, y^{*}(x_{1}))]^{-1} - \nabla_{xy}^{2}g(x_{2}, y^{*}(x_{2}))[\nabla_{yy}^{2}g(x_{2}, y^{*}(x_{2}))]^{-1}\| \\ &\leq \|\nabla_{xy}^{2}g(x_{1}, y^{*}(x_{1})) - \nabla_{xy}^{2}g(x_{2}, y^{*}(x_{2}))\|\|[\nabla_{yy}^{2}g(x_{1}, y^{*}(x_{1}))]^{-1}\| \\ &+ \|\nabla_{xy}^{2}g(x_{2}, y^{*}(x_{2}))\|\|[\nabla_{yy}^{2}g(x_{1}, y^{*}(x_{1}))]^{-1} - [\nabla_{yy}^{2}g(x_{2}, y^{*}(x_{2}))]^{-1}\| \\ &\leq \frac{1}{\mu_{g}}\|\nabla_{xy}^{2}g(x_{1}, y^{*}(x_{1})) - \nabla_{xy}^{2}g(x_{2}, y^{*}(x_{2}))\| \\ &+ \ell_{g,1}\|[\nabla_{yy}^{2}g(x_{1}, y^{*}(x_{1}))]^{-1} \left(\nabla_{yy}^{2}g(x_{1}, y^{*}(x_{1})) - \nabla_{yy}^{2}g(x_{2}, y^{*}(x_{2}))\right)[\nabla_{yy}^{2}g(x_{2}, y^{*}(x_{2}))]^{-1}\| \\ &\leq \frac{1}{\mu_{g}}\|\nabla_{xy}^{2}g(x_{1}, y^{*}(x_{1})) - \nabla_{xy}^{2}g(x_{2}, y^{*}(x_{2}))\| + \frac{\ell_{g,1}}{\mu_{g}^{2}}\|\nabla_{yy}^{2}g(x_{1}, y^{*}(x_{1})) - \nabla_{yy}^{2}g(x_{2}, y^{*}(x_{2}))\| \\ &\leq \frac{1}{\mu_{g}}\|\nabla_{xy}^{2}g(x_{1}, y^{*}(x_{1})) - \nabla_{xy}^{2}g(x_{2}, y^{*}(x_{2}))\| + \frac{\ell_{g,1}}{\mu_{g}^{2}}\|\nabla_{yy}^{2}g(x_{1}, y^{*}(x_{1})) - \nabla_{yy}^{2}g(x_{2}, y^{*}(x_{2}))\| \end{aligned}$$

where both (a) and (b) follow from Assumption 1 and 2.

In addition, we have that

$$\frac{1}{\mu_{g}} \|\nabla_{xy}^{2} g(x_{1}, y^{*}(x_{1})) - \nabla_{xy}^{2} g(x_{2}, y^{*}(x_{2}))\| + \frac{\ell_{g,1}}{\mu_{g}^{2}} \|\nabla_{yy}^{2} g(x_{1}, y^{*}(x_{1})) - \nabla_{yy}^{2} g(x_{2}, y^{*}(x_{2}))\| \\
\leq \frac{\ell_{g,2}}{\mu_{g}} \|x_{1} - x_{2}\| + \frac{\ell_{g,2}}{\mu_{g}} \|y^{*}(x_{1}) - y^{*}(x_{2})\| + \frac{\ell_{g,1}\ell_{g,2}}{\mu_{g}^{2}} \|x_{1} - x_{2}\| + \frac{\ell_{g,1}\ell_{g,2}}{\mu_{g}^{2}} \|y^{*}(x_{1}) - y^{*}(x_{2})\| \\
\leq \left(\frac{\ell_{g,2} + \ell_{g,2}L_{y}}{\mu_{g}} + \frac{\ell_{g,1}(\ell_{g,2} + \ell_{g,2}L_{y})}{\mu_{g}^{2}}\right) \|x_{1} - x_{2}\| \tag{40}$$

where (c) follows from Lemma 4.

Next we derive the bound of h_f^k ,

$$\mathbb{E}[\|h_{f}^{k}\|^{2}|\mathcal{F}_{k}'] = \|\bar{h}_{f}^{k}\|^{2} + \mathbb{E}[\|h_{f}^{k} - \bar{h}_{f}^{k}\|^{2}|\mathcal{F}_{k}'] \\
\stackrel{(d)}{\leq} (\|\bar{\nabla}f(x^{k}, y^{k+1})\| + \|\bar{h}_{f}^{k} - \bar{\nabla}f(x^{k}, y^{k+1})\|)^{2} + \tilde{\sigma}_{f}^{2} \\
\stackrel{(e)}{\leq} \left(\ell_{f,0} + \frac{\ell_{f,0}\ell_{g,1}}{\mu_{g}} + \frac{\ell_{g,1}\ell_{f,1}}{\mu_{g}} \left(1 - \frac{\mu_{g}}{\ell_{g,1}}\right)^{N}\right)^{2} + \tilde{\sigma}_{f}^{2} \\
\stackrel{\leq}{\leq} \left(\ell_{f,0} + \frac{\ell_{f,0}\ell_{g,1}}{\mu_{g}} + \frac{\ell_{g,1}\ell_{f,1}}{\mu_{g}}\right)^{2} + \tilde{\sigma}_{f}^{2} \tag{41}$$

where (d) is from Lemma 5, and (e) is due to

$$\|\overline{\nabla}_{x}f(x,y)\| = \|\nabla_{x}f(x,y) - \nabla_{xy}^{2}g(x,y) \left[\nabla_{yy}^{2}g(x,y)\right]^{-1} \nabla_{y}f(x,y)\|$$

$$\leq \|\nabla_{x}f(x,y)\| + \|\nabla_{xy}^{2}g(x,y)\| \left\| \left[\nabla_{yy}^{2}g(x,y)\right]^{-1} \right\| \|\nabla_{y}f(x,y)\|$$

$$\leq \ell_{f,0} + \ell_{g,1}\frac{1}{\mu_{g}}\ell_{f,0}.$$

As a result, we have

$$L_{yx} := \frac{\ell_{g,2} + \ell_{g,2} L_y}{\mu_g} + \frac{\ell_{g,1}(\ell_{g,2} + \ell_{g,2} L_y)}{\mu_g^2} = \mathcal{O}(\kappa^3)$$
 (42)

$$\tilde{C}_f^2 := \left(l_{f,0} + \frac{\ell_{g,1}}{\mu_g} \ell_{f,1} + \ell_{g,1} \ell_{f,1} \frac{1}{\mu_g}\right)^2 + \tilde{\sigma}_f^2 = \mathcal{O}(\kappa^2) \tag{43}$$

from which the proof is complete.

A.4 Proof of Lemma 3

This part of analysis is very important to obtain our improved results. We start by decomposing the error of the lower level variable as

$$||y^{k+1} - y^*(x^{k+1})||^2 = \underbrace{||y^{k+1} - y^*(x^k)||^2}_{J_1} + \underbrace{||y^*(x^{k+1}) - y^*(x^k)||^2}_{J_2} + 2\underbrace{\langle y^{k+1} - y^*(x^k), y^*(x^k) - y^*(x^{k+1}) \rangle}_{J_2}.$$
(44)

Notice that $y^{k+1} = y^{k,T}$ as defined in (9a). We first analyze

$$\mathbb{E}[\|y^{k,t+1} - y^*(x^k)\|^2 | \mathcal{F}_k^t] \\
= \mathbb{E}[\|y^{k,t} - \beta_k h_g^{k,t} - y^*(x^k)\|^2 | \mathcal{F}_k^t] \\
= \|y^{k,t} - y^*(x^k)\|^2 - 2\beta_k \langle y^{k,t} - y^*(x^k), \mathbb{E}[h_g^{k,t} | \mathcal{F}_k^t] \rangle + \beta_k^2 \mathbb{E}[\|h_g^{k,t}\|^2 | \mathcal{F}_k^t] \\
\leq \|y^{k,t} - y^*(x^k)\|^2 - 2\beta_k \langle y^{k,t} - y^*(x^k), \nabla g(x^k, y^{k,t}) \rangle + \beta_k^2 \|\nabla g(x^k, y^{k,t})\|^2 + \beta_k^2 \sigma_{g,1}^2 \\
\stackrel{(b)}{\leq} \left(1 - \frac{2\mu_g \ell_{g,1}}{\mu_g + \ell_{g,1}} \beta_k\right) \|y^{k,t} - y^*(x^k)\|^2 + \beta_k \left(\beta_k - \frac{2}{\mu_g + \ell_{g,1}}\right) \|\nabla_y g(x^k, y^{k,t})\|^2 + \beta_k^2 \sigma_{g,1}^2 \\
\stackrel{(c)}{\leq} (1 - \rho_g \beta_k) \|y^{k,t} - y^*(x^k)\|^2 + \beta_k^2 \sigma_{g,1}^2$$
(45)

where (a) comes from the fact that $\mathrm{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$, (b) follows from the μ_g -strong convexity and $\ell_{g,1}$ smoothness of g(x,y) [53, Theorem 2.1.11], and (c) follows from the choice of stepsize $\beta_k \leq \frac{2}{\mu_g + \ell_{g,1}}$ in (12) and the definition of $\rho_g := \frac{2\mu_g \ell_{g,1}}{\mu_g + \ell_{g,1}}$.

Taking expectation over \mathcal{F}_k^t on both sides of (45) and using induction, we are able to get

$$\mathbb{E}[J_1] = \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2] \le (1 - \rho_q \beta_k)^T \mathbb{E}[\|y^k - y^*(x^k)\|^2] + T\beta_k^2 \sigma_{q,1}^2. \tag{46}$$

The upper bound of J_2 can be derived as

$$\mathbb{E}[J_{2}] = \mathbb{E}[\|y^{*}(x^{k+1}) - y^{*}(x^{k})\|^{2}] \leq L_{y}^{2}\mathbb{E}[\|x^{k+1} - x^{k}\|^{2}]$$

$$= L_{y}^{2}\alpha_{k}^{2}\mathbb{E}\left[\mathbb{E}[\|h_{f}^{k} - \bar{h}_{f}^{k} + \bar{h}_{f}^{k}\|^{2}|\mathcal{F}_{k}']\right]$$

$$\leq L_{y}^{2}\alpha_{k}^{2}(\mathbb{E}[\|\bar{h}_{f}^{k}\|^{2}] + \tilde{\sigma}_{f}^{2})$$
(47)

where the inequality follows from Lemma 5.

Our analysis of the term J_3 is very different from existing bilevel optimization literature [16, 18, 17, 25, 26]. The term J_3 can be decomposed as

$$\mathbb{E}[J_{3}] = -\mathbb{E}[\langle y^{k+1} - y^{*}(x^{k}), \nabla y^{*}(x^{k})(x^{k+1} - x^{k})\rangle] - \mathbb{E}[\langle y^{k+1} - y^{*}(x^{k}), y^{*}(x^{k+1}) - y^{*}(x^{k}) - \nabla y^{*}(x^{k})(x^{k+1} - x^{k})\rangle].$$

$$(48)$$

Using the alternating update of x and y, e.g., $x^k \to y^{k+1} \to x^{k+1}$, we can bound J_3^1 by

$$-\mathbb{E}[\langle y^{k+1} - y^{*}(x^{k}), \nabla y^{*}(x^{k})(x^{k+1} - x^{k})\rangle] = -\mathbb{E}[\langle y^{k+1} - y^{*}(x^{k}), \mathbb{E}[\nabla y^{*}(x^{k})(x^{k+1} - x^{k}) \mid \mathcal{F}'_{k}]\rangle]$$

$$\stackrel{(d)}{=} -\alpha_{k}\mathbb{E}[\langle y^{k+1} - y^{*}(x^{k}), \nabla y^{*}(x^{k})\bar{h}_{f}^{k}\rangle]$$

$$\leq \alpha_{k}\mathbb{E}[\|y^{k+1} - y^{*}(x^{k})\|\|\nabla y^{*}(x^{k})\bar{h}_{f}^{k}\|]$$

$$\stackrel{(e)}{\leq} \alpha_{k}L_{y}\mathbb{E}[\|y^{k+1} - y^{*}(x^{k})\|\|\bar{h}_{f}^{k}\|]$$

$$\stackrel{(f)}{\leq} 2\gamma_{k}\mathbb{E}[\|y^{k+1} - y^{*}(x^{k})\|^{2}] + \frac{L_{y}^{2}\alpha_{k}^{2}}{8\gamma_{k}}\mathbb{E}[\|\bar{h}_{f}^{k}\|^{2}]$$

$$(49)$$

where (d) uses the fact that $\bar{h}_f^k = \mathbb{E}[h_f^k | \mathcal{F}_k']$; (e) follows from Lemma 4; and (f) uses the Young's inequality such that $ab \leq 2\gamma_k a^2 + \frac{b^2}{8\gamma_k}$.

Next we will use the smoothness of $y^*(x)$ in Lemma 2. We can bound J_3^2 by

$$-\mathbb{E}[\langle y^{k+1} - y^{*}(x^{k}), y^{*}(x^{k+1}) - y^{*}(x^{k}) - \nabla y^{*}(x^{k})(x^{k+1} - x^{k})\rangle]$$

$$\leq \mathbb{E}[\|y^{k+1} - y^{*}(x^{k})\|\|y^{*}(x^{k+1}) - y^{*}(x^{k}) - \nabla y^{*}(x^{k})(x^{k+1} - x^{k})\|]$$

$$\stackrel{(g)}{\leq} \frac{L_{yx}}{2} \mathbb{E}\left[\|y^{k+1} - y^{*}(x^{k})\|\|x^{k+1} - x^{k}\|^{2}\right]$$

$$\stackrel{(h)}{\leq} \frac{\eta L_{yx}}{4} \mathbb{E}\left[\|y^{k+1} - y^{*}(x^{k})\|^{2} \mathbb{E}[\|x^{k+1} - x^{k}\|^{2} | \mathcal{F}'_{k}]\right] + \frac{L_{yx}}{4\eta} \mathbb{E}\left[\mathbb{E}[\|x^{k+1} - x^{k}\|^{2} | \mathcal{F}'_{k}]\right]$$

$$\stackrel{(i)}{\leq} \frac{\eta L_{yx} \tilde{C}_{f}^{2} \alpha_{k}^{2}}{4} \mathbb{E}[\|y^{k+1} - y^{*}(x^{k})\|^{2}] + \frac{L_{yx} \alpha_{k}^{2}}{4\eta} (\mathbb{E}[\|\bar{h}_{f}^{k}\|^{2}] + \tilde{\sigma}_{f}^{2})$$

$$(50)$$

where (g) uses the smoothness of $y^*(x)$; (h) follows from the Young's inequality such that $1 \leq \frac{\eta}{2} + \frac{1}{2\eta}$; and (i) uses the fact that $\mathbb{E}[\|h_f^k\|^2|\mathcal{F}_k'] \leq \tilde{C}_f^2$ in Lemma 2 and the variance bound in Lemma 5.

Plugging (49) and (50) into (48), we have

$$\mathbb{E}[J_3] \le \left(2\gamma_k + \frac{\eta L_{yx}\tilde{C}_f^2}{4}\alpha_k^2\right) \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2] + \left(\frac{L_y^2\alpha_k^2}{8\gamma_k} + \frac{L_{yx}\alpha_k^2}{4\eta}\right) \mathbb{E}[\|\bar{h}_f^k\|^2] + \frac{L_{yx}\alpha_k^2}{4\eta}\tilde{\sigma}_f^2.$$
(51)

Plugging (47), (51) into (44), we get

$$\mathbb{E}[\|y^{k+1} - y^*(x^{k+1})\|^2] \le \left(1 + 4\gamma_k + \frac{\eta L_{yx}\tilde{C}_f^2}{2}\alpha_k^2\right) \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2] \\ + \left(L_y^2\alpha_k^2 + \frac{L_y^2\alpha_k^2}{4\gamma_k} + \frac{L_{yx}\alpha_k^2}{2\eta}\right) \mathbb{E}[\|\bar{h}_f^k\|^2] + \left(L_y^2\alpha_k^2 + \frac{L_{yx}\alpha_k^2}{2\eta}\right)\tilde{\sigma}_f^2$$

from which the proof is complete by choosing $\gamma_k = L_f L_y \alpha_k$.

A.5 Proof of Theorem 1

Using Lemmas 1 and 3, we, respectively, bound the two difference terms in (15) and obtain

$$\begin{split} &\mathbb{E}[\mathbb{V}^{k+1}] - \mathbb{E}[\mathbb{V}^{k}] \\ &\leq -\frac{\alpha_{k}}{2} \mathbb{E}[\|\nabla F(x^{k})\|^{2}] - \left(\frac{\alpha_{k}}{2} - \frac{L_{F}\alpha_{k}^{2}}{2} - \frac{L_{f}}{L_{y}}L_{y}^{2}\alpha_{k}^{2} - \frac{L_{f}}{L_{y}}\frac{\alpha_{k}^{2}L_{y}^{2}}{4\gamma_{k}} - \frac{L_{f}}{L_{y}}\frac{L_{yx}\alpha_{k}^{2}}{2\eta}\right) \mathbb{E}[\|\bar{h}_{f}^{k}\|^{2}] \\ &+ \frac{L_{f}}{L_{y}} \left(1 + 4\gamma_{k} + L_{f}L_{y}\alpha_{k} + \frac{\eta L_{yx}\tilde{C}_{f}^{2}}{2}\alpha_{k}^{2}\right) \mathbb{E}[\|y^{k+1} - y^{*}(x^{k})\|^{2}] - \frac{L_{f}}{L_{y}} \mathbb{E}[\|y^{k} - y^{*}(x^{k})\|^{2}] \\ &+ \alpha_{k}b_{k}^{2} + \left(\frac{L_{F}}{2} + \frac{L_{f}}{L_{y}}L_{y}^{2} + \frac{L_{f}}{L_{y}}\frac{L_{yx}}{2\eta}\right)\alpha_{k}^{2}\tilde{\sigma}_{f}^{2} \\ &\stackrel{(a)}{\leq} - \frac{\alpha_{k}}{2} \mathbb{E}[\|\nabla F(x^{k})\|^{2}] - \left(\frac{\alpha_{k}}{2} - \frac{L_{F}\alpha_{k}^{2}}{2} - L_{f}L_{y}\alpha_{k}^{2} - \frac{L_{f}}{L_{y}}\frac{\alpha_{k}^{2}L_{y}^{2}}{4\gamma_{k}} - \frac{L_{f}}{L_{y}}\frac{L_{yx}\alpha_{k}^{2}}{2\eta}\right) \mathbb{E}[\|\bar{h}_{f}^{k}\|^{2}] \\ &+ \frac{L_{f}}{L_{y}} \left(\left(1 + 4\gamma_{k} + L_{f}L_{y}\alpha_{k} + \frac{\eta L_{yx}\tilde{C}_{f}^{2}}{2}\alpha_{k}^{2}\right)(1 - \rho_{g}\beta_{k})^{T} - 1\right) \mathbb{E}[\|y^{k} - y^{*}(x^{k})\|^{2}] \\ &+ \frac{L_{f}}{L_{y}} \left(1 + 4\gamma_{k} + L_{f}L_{y}\alpha_{k} + \frac{\eta L_{yx}\tilde{C}_{f}^{2}}{2}\alpha_{k}^{2}\right)T\beta_{k}^{2}\sigma_{g,1}^{2} + \alpha_{k}b_{k}^{2} + \left(\frac{L_{F}}{2} + L_{f}L_{y} + \frac{L_{f}}{L_{y}}\frac{L_{yx}}{2\eta}\right)\alpha_{k}^{2}\tilde{\sigma}_{f}^{2} \\ &\qquad \qquad (52) \end{split}$$

where (a) uses (18a) in Lemma 3.

Selecting $\gamma_k = L_f L_u \alpha_k$, we can simplify (52) as

$$\mathbb{E}[\mathbb{V}^{k+1}] - \mathbb{E}[\mathbb{V}^{k}] \leq -\frac{\alpha_{k}}{2} \mathbb{E}[\|\nabla F(x^{k})\|^{2}] - \left(\frac{\alpha_{k}}{2} - \frac{L_{F}\alpha_{k}^{2}}{2} - L_{f}L_{y}\alpha_{k}^{2} - \frac{\alpha_{k}}{4} - \frac{L_{f}}{L_{y}} \frac{L_{yx}\alpha_{k}^{2}}{2\eta}\right) \mathbb{E}[\|\bar{h}_{f}^{k}\|^{2}]
+ \frac{L_{f}}{L_{y}} \left(\left(1 + 2L_{f}L_{y}\alpha_{k} + \frac{\eta L_{yx}\tilde{C}_{f}^{2}}{2}\alpha_{k}^{2}\right)(1 - \rho_{g}\beta_{k})^{T} - 1\right) \mathbb{E}[\|y^{k} - y^{*}(x^{k})\|^{2}]
+ \frac{L_{f}}{L_{y}} \left(1 + 5L_{f}L_{y}\alpha_{k} + \frac{\eta L_{yx}\tilde{C}_{f}^{2}}{4}\alpha_{k}^{2}\right) T\beta_{k}^{2}\sigma_{g,1}^{2}
+ \alpha_{k}b_{k}^{2} + \left(\frac{L_{F}}{2} + L_{f}L_{y} + \frac{L_{yx}L_{f}}{2\eta L_{y}}\right)\alpha_{k}^{2}\tilde{\sigma}_{f}^{2}.$$
(53)

To guarantee the descent of \mathbb{V}^k , the following constraints need to be satisfied

$$\alpha_k \le \frac{1}{2L_F + 4L_f L_y + \frac{2L_f L_{yx}}{L_y \eta}} \tag{54a}$$

$$T\rho_g\beta_k \ge 2L_f L_y \alpha_k + \frac{\eta L_{yx} \tilde{C}_f^2}{2} \alpha_k^2 \tag{54b}$$

$$\beta_k \le \frac{2}{\mu_g + \ell_{g,1}}.\tag{54c}$$

Finally, we define (with $ho_g := rac{2\mu_g\ell_{g,1}}{\mu_g+\ell_{g,1}}$)

$$\bar{\alpha}_1 = \frac{1}{2L_F + 4L_f L_y + \frac{2L_f L_{yx}}{L_y n}}, \quad \bar{\alpha}_2 = \frac{8T\rho_g}{(\mu_g + \ell_{g,1})(8L_f L_y + 2\eta L_{yx}\tilde{C}_f^2\bar{\alpha}_1)}$$
(55)

and, to satisfy the condition (54), we select the following stepsizes as

$$\alpha_k = \min\left\{\bar{\alpha}_1, \bar{\alpha}_2, \frac{\alpha}{\sqrt{K}}\right\}, \qquad \beta_k = \frac{8L_f L_y + 2\eta L_{yx} \tilde{C}_f^2 \bar{\alpha}_1}{4T\rho_a} \alpha_k. \tag{56}$$

With the above choice of stepsizes, (53) can be simplified as

$$\mathbb{E}[\mathbb{V}^{k+1}] - \mathbb{E}[\mathbb{V}^k] \le -\frac{\alpha_k}{2} \mathbb{E}[\|\nabla F(x^k)\|^2] + c_1 \alpha_k^2 \sigma_{g,1}^2 + \alpha_k b_k^2 + c_2 \alpha_k^2 \tilde{\sigma}_f^2$$
 (57)

where the constants c_1 and c_2 are defined as

$$c_{1} = \frac{L_{f}}{L_{y}} \left(1 + 5L_{f}L_{y}\bar{\alpha}_{1} + \frac{\eta L_{yx}\tilde{C}_{f}^{2}}{4}\bar{\alpha}_{1}^{2} \right) \left(\frac{8L_{f}L_{y} + 2\eta L_{yx}\tilde{C}_{f}^{2}\bar{\alpha}_{1}}{4\rho_{g}} \right)^{2} \frac{1}{T}$$

$$c_{2} = \left(\frac{L_{F}}{2} + L_{f}L_{y} + \frac{L_{yx}L_{f}}{2\eta L_{y}} \right). \tag{58}$$

Then telescoping leads to

$$\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla F(x^k)\|^2] \le \frac{\mathbb{V}^0 + \sum_{k=0}^{K-1} \alpha_k b_k^2 + c_1 \alpha_k^2 \sigma_{g,1}^2 + c_2 T \beta_k^2 \tilde{\sigma}_f^2}{\frac{1}{2} \sum_{k=0}^{K-1} \alpha_k} \\
\le \frac{2\mathbb{V}^0}{K \min{\{\bar{\alpha}_1, \bar{\alpha}_2\}}} + \frac{2\mathbb{V}^0}{\alpha \sqrt{K}} + 2b_k^2 + \frac{2c_1 \alpha}{\sqrt{K}} \sigma_{g,1}^2 + \frac{2c_2 \alpha}{\sqrt{K}} \tilde{\sigma}_f^2. \tag{59}$$

To obtain the best κ -dependence, we choose the balancing constant $\eta = \frac{L_f}{L_y} = \mathcal{O}(\kappa)$, and then we can get $\bar{\alpha}_1 = \mathcal{O}(\kappa^{-3})$, $\bar{\alpha}_2 = \mathcal{O}(T\kappa^{-3})$, $c_1 = \mathcal{O}(\kappa^9/T)$, $c_2 = \mathcal{O}(\kappa^3)$. To obtain $b_k^2 = \frac{1}{\sqrt{K}}$, we need $N = \mathcal{O}(\kappa \log K)$. Select $\alpha = \Theta(\kappa^{-5/2})$ and $T = \mathcal{O}(\kappa^4)$, we are able to get

$$\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla F(x^k)\|^2] = \mathcal{O}\left(\frac{\kappa^3}{K} + \frac{\kappa^{5/2}}{\sqrt{K}}\right).$$

To achieve ϵ -optimal solution, we need $K=\mathcal{O}(\kappa^5\epsilon^{-2})$, and the number of evaluations of h_f^k, h_g^k are $\mathcal{O}(\kappa^5\epsilon^{-2}), \mathcal{O}(\kappa^9\epsilon^{-2})$ respectively.

B Proof for stochastic min-max problem

Recall that the lower-level function for the min-max problem is $g(x, y; \phi) = -f(x, y; \xi)$. Then we rewrite the bilevel problem (1) as

$$\min_{x \in \mathbb{R}^d} F(x) := \mathbb{E}_{\xi} \left[f\left(x, y^*(x); \xi \right) \right] \tag{60a}$$

s.t.
$$y^*(x) = \underset{y \in \mathbb{R}^{d'}}{\min} -\mathbb{E}_{\xi}[f(x, y; \xi)].$$
 (60b)

In this case, the bilevel gradient in (6) reduces to

$$\nabla F(x) := \nabla_x f(x, y^*(x)) + \nabla_x y^*(x)^\top \nabla_y f(x, y^*(x)) = \nabla_x f(x, y^*(x)) \tag{61}$$

where the second equality follows from the optimality condition of the lower-level problem, i.e., $\nabla_y f(x, y^*(x)) = 0$. We approximate $\nabla F(x)$ on a vector y in place of $y^*(x)$, denoted as $\overline{\nabla} f(x, y) := \nabla_x f(x, y)$. Therefore, the alternating stochastic gradients for this special case are given by

$$h_g^{k,t} = -\nabla_y f(x^k, y^{k,t}; \xi_1^k) \text{ and } h_f^k = \nabla_x f(x^k, y^{k+1}; \xi_2^k).$$
 (62)

B.1 Verifying lemmas

We make the following assumptions that are counterparts of Assumptions 1–3, most of which are common in the min-max optimization literature [9, 10, 30, 28].

Assumption 4 (Lipschitz continuity). *Assume that* $f(\cdot,y)$ *is Lipschitz over* $x \in \mathbb{R}^d$; *that is, we have* $||f(x_1,y) - f(x_2,y)|| \le \ell_{f,0} ||x_1 - x_2||$. *Assume* $\nabla f, \nabla^2 f$ *are* $\ell_{f,1}, \ell_{f,2}$ -Lipschitz continuous; that is, for $z_1 := [x_1; y_1], \ z_2 := [x_2; y_2]$, we have $||\nabla f(x_1, y_1) - \nabla f(x_2, y_2)|| \le \ell_{f,1} ||z_1 - z_2||$, $||\nabla^2 f(x_1, y_1) - \nabla^2 f(x_2, y_2)|| \le \ell_{f,2} ||z_1 - z_2||$.

Assumption 5 (Strong convexity of f in y). For any fixed x, f(x,y) is μ_f -strongly convex in y.

Assumptions 1 and 2 together ensure that the first- and second-order derivations of f(x,y) as well as the solution mapping $y^*(x)$ are well-behaved. Define the condition number $\kappa := \ell_{f,1}/\mu_f$.

Assumption 6 (Stochastic derivatives). The stochastic gradient $\nabla f(x, y; \xi)$ is an unbiased estimators of $\nabla f(x, y)$; and its variances is bounded by σ_f^2 .

Next we re-derive Lemmas 2, 4 and 5 for this special case.

Lemma 6 (Counterparts of Lemmas 2, 4 and 5). *Under Assumptions 1–3, we have*

(Lemma 2)
$$\|\nabla y^*(x_1) - \nabla y^*(x_2)\| \le L_{yx} \|x_1 - x_2\|, \quad \mathbb{E}[\|h_f^k\|^2 | \mathcal{F}_k'] \le \tilde{C}_f^2$$

(Lemma 4)
$$\|\overline{\nabla}f(x,y^*(x)) - \overline{\nabla}f(x,y)\| \le L_f\|y^*(x) - y\|$$
 $\|\nabla F(x_1) - \nabla F(x_2)\| \le L_f\|x_1 - x_2\|, \|y^*(x_1) - y^*(x_2)\| \le L_y\|x_1 - x_2\|$

$$(\textit{Lemma 5}) \quad \bar{h}_f^k = \overline{\nabla} f(x^k, y^{k+1}), \quad \mathbb{E}[\|h_f^k - \bar{h}_f^k\|^2 | \mathcal{F}_k'] \leq \tilde{\sigma}_f^2$$

where the constants are defined as

$$L_{yx} = \frac{\ell_{f,2} + \ell_{f,2} L_y}{\mu_f} + \frac{\ell_{f,1} (\ell_{f,2} + \ell_{f,2} L_y)}{\mu_f^2} = \mathcal{O}(\kappa^3), \quad \tilde{C}_f^2 = \ell_{l,0}^2 + \sigma_f^2$$

$$L_f = \ell_{f,1} = \mathcal{O}(1), \quad L_F = (\ell_{f,1} + \frac{\ell_{f,1}^2}{\mu_f}) = \mathcal{O}(\kappa), \quad L_y = \frac{\ell_{f,1}}{\mu_f} = \mathcal{O}(\kappa), \quad \tilde{\sigma}_f^2 = \sigma_f^2.$$

Proof: We first calculate L_f by

$$\|\overline{\nabla}f(x,y^{*}(x)) - \overline{\nabla}f(x,y)\| = \|\nabla_{x}f(x,y^{*}(x)) - \nabla_{x}f(x,y)\|$$

$$\leq \ell_{f,1}\|y^{*}(x) - y\| := L_{f}\|y^{*}(x) - y\|.$$
(63)

We then calculate L_F by

$$\|\nabla F(x_{1}) - \nabla F(x_{2})\| = \|\nabla_{x} f(x_{1}, y^{*}(x_{1})) - \nabla_{x} f(x_{2}, y^{*}(x_{2}))\|$$

$$\leq \|\nabla_{x} f(x_{1}, y^{*}(x_{1})) - \nabla_{x} f(x_{2}, y^{*}(x_{1}))\| + \|\nabla_{x} f(x_{2}, y^{*}(x_{1})) - \nabla_{x} f(x_{2}, y^{*}(x_{2}))\|$$

$$\leq \ell_{f,1} \|x_{1} - x_{2}\| + \ell_{f,1} \|y^{*}(x_{1}) - y^{*}(x_{2})\|$$

$$\leq \left(\ell_{f,1} + \frac{\ell_{f,1}^{2}}{\mu_{f}}\right) \|x_{1} - x_{2}\| := L_{F} \|x_{1} - x_{2}\|.$$

$$(64)$$

The calculation of L_y, L_{yx} follows the proof of Lemma 2 and Lemma 4, and $\tilde{\sigma}_f^2, \tilde{C}_f^2, \sigma_g^2$ follows from the fact $h_f^k = \nabla_x f(x^k, y^{k+1}; \xi_2^k), h_g^{k,t} = -\nabla_y f(x^k, y^{k,t}; \xi_2^{k,t})$. Note that different from the bilevel case, the upper-level gradients h_f^k in the min-max case only contain $\nabla_x f$ not $\nabla_y f$, which only needs the lipschitz continuity of x.

B.2 Reduction from Theorem 1 to Proposition 3

In the min-max case, we apply Theorem 1 with $\eta = 1$. We define

$$\bar{\alpha}_1 = \frac{1}{2L_F + 4L_fL_y + \frac{L_fL_{yx}}{L_y}}, \quad \bar{\alpha}_2 = \frac{8T\rho_g}{(\mu_g + \ell_{g,1})(8L_fL_y + L_{yx}\tilde{C}_f^2\bar{\alpha}_1)}$$

and, to satisfy the condition (54), we select

$$\alpha_k = \min\{\bar{\alpha}_1, \bar{\alpha}_2, \frac{\alpha}{\sqrt{K}}\}$$
 and $\beta_k = \frac{8L_f L_y + L_{yx} \tilde{C}_f^2 \bar{\alpha}_1}{4T\rho_q} \alpha_k$.

With the above choice of stepsizes, (59) can be simplified as

$$\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla F(x^k)\|^2] \le \frac{2\mathbb{V}^0}{K \min\{\bar{\alpha}_1, \bar{\alpha}_2\}} + \frac{2\mathbb{V}^0}{\alpha \sqrt{K}} + \frac{2c_1 \alpha}{\sqrt{K}} \sigma_f^2 + \frac{2c_2 \alpha}{\sqrt{K}} \sigma_f^2, \tag{65}$$

where the constants can be defined as

$$c_{1} = \frac{L_{f}}{L_{y}} \left(1 + 2L_{f}L_{y}\alpha_{k} + \frac{L_{yx}\tilde{C}_{f}^{2}}{4}\alpha_{k}^{2} \right) \left(\frac{8L_{f}L_{y} + \eta L_{yx}\tilde{C}_{f}^{2}\bar{\alpha}_{1}}{4\rho_{g}} \right)^{2} \frac{1}{T} = \mathcal{O}(\frac{\kappa^{3}}{T})$$

$$c_{2} = \left(\frac{L_{F}}{2} + L_{f}L_{y} + \frac{L_{yx}L_{f}}{4L_{y}} \right) = \mathcal{O}(\kappa^{2}).$$

Note that $\bar{\alpha}_1 = \mathcal{O}(\kappa^{-2})$, $\bar{\alpha}_2 = \mathcal{O}(T\kappa^{-2})$. Select $\alpha = \Theta(\kappa^{-1})$, $T = \Theta(\kappa)$, then

$$\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla F(x^k)\|^2] = \mathcal{O}\left(\frac{\kappa^2}{K} + \frac{\kappa}{\sqrt{K}}\right). \tag{66}$$

To achieve ϵ -accuracy, we need $K = \mathcal{O}(\kappa^2 \epsilon^{-2})$. And the number of gradient evaluations for h_f^k, h_g^k are $\mathcal{O}(\kappa^2 \epsilon^{-2})$, $\mathcal{O}(\kappa^3 \epsilon^{-2})$ respectively.

C Proof for stochastic compositional problem

Recall that in the stochastic compositional problem, the upper-level function is defined as $f(x,y;\xi) := f(y;\xi)$, and the lower-level function is defined as $g(x,y;\phi) := \frac{1}{2} \|y - h(x;\phi)\|^2$. Then we rewrite the bilevel problem (1) as

$$\min_{x \in \mathbb{R}^d} F(x) := \mathbb{E}_{\xi} \left[f\left(y^*(x); \xi \right) \right]$$
 (67a)

s.t.
$$y^*(x) = \underset{y \in \mathbb{R}^{d'}}{\arg\min} \frac{1}{2} \mathbb{E}_{\phi}[\|y - h(x; \phi)\|^2].$$
 (67b)

In this case, the bilevel gradient in (6) reduces to

$$\nabla F(x) := \nabla_{xy}^{2} g(x, y^{*}(x)) \left[\nabla_{yy}^{2} g(x, y^{*}(x)) \right]^{-1} \nabla_{y} f(x, y^{*}(x))$$
$$= \nabla h(x; \phi)^{\top} \nabla_{y} f(y^{*}(x))$$
(68)

where we use the fact that $\nabla^2_{yy}g(x,y;\phi) = \mathbf{I}_{d'\times d'}$ and $\nabla^2_{xy}g(x,y;\phi) = -\nabla h(x;\phi)^{\top}$.

Similar to Section 2, we again evaluate $\nabla F(x)$ on a certain vector y in place of $y^*(x)$, which is denoted as $\overline{\nabla} f(x,y) = \nabla h(x) \nabla f(y)$. Therefore, the alternating stochastic gradients $h_f^k, h_g^{k,t}$ for this special case are much simpler, given by

$$h_g^{k,t} = y^{k,t} - h(x^k; \phi^{k,t}) \text{ and } h_f^k = \nabla h(x^k; \phi^k) \nabla f(y^{k+1}; \xi^k).$$
 (69)

It can be observed that h_f^k is an unbiased estimate of $\overline{\nabla} f(x^k,y^{k+1})$, that is, $\bar{h}_f^k = \overline{\nabla} f(x,y), b_k = 0$.

C.1 Verifying lemmas

We make the following assumptions that are counterparts of Assumptions 1–3, all of which are common in compositional optimization literature [12, 37, 14, 41, 38].

Assumption 7 (Lipschitz continuity). *Assume that* $f, \nabla f, h, \nabla h$ *are respectively* $\ell_{f,0}, \ell_{f,1}, \ell_{h,0}, \ell_{h,1}$ -Lipschitz continuous; that is, for $z_1 := [x_1; y_1], z_2 := [x_2; y_2],$ we have $||f(x_1, y_1) - f(x_2, y_2)|| \le \ell_{f,0}||z_1 - z_2||, ||\nabla f(x_1, y_1) - \nabla f(x_2, y_2)|| \le \ell_{f,1}||z_1 - z_2||, ||h(x_1) - h(x_2)|| \le \ell_{h,0}||x_1 - x_2||, ||\nabla h(x_1) - \nabla h(x_2)|| \le \ell_{h,1}||x_1 - x_2||.$

Note that the Lipschitz continuity of $\nabla g, \nabla^2 g$ in Assumption 1 can be implied by the Lipschitz continuity of $h, \nabla h$ in the above assumption. Assumption 2 is automatically satisfied for stochastic compositional problems since $\nabla_{yy}g(x,y;\phi)=\mathbf{I}_{d'\times d'}$ and the condition number $\kappa:=1$.

Assumption 8 (Stochastic derivatives). The stochastic quantities $\nabla f(x,y;\xi)$, $h(x;\phi)$, $\nabla h(x;\phi)$ are unbiased estimators of $\nabla f(x,y)$, h(x), $\nabla h(x)$, respectively; and their variances are bounded by $\sigma_f^2, \sigma_{h,0}^2, \sigma_{h,1}^2$, respectively.

The unbiasedness and bounded variance of $\nabla g(x, y; \phi)$, $\nabla^2 g(x, y, \phi)$ in Assumption 3 can be implied by the unbiasedness and bounded variance of $h(x; \phi)$, $\nabla h(x; \phi)$.

Next we re-derive Lemmas 2, 4 and 5 for this special case.

Lemma 7 (Counterparts of Lemmas 2, 4 and 5). *Under Assumptions 1–3, we have*

$$\begin{array}{ll} \textit{(Lemma 2)} & \|\nabla y^*(x_1) - \nabla y^*(x_2)\| \leq L_{yx} \|x_1 - x_2\|, \quad \mathbb{E}[\|h_f^k\|^2 |\mathcal{F}_k'] \leq \tilde{C}_f^2 \\ \textit{(Lemma 4)} & \|\overline{\nabla} f(x,y^*(x)) - \overline{\nabla} f(x,y)\| \leq L_f \|y^*(x) - y\| \\ & \|\nabla F(x_1) - \nabla F(x_2)\| \leq L_F \|x_1 - x_2\|, \quad \|y^*(x_1) - y^*(x_2)\| \leq L_y \|x_1 - x_2\| \\ \textit{(Lemma 5)} & \mathbb{E}[\|h_f^k - \bar{h}_f^k\|^2 |\mathcal{F}_k'| \leq \tilde{\sigma}_f^2, \quad \bar{h}_f^k = \overline{\nabla} f(x^k, y^{k+1}) \\ \end{array}$$

where the constants are defined as

$$L_{f} = \ell_{h,0}\ell_{f,1}, \quad L_{y} = \ell_{h,0}, \quad L_{F} = \ell_{h,0}^{2}\ell_{f,1} + \ell_{f,0}\ell_{h,1}, \quad L_{yx} = \ell_{h,1}$$

$$\tilde{\sigma}_{f}^{2} = \ell_{h,0}^{2}\sigma_{f}^{2} + (\ell_{f,0}^{2} + \sigma_{f}^{2})\sigma_{h,1}^{2}, \quad \tilde{C}_{f}^{2} = (\ell_{f,0}^{2} + \sigma_{f}^{2})(\ell_{h,0}^{2} + \sigma_{h,1}^{2}). \tag{70}$$

Proof: We first calculate L_f by

$$\begin{aligned} \|\overline{\nabla}f(x,y^{*}(x)) - \overline{\nabla}f(x,y)\| &= \|\nabla h(x)\nabla f(y^{*}(x)) - \nabla h(x)\nabla f(y)\| \\ &\leq \|\nabla h(x)\| \|\nabla f(y^{*}(x)) - \nabla f(y)\| \\ &\leq \ell_{h,0}\ell_{f,1} \|y^{*}(x) - y\| := L_{f} \|y^{*}(x) - y\|. \end{aligned}$$

We then calculate L_F by

$$\|\nabla F(x_1) - \nabla F(x_2)\| = \|\nabla h(x_1)\nabla f(h(x_1)) - \nabla h(x_2)\nabla f(h(x_2))\|$$

$$\leq \|\nabla h(x_1)\|\|\nabla f(h(x_1)) - \nabla f(h(x_2))\| + \|\nabla f(h(x_2))\|\|\nabla h(x_1) - \nabla h(x_2)\|$$

$$\leq \ell_{h,0}^2 \ell_{f,1} \|x_1 - x_2\| + \ell_{f,0}\ell_{h,1} \|x_1 - x_2\|$$

$$:= L_F \|x_1 - x_2\|. \tag{71}$$

We then calculate L_y and L_{yx} by

$$||y^*(x_1) - y^*(x_2)|| = ||h(x_1) - h(x_2)|| \le \ell_{h,0} ||x_1 - x_2|| := L_y ||x_1 - x_2||$$

$$||\nabla y^*(x_1) - \nabla y^*(x_2)|| = ||\nabla h(x_1) - \nabla h(x_2)|| \le \ell_{h,1} ||x_1 - x_2|| := L_{yx} ||x_1 - x_2||.$$

We then calculate $\tilde{\sigma}_f^2$ by

$$\mathbb{E}[\|h_{f}^{k} - \bar{h}_{f}^{k}\|^{2} | \mathcal{F}'_{k}] \leq \mathbb{E}[\|\nabla h(x^{k}; \phi_{2}^{k}) \nabla f(y^{k+1}; \xi^{k}) - \nabla h(x^{k}) \nabla f(y^{k+1})\|^{2} | \mathcal{F}'_{k}] \\
\leq \mathbb{E}[\|\nabla f(y^{k+1}; \xi^{k})\|^{2} \|\nabla h(x^{k}; \phi_{2}^{k}) - \nabla h(x^{k})\|^{2} | \mathcal{F}'_{k}] \\
+ \mathbb{E}[\|\nabla h(x^{k})\|^{2} \|\nabla f(y^{k+1}; \xi^{k}) - \nabla f(y^{k+1})\|^{2} | \mathcal{F}'_{k}] \\
\leq (\ell_{f, 0}^{k} + \sigma_{f}^{2}) \sigma_{h, 1}^{2} + \ell_{h, 0}^{2} \sigma_{f}^{2} := \tilde{\sigma}_{f}^{2}. \tag{72}$$

We then calculate \tilde{C}_f^2 by

$$\mathbb{E}[\|h_f^k\|^2 | \mathcal{F}_k'] = \mathbb{E}[\|\nabla h(x^k; \phi_2^k) \nabla f(y^{k+1}; \xi^k)\|^2 | \mathcal{F}_k']$$

$$\leq \mathbb{E}[\|\nabla f(y^{k+1}; \xi^k)\|^2 | \mathcal{F}_k'] \mathbb{E}[\|\nabla h(x^k; \phi_2^k)\|^2 | \mathcal{F}_k']$$

$$\leq (\ell_{f,0}^2 + \sigma_f^2)(\ell_{h,0}^2 + \sigma_{h,1}^2) := \tilde{C}_f^2.$$
(73)

C.2 Reduction from Theorem 1 to Proposition 4

In the compositional case, we apply Theorem 1 by setting $T=1, \alpha=1, \eta=\frac{1}{\ell_{h,1}}$. We define

$$\bar{\alpha}_1 = \frac{1}{6\ell_{h,0}^2\ell_{f,1} + 2\ell_{f,0}\ell_{h,1} + \ell_{f,1}\ell_{h,1}^2}, \quad \bar{\alpha}_2 = \frac{8}{(\mu_g + \ell_{g,1})(8\ell_{f,1}\ell_{h,0}^2 + \tilde{C}_f^2\bar{\alpha}_1)}$$

and, to satisfy the condition (54), we select

$$\alpha_k = \min\left\{\bar{\alpha}_1, \bar{\alpha}_2, \frac{\alpha}{\sqrt{K}}\right\} \quad \text{and} \quad \beta_k = \frac{8\ell_{f,1}\ell_{h,0}^2 + \tilde{C}_f^2\bar{\alpha}_1}{4}\alpha_k. \tag{74}$$

And the constants c_1, c_2 in (58) reduce to

$$c_{1} = \ell_{f,1} \left(1 + 2\ell_{f,1}\ell_{h,0}^{2} \bar{\alpha}_{1} + \frac{\tilde{C}_{f}^{2}}{4} \bar{\alpha}_{1}^{2} \right) \left(\frac{8\ell_{h,0}^{2}\ell_{f,1} + \tilde{C}_{f}^{2} \bar{\alpha}_{1}}{4} \right)^{2}$$

$$c_{2} = \left(\frac{\ell_{h,0}^{2}\ell_{f,1} + \ell_{f,0}\ell_{h,1}}{2} + \ell_{h,0}^{2}\ell_{f,1} + \frac{\ell_{f,1}\ell_{h,1}^{2}}{4} \right). \tag{75}$$

We apply (59) and get

$$\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla F(x^k)\|^2] \le \frac{2\mathbb{V}^0}{K \min\{\bar{\alpha}_1, \bar{\alpha}_2\}} + \frac{2\mathbb{V}^0}{\alpha\sqrt{K}} + \frac{2c_1}{\sqrt{K}}\sigma_{h,1}^2 + \frac{2c_2}{\sqrt{K}}\tilde{\sigma}_f^2 = \mathcal{O}\left(\frac{1}{\sqrt{K}}\right)$$
(76)

from which the proof is complete.

D Proof for actor-critic method

Recall the state feature mapping $\phi(\cdot): \mathcal{S} \to \mathbb{R}^{d'}$. Define

$$A_{\theta,\phi} := \mathbb{E}_{s \sim \mu_{\theta}, s' \sim \mathcal{P}_{\pi_{\theta}}} [\phi(s)(\gamma \phi(s') - \phi(s))^{\top}], \tag{77a}$$

$$b_{\theta,\phi} := \mathbb{E}_{s \sim \mu_{\theta}, a \sim \pi_{\theta}, s' \sim \mathcal{P}}[r(s, a, s')\phi(s)]. \tag{77b}$$

It is known that for a given θ , the stationary point $y^*(\theta)$ of the TD update in (29) satisfies

$$A_{\theta,\phi}y^*(\theta) + b_{\theta,\phi} = 0. \tag{78}$$

Due to the special nature of the policy gradient, we make the following assumptions that will lead to the counterparts of Lemmas 2, 4 and 5 in reinforcement learning. These assumptions are mostly common in analyzing actor-critic method with linear value function approximation [50–52].

Assumption 9. For all $s \in \mathcal{S}$, the feature vector $\phi(s)$ is normalized so that $\|\phi(s)\|_2 \leq 1$. For all eligible θ , $A_{\theta,\phi}$ is negative definite and its maximum eigenvalue is upper bounded by constant $-\lambda$.

Assumption 9 is common in analyzing TD with linear function approximation; see e.g., [54, 55, 50]. With this assumption, $A_{\theta,\phi}$ is invertible, so we have $y^*(\theta) = -A_{\theta,\phi}^{-1}b_{\theta,\phi}$. Defining $R_y := r_{\text{max}}/\lambda$, we have $\|y^*(\theta)\|_2 \le R_y$. It justifies the projection introduced in the critic update (29).

Assumption 10. For any $\theta, \theta' \in \mathbb{R}^d$, $s \in \mathcal{S}$ and $a \in \mathcal{A}$, there exist constants $C_{\psi}, L_{\psi}, L_{\pi}$ such that: i) $\|\psi_{\theta}(s, a)\|_2 \leq C_{\psi}$; ii) $\|\psi_{\theta}(s, a) - \psi_{\theta'}(s, a)\|_2 \leq L_{\psi} \|\theta - \theta'\|_2$; iii) $|\pi_{\theta}(a|s) - \pi_{\theta'}(a|s)| \leq L_{\pi} \|\theta - \theta'\|_2$.

Assumption 10 is common in analyzing policy gradient-type algorithms which has also been made by e.g., [56, 57]. This assumption holds for many policy parameterization methods such as tabular softmax policy [57], Gaussian policy [58] and Boltzmann policy [44].

Assumption 11. For any $\theta, \theta' \in \mathbb{R}^d$, there exist constants such that: i) $\|\nabla \mu_{\theta}(s)\|_{2} \leq C_{\mu}$; ii) $\|\nabla \mu_{\theta}(s) - \nabla \mu_{\theta'}(s)\|_{2} \leq L_{\mu,1} \|\theta - \theta'\|_{2}$; iii) $|\mu_{\theta}(s) - \mu_{\theta'}(s)| \leq L_{\mu,0} \|\theta - \theta'\|_{2}$.

Assumption 11 is the counterpart of Assumption 10 that is made for the stationary distribution $\mu_{\theta}(a|s)$. Note that the existence of $\nabla \mu_{\theta}(s)$ has been shown in [59]. In this case, under Assumption 10, i) and iii) of Assumption 11 can be obtained from the sensitivity analysis of Markov chain; see e.g., [60, Theorem 3.1]. While we cannot provide a justification of (ii), we found it necessary to ensure the smoothness of the lower-level critic solution $y^*(\theta)$.

Assumption 12. For any θ , the Markov chain under π_{θ} and transition kernel $\mathcal{P}(\cdot|s,a)$ is irreducible and aperiodic. Then there exist constants $\kappa > 0$ and $\rho \in (0,1)$ such that

$$\sup_{s \in \mathcal{S}} d_{TV} \left(\mathbb{P}(s_t \in \cdot | s_0 = s, \pi_\theta), \mu_\theta \right) \leq \kappa \rho^t, \quad \forall t$$
 (79)

where μ_{θ} is the stationary state distribution under π_{θ} , and s_t is the state of Markov chain at time t.

Assumption 12 assumes the Markov chain mixes at a geometric rate; see also [54, 55].

We define the critic approximation error as

$$\epsilon_{app} := \max_{\theta \in \mathbb{R}^d} \sqrt{\mathbb{E}_{s \sim \mu_{\theta}} |V_{\pi_{\theta}}(s) - \hat{V}_{y_{\theta}^*}(s)|^2}.$$
(80)

This error captures the quality of the critic function approximation; see also [61, 50, 51]. It becomes zero when the value function $V_{\pi_{\theta}}$ belongs to the linear function space for any θ .

D.1 Auxiliary lemmas

We give a proposition regarding the L_F -Lipschitz of the policy gradient under proper assumptions. **Proposition 6** (Smoothness of policy gradiemt [56]). Suppose Assumption 10 holds. For any $\theta, \theta' \in \mathbb{R}^d$, we have $\|\nabla F(\theta) - \nabla F(\theta')\|_2 \le L_F \|\theta - \theta'\|_2$, where L_F is a positive constant.

We provide a justification for Lipschitz continuity of $y^*(\theta)$ in the next proposition.

Proposition 7 (Lipschitz continuity of $y^*(\theta)$). Suppose Assumption 10 and 12 hold. For any $\theta_1, \theta_2 \in \mathbb{R}^d$, we have $\|y^*(\theta_1) - y^*(\theta_2)\|_2 \le L_y \|\theta_1 - \theta_2\|_2$, where L_y is a positive constant.

Proof. We use y_1^*, y_2^*, A_1 , A_2 , b_1 and b_2 as shorthand notations of $y^*(\theta_1)$, $y^*(\theta_2)$, $A_{\pi_{\theta_1}}$, $A_{\pi_{\theta_2}}$, $b_{\pi_{\theta_1}}$ and $b_{\pi_{\theta_2}}$ respectively. By Assumption 9, $A_{\theta,\phi}$ is invertible for any $\theta \in \mathbb{R}^d$, so we can write $y^*(\theta) = -A_{\theta,\phi}^{-1}b_{\theta,\phi}$. Then we have

$$||y_{1}^{*} - y_{2}^{*}||_{2} = || - A_{1}^{-1}b_{1} + A_{2}^{-1}b_{2}||_{2}$$

$$= || - A_{1}^{-1}b_{1} - A_{1}^{-1}b_{2} + A_{1}^{-1}b_{2} + A_{2}^{-1}b_{2}||_{2}$$

$$= || - A_{1}^{-1}(b_{1} - b_{2}) - (A_{1}^{-1} - A_{2}^{-1})b_{2}||_{2}$$

$$\leq ||A_{1}^{-1}(b_{1} - b_{2})||_{2} + ||(A_{1}^{-1} - A_{2}^{-1})b_{2}||_{2}$$

$$\leq ||A_{1}^{-1}||_{2}||b_{1} - b_{2}||_{2} + ||A_{1}^{-1} - A_{2}^{-1}||_{2}||b_{2}||_{2}$$

$$= ||A_{1}^{-1}||_{2}||b_{1} - b_{2}||_{2} + ||A_{1}^{-1}(A_{2} - A_{1})A_{2}^{-1}||_{2}||b_{2}||_{2}$$

$$\leq ||A_{1}^{-1}||_{2}||b_{1} - b_{2}||_{2} + ||A_{1}^{-1}||_{2}||A_{2}^{-1}||_{2}||b_{2}||_{2}||(A_{2} - A_{1})||_{2}$$

$$\leq \lambda^{-1} ||b_{1} - b_{2}||_{2} + \lambda^{-2}r_{\max} ||A_{1} - A_{2}||_{2},$$
(81)

where the last inequality follows Assumption 9, and the fact that

 $||b_2||_2 = ||\mathbb{E}[r(s, a, s')\phi(s)]||_2 \le \mathbb{E}||r(s, a, s')\phi(s)||_2 \le \mathbb{E}[|r(s, a, s')|||\phi(s)||_2] \le r_{\text{max}}.$ (82) Denote (s^1, a^1, s'^1) and (s^2, a^2, s'^2) as samples drawn with θ_1 and θ_2 respectively, i.e. $s^1 \sim \mu_{\theta_1}$, $a^1 \sim \pi_{\theta_1}$, $s'^1 \sim \mathcal{P}$ and $s^2 \sim \mu_{\theta_2}$, $a^2 \sim \pi_{\theta_2}$, $s'^2 \sim \mathcal{P}$. Then we have

$$||b_{1} - b_{2}||_{2} = ||\mathbb{E}\left[r(s^{1}, a^{1}, s'^{1})\phi(s^{1})\right] - \mathbb{E}\left[r(s^{2}, a^{2}, s'^{2})\phi(s^{2})\right]||_{2}$$

$$\leq \sup_{s, a, s'} ||r(s, a, s')\phi(s)||_{2} ||\mathbb{P}((s^{1}, a^{1}, s'^{1}) \in \cdot) - \mathbb{P}((s^{2}, a^{2}, s'^{2}) \in \cdot)||_{TV}$$

$$\leq r_{\max} ||\mathbb{P}((s^{1}, a^{1}, s'^{1}) \in \cdot) - \mathbb{P}((s^{2}, a^{2}, s'^{2}) \in \cdot)||_{TV}$$

$$= 2r_{\max} d_{TV} \left(\mu_{\theta_{1}} \otimes \pi_{\theta_{1}} \otimes \mathcal{P}, \mu_{\theta_{2}} \otimes \pi_{\theta_{2}} \otimes \mathcal{P}\right)$$

$$\leq 2r_{\max} |\mathcal{A}|L_{\pi} (1 + \log_{\rho} \kappa^{-1} + (1 - \rho)^{-1})||\theta_{1} - \theta_{2}||_{2}, \tag{83}$$

where the first inequality follows the definition of total variation (TV) norm, and the last inequality follows in [50, Lemma A.1]. Similarly we have:

$$||A_{1} - A_{2}||_{2} \leq 2(1 + \gamma)d_{TV} \left(\mu_{\theta_{1}} \otimes \pi_{\theta_{1}}, \mu_{\theta_{2}} \otimes \pi_{\theta_{2}}\right)$$

$$= (1 + \gamma)|\mathcal{A}|L_{\pi}(1 + \log_{\rho} \kappa^{-1} + (1 - \rho)^{-1})||\theta_{1} - \theta_{2}||_{2}$$

$$:= L_{A,0}||\theta_{1} - \theta_{2}||_{2}.$$
(84)

Substituting (83) and (84) into (81) completes the proof.

We prove the Lipschitz continuity of $\nabla_{\theta} y^*(\theta)$ next, for which we will use the following fact.

Fact. If the functions $f(\theta)$, $g(\theta)$ are bounded by C_f and C_g ; and are L_f - and L_g -Lipschitz continuous, then $f(\theta)g(\theta)$ is also bounded by C_fC_g and is $(C_fL_g+C_gL_f)$ -Lipschitz continuous.

Proof. Using the Cauchy-Schwartz inequality, it is easy to see that $f(\theta)$, $g(\theta)$ are bounded by C_fC_g . In addition, we have that

$$\begin{split} \|f(\theta_1)g(\theta_1) - f(\theta_2)g(\theta_2)\| &= \|f(\theta_1)g(\theta_1) - f(\theta_1)g(\theta_2) + f(\theta_1)g(\theta_2) - f(\theta_2)g(\theta_2)\| \\ &\leq \|f(\theta_1)\| \|g(\theta_1) - g(\theta_2)\| + \|f(\theta_1) - f(\theta_2)\| \|g(\theta_2)\| \\ &\leq (C_f L_q + C_q L_f) \|\theta_1 - \theta_2\|_2 \end{split}$$

which implies that $f(\theta)$, $g(\theta)$ is $(C_f L_q + C_q L_f)$ -Lipschitz continuous.

Proposition 8 (Lipschitz continuity of $\nabla_{\theta}y^*(\theta)$). Suppose Assumption 10-12 hold. For any $\theta_1, \theta_2 \in \mathbb{R}^d$, we have $\|\nabla_{\theta}y^*(\theta_1) - \nabla_{\theta}y^*(\theta_2)\|_2 \le L_{yx}\|\theta_1 - \theta_2\|_2$, where L_{yx} is a positive constant.

Proof. With $y^*(\theta) = -A_{\theta,\phi}^{-1}b_{\theta,\phi}$, we have

$$\nabla_{\theta} y^*(\theta) = -\nabla_{\theta} (A_{\theta,\phi}^{-1} b_{\theta,\phi}) = -A_{\theta,\phi}^{-1} (\nabla_{\theta} A_{\theta,\phi}) A_{\theta,\phi}^{-1} b_{\theta,\phi} - A_{\theta,\phi} (\nabla_{\theta} b_{\theta,\phi}). \tag{85}$$

To validate the Lipschitz continuity of $\nabla_{\theta} y^*(\theta)$, we need to show the boundedness and Lipschitz continuity of $A_{\theta,\phi}^{-1}$, $b_{\theta,\phi}$, $\nabla_{\theta} A_{\theta,\phi}$ and $\nabla_{\theta} b_{\theta,\phi}$.

From (83) and (84), we have that there exist constants $L_{A,0}$ and $L_{b,0}$ such that $A_{\theta,\phi}$ is $L_{A,0}$ -Lipschitz continuous, and $b_{\theta,\phi}$ is $L_{b,0}$ -Lipschitz continuous. From Assumption 9 and (82), we have that there exist constants $C_{A,0}$ and $C_{b,0}$ such that $||A_{\theta,\phi}||_2 \leq C_{A,0}$, and $||b_{\theta,\phi}||_2 \leq C_{b,0}$.

In addition, using A_1 and A_2 as shorthand notations of $A_{\pi_{\theta_1}}$ and $A_{\pi_{\theta_2}}$, respectively, we have

$$||A_{1}^{-1} - A_{2}^{-1}||_{2} = ||A_{1}^{-1}(A_{2} - A_{1})A_{2}^{-1}||_{2}$$

$$\leq ||A_{1}^{-1}||_{2}||A_{2}^{-1}||_{2}||(A_{2} - A_{1})||_{2}$$

$$\leq \lambda^{-2} ||A_{1} - A_{2}||_{2}$$

$$\stackrel{(84)}{\leq} \lambda^{-2} L_{A,0} ||\theta_{1} - \theta_{2}||_{2}.$$
(86)

Therefore, $A_{\theta,\phi}^{-1}$ is $\lambda^{-2}L_{A,0}$ -Lipschitz continuous, and is bounded by λ^{-1} due to Assumption 9.

For simplicity, denote

$$A(s,s') := \phi(s)(\gamma\phi(s') - \phi(s))^{\top}, \quad b(s,a,s') := r(s,a,s')\phi(s)$$
(87)

and then $b_{\theta,\phi} \coloneqq \mathbb{E}_{s \sim \mu_{\theta}, a \sim \pi_{\theta}, s' \sim \mathcal{P}}[b(s, a, s')]$ and $A_{\theta,\phi} \coloneqq \mathbb{E}_{s \sim \mu_{\theta}, s' \sim \mathcal{P}_{\pi_{\theta}}}[A(s, s')]$.

Next we analyze $\nabla_{\theta} A_{\theta,\phi}$ and $\nabla_{\theta} b_{\theta,\phi}$, which is given by

$$\nabla_{\theta} A_{\theta,\phi} = \nabla_{\theta} \left(\sum_{s,a,s'} \mu_{\theta}(s) \pi_{\theta}(a|s) P(s'|s,a) A(s,s') \right)$$

$$= \sum_{s,a,s'} \left[\nabla_{\theta} \mu_{\theta}(s) \pi_{\theta}(a|s) P(s'|s,a) A(s,s') + \mu_{\theta}(s) \nabla_{\theta} \pi_{\theta}(a|s) P(s'|s,a) A(s,s') \right]. \tag{88}$$

From Assumption 10 and 11, $\mu_{\theta}(s)$, $\pi_{\theta}(a|s)$, $\nabla_{\theta}\mu_{\theta}(s)$, $\nabla_{\theta}\pi_{\theta}(a|s)$ are Lipschitz continuous and bounded. Using the **Fact**, we can show that there exist constants $C_{A,1}$ and $L_{A,1}$ such that $\nabla_{\theta}A_{\theta,\phi}$ is $L_{A,1}$ -Lipschitz continuous and bounded by $C_{A,1}$.

Likewise, we have

$$\nabla_{\theta} b_{\theta,\phi} = \nabla_{\theta} \left(\sum_{s,a,s'} \mu_{\theta}(s) \pi_{\theta}(a|s) P(s'|s,a) b(s,a,s') \right)$$

$$= \sum_{s,a,s'} \left[\nabla_{\theta} \mu_{\theta}(s) \pi_{\theta}(a|s) P(s'|s,a) b(s,a,s') + \mu_{\theta}(s) \nabla_{\theta} \pi_{\theta}(a|s) P(s'|s,a) b(s,a,s') \right].$$
(89)

From Assumption 10 and 11, $\mu_{\theta}(s)$, $\pi_{\theta}(a|s)$, $\nabla_{\theta}\mu_{\theta}(s)$, $\nabla_{\theta}\pi_{\theta}(a|s)$ are Lipschitz continuous and bounded. Using the **Fact**, we are able to show that there exist constants $C_{b,1}$ and $L_{b,1}$ such that $\nabla_{\theta}b_{\theta,\phi}$ is $L_{b,1}$ -Lipschitz continuous and bounded by $C_{b,1}$.

Therefore, since $A_{\theta,\phi}^{-1}$, $b_{\theta,\phi}$, $\nabla_{\theta}A_{\theta,\phi}$ and $\nabla_{\theta}b_{\theta,\phi}$ are all Lipschitz continuous, using **Fact**, we can show that $\nabla_{\theta}y^*(\theta)$ in (85) is L_{yx} -Lipschitz continuous, where L_{yx} depends on the constants $C_{\mu}, C_{\psi}, L_{\pi}, L_{\mu,0}, L_{\mu,1}, \lambda$ defined in Assumptions 10-12.

D.2 Convergence of critic variables

For brevity, we first define the following notations (cf. $\xi := (s, a, s')$):

$$\hat{\delta}(\xi, y) := r(s, a, s') + \gamma \phi(s')^{\top} y - \phi(s)^{\top} y,$$

$$h_g(\xi, y) := \hat{\delta}(\xi, y) \phi(s),$$

$$\overline{h}_g(\theta, y) := \mathbb{E}_{s \sim \mu_{\theta}, a \sim \pi_{\theta}, s' \sim \mathcal{P}} [h_g(\xi, y)].$$

We also define constant $C_{\delta} := r_{\max} + (1 + \gamma) \max\{R_{\max}, R_u\}$, and we immediately have

$$||h_g(\xi, y)||_2 \le |r(\xi) + \gamma \phi(s')^\top y - \phi(s)^\top y| \le r_{\text{max}} + (1 + \gamma)R_y \le C_g$$
 (90)

and likewise, we have $\|\overline{h}_g(\xi, y)\|_2 \leq C_g$.

The critic update can be written compactly as:

$$y_{k+1} = \Pi_{R_n} (y_k + \beta_k g(\xi_k, y_k)), \qquad (91)$$

where $\xi_k := (s_k, a_k, s_k')$ is the sample used to evaluate the stochastic gradient at kth update.

Proof. Using $y^*(\theta_k)$ as shorthand notation of $y^*_{\theta_k}$, we start with the optimality gap

$$||y_{k+1} - y^*(\theta_{k+1})||_2^2$$

$$= ||y_{k+1} - y^*(\theta_k) + y^*(\theta_k) - y^*(\theta_{k+1})||_2^2$$

$$= ||y_{k+1} - y^*(\theta_k)||_2^2 + ||y^*(\theta_k) - y^*(\theta_{k+1})||_2^2 + 2\langle y_{k+1} - y^*(\theta_k), y^*(\theta_k) - y^*(\theta_{k+1})\rangle.$$
(92)

We first bound

$$||y_{k+1} - y^*(\theta_k)||_2^2 = ||\Pi_{R_y} (y_k + \beta_k g(\xi_k, y_k)) - y^*(\theta_k)||_2^2$$

$$\leq ||y_k + \beta_k g(\xi_k, y_k) - y^*(\theta_k)||_2^2$$

$$= ||y_k - y^*(\theta_k)||_2^2 + 2\beta_k \langle y_k - y^*(\theta_k), g(\xi_k, y_k) \rangle + ||\beta_k g(\xi_k, y_k)||_2^2.$$
(93)

We first bound $\mathbb{E}[\langle y_k - y^*(\theta_k), g(\theta_k, y_k) \rangle | y_k]$ in (92) as

$$\mathbb{E}[\langle y_k - y^*(\theta_k), g(\theta_k, y_k) \rangle | y_k] = \langle y_k - y^*(\theta_k), \overline{h}_g(\theta_k, y_k) - \overline{h}_g(\theta_k, y^*(\theta_k)) \rangle$$

$$= \langle y_k - y^*(\theta_k), \mathbb{E}\left[(\gamma \phi(s') - \phi(s))^\top (y_k - y^*(\theta_k)) \phi(s) \right] \rangle$$

$$= \langle y_k - y^*(\theta_k), \mathbb{E}\left[\phi(s) (\gamma \phi(s') - \phi(s))^\top \right] (y_k - y^*(\theta_k)) \rangle$$

$$= \langle y_k - y^*(\theta_k), A_{\pi_{\theta_k}}(y_k - y^*(\theta_k)) \rangle$$

$$\leq -\lambda \|y_k - y^*(\theta_k)\|_{2}^{2}, \tag{94}$$

where the first equality is due to $\overline{h}_g(\theta, y_{\theta}^*) = A_{\theta,\phi} y^*(\theta) + b = 0$, and the last inequality follows Assumption 9.

Substituting (94) into (93), then taking expectation on both sides of (93) yields

$$\mathbb{E}\|y_{k+1} - y^*(\theta_k)\|_2^2 \le (1 - 2\lambda\beta_k)\mathbb{E}\|y_k - y^*(\theta_k)\|_2^2 + C_a^2\beta_k^2 \tag{95}$$

and plugging into into (92) yields

$$\mathbb{E}\|y_{k+1} - y^*(\theta_{k+1})\|_2^2 \le (1 - 2\lambda\beta_k)\mathbb{E}\|y_k - y^*(\theta_k)\|_2^2 + 2\mathbb{E}\langle y_{k+1} - y^*(\theta_k), y^*(\theta_k) - y^*(\theta_{k+1})\rangle + \mathbb{E}\|y^*(\theta_k) - y^*(\theta_{k+1})\|_2^2 + C_g^2\beta_k^2.$$
(96)

Next we bound the third and fourth terms in (96) as

$$\mathbb{E}\left\langle y_{k+1} - y^{*}(\theta_{k}), y^{*}(\theta_{k}) - y^{*}(\theta_{k+1})\right\rangle \\
= \mathbb{E}\left\langle y_{k+1} - y^{*}(\theta_{k}), y^{*}(\theta_{k}) - y^{*}(\theta_{k+1}) - (\nabla y^{*}(\theta_{k}))^{\top}(\theta_{k+1} - \theta_{k})\right\rangle \\
+ \mathbb{E}\left\langle y_{k+1} - y^{*}(\theta_{k}), (\nabla y^{*}(\theta_{k}))^{\top}(\theta_{k+1} - \theta_{k})\right\rangle \\
\stackrel{(a)}{\leq} \frac{L_{y,2}^{2}}{2} \mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|_{2}\|\theta_{k+1} - \theta_{k}\|_{2}^{2} + \mathbb{E}\left[\left\langle y_{k+1} - y^{*}(\theta_{k}), \mathbb{E}\left[(\nabla y^{*}(\theta_{k}))^{\top}(\theta_{k+1} - \theta_{k}) \mid y_{k+1}\right]\right\rangle\right] \\
\stackrel{(b)}{\leq} \frac{L_{y,2}^{2}}{2} \mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|_{2}\|\theta_{k+1} - \theta_{k}\|_{2}^{2} + \alpha_{k}L_{y}\mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|\|\bar{h}_{f}(\theta_{k}, y_{k+1})\| \\
\stackrel{(c)}{\leq} \frac{L_{y,2}^{2}}{4} \mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|_{2}^{2}\|\theta_{k+1} - \theta_{k}\|_{2}^{2} + \frac{L_{y,2}^{2}}{4} \mathbb{E}\|\theta_{k+1} - \theta_{k}\|_{2}^{2} + \alpha_{k}L_{y}\mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|\|\bar{h}_{f}(\theta_{k}, y_{k+1})\| \\
\stackrel{(d)}{\leq} \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{2} \mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|_{2} + \frac{L_{y,2}^{2}}{4} \mathbb{E}\|\theta_{k+1} - \theta_{k}\|_{2}^{2} + \alpha_{k}L_{y}\mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|_{2}^{2} + \frac{\alpha_{k}}{4} \mathbb{E}\|\bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} \\
\stackrel{(d)}{\leq} \left(\alpha_{k}L_{y,2}^{2} + \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{4}\right) \mathbb{E}\|y_{k+1} - y^{*}(\theta_{k})\|_{2}^{2} + \frac{\alpha_{k}}{4} \mathbb{E}\|\bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} + \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{4}$$

$$(97)$$

where (a) follows from the $L_{y,2}$ -smoothness of y^* with respect to θ ; (b) follows from L_y is the Lipschitz constant of y^* in Proposition 7 and

$$\mathbb{E}[(\nabla y^*(\theta_k))^{\top}(\theta_{k+1} - \theta_k) \mid y_{k+1}] = \nabla y^*(\theta_k))^{\top} \bar{h}_f(\theta_k, y_{k+1});$$

(c) uses the Young's inequality; (d) uses the Young's inequality and the fact that $\|\theta_{k+1} - \theta_k\|_2 = \alpha_k \|h_f(\xi_k', \theta_k, y_{k+1})\| \le C_g C_\psi = C_f$ and $\|\bar{h}_f(\theta_k, y_{k+1})\| \le C_f$.

We bound

$$\mathbb{E} \|y^*(\theta_k) - y^*(\theta_{k+1})\|_2^2 \le L_y^2 \mathbb{E} \|\theta_k - \theta_{k+1}\|_2^2$$

$$\le L_y^2 \alpha_k^2 \mathbb{E} \|\hat{\delta}(\xi_k, y_k) \psi_{\theta_k}(s_k, a_k)\|_2^2 \le L_y^2 C_f^2 \alpha_k^2 \tag{98}$$

where the inequality is due to the L_y -Lipschitz of $y^*(\theta)$ shown in Proposition 7, and the last inequality follows the fact that

$$\|\hat{\delta}(\xi_k, y_k)\psi_{\theta_k}(s_k, a_k)\|_2 \le C_g C_{\psi} = C_f.$$
 (99)

Substituting (97)-(98) into (92) yields

$$\mathbb{E}\|y_{k+1} - y^*(\theta_{k+1})\|_2^2 \le \left(1 + \alpha_k L_{y,2}^2 + \frac{\alpha_k^2 C_f^2 L_{y,2}^2}{4}\right) \mathbb{E}\left[\|y_{k+1} - y^*(\theta_k)\|_2^2\right] + \frac{\alpha_k}{4} \mathbb{E}\left\|\bar{h}_f(\theta_k, y_{k+1})\right\|^2 + \frac{\alpha_k^2 C_f^2 L_{y,2}^2}{4} + L_y^2 C_f^2 \alpha_k^2.$$
 (100)

D.3 Proof of Theorem 2

Recall the notations:

$$\hat{\delta}(\xi, y) \coloneqq r(s, a, s') + \gamma \phi(s')^{\top} y - \phi(s)^{\top} y,$$

$$\bar{\delta}(\xi, y) \coloneqq \mathbb{E}_{s \sim d_{\theta}, a \sim \pi_{\theta}, s' \sim \mathcal{P}} \left[r(s, a, s') + \gamma \phi(s')^{\top} y - \phi(s)^{\top} y \mid y \right]$$

$$\delta(\xi, \theta) \coloneqq r(s, a, s') + \gamma V_{\pi_{\theta}}(s') - V_{\pi_{\theta}}(s).$$

The actor update can be written compactly as:

$$\theta_{k+1} = \theta_k + \alpha_k h_f(\xi_k', \theta_k, y_{k+1}) \tag{101}$$

where $h_f(\xi_k', \theta_k, y_{k+1}) := \hat{\delta}(\xi_k', y_{k+1}) \psi_{\theta_k}(s_k, a_k)$. Define $\bar{h}_f(\theta_k, y_{k+1}) := \mathbb{E}[\hat{\delta}(\xi_k', y_{k+1}) \psi_{\theta_k}(s_k, a_k) | y_{k+1}]$. Then we are ready to give the convergence proof.

Proof. From L_F -Lipschitz of policy gradient in Proposition 6, taking expectation conditioned on θ_k, y_{k+1} , we have:

$$\begin{split} & \mathbb{E}[F(\theta_{k+1})] - F(\theta_{k}) \\ & \geq \mathbb{E} \left\langle \nabla F(\theta_{k}), \theta_{k+1} - \theta_{k} \right\rangle - \frac{L_{F}}{2} \mathbb{E} \|\theta_{k+1} - \theta_{k}\|_{2}^{2} \\ & \geq \alpha_{k} \mathbb{E} \left\langle \nabla F(\theta_{k}), \bar{h}_{f}(\theta_{k}, y_{k+1}) \right\rangle - \frac{L_{F}}{2} \mathbb{E} \|\theta_{k+1} - \theta_{k}\|_{2}^{2} \\ & = \frac{\alpha_{k}}{2} \mathbb{E} \left\| \nabla F(\theta_{k}) \right\|^{2} + \frac{\alpha_{k}}{2} \mathbb{E} \left\| \bar{h}_{f}(\theta_{k}, y_{k+1}) \right\|^{2} - \frac{\alpha_{k}}{2} \mathbb{E} \left\| \nabla F(\theta_{k}) - \bar{h}_{f}(\theta_{k}, y_{k+1}) \right\|^{2} - \frac{L_{F}}{2} \mathbb{E} \|\theta_{k+1} - \theta_{k}\|_{2}^{2} \\ & \geq \frac{\alpha_{k}}{2} \mathbb{E} \left\| \nabla F(\theta_{k}) \right\|^{2} + \frac{\alpha_{k}}{2} \mathbb{E} \left\| \bar{h}_{f}(\theta_{k}, y_{k+1}) \right\|^{2} - \frac{\alpha_{k}}{2} \mathbb{E} \left\| \nabla F(\theta_{k}) - \bar{h}_{f}(\theta_{k}, y_{k+1}) \right\|^{2} \\ & - \frac{L_{F} \alpha_{k}^{2}}{2} \mathbb{E} \|\bar{h}_{f}(\theta_{k}, y_{k+1}) \|_{2}^{2} - \frac{L_{F} \alpha_{k}^{2}}{2} \mathbb{E} \|\bar{h}_{f}(\theta_{k}, y_{k+1}) - h_{f}(\xi_{k}', \theta_{k}, y_{k+1}) \|_{2}^{2} \\ & \geq \frac{\alpha_{k}}{2} \mathbb{E} \left\| \nabla F(\theta_{k}) \right\|^{2} + \left(\frac{\alpha_{k}}{2} - \frac{L_{F} \alpha_{k}^{2}}{2} \right) \mathbb{E} \left\| \bar{h}_{f}(\theta_{k}, y_{k+1}) \right\|^{2} - \frac{\alpha_{k}}{2} \mathbb{E} \left\| \nabla F(\theta_{k}) - \bar{h}_{f}(\theta_{k}, y_{k+1}) \right\|^{2} - \frac{L_{F} C_{f}^{2} \alpha_{k}^{2}}{2} \end{split}$$

where the last inequality follows the definition of C_f in (99).

We next bound the gradient bias as

$$\|\nabla F(\theta_{k}) - \bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} = \|\nabla F(\theta_{k}) - \mathbb{E}[\hat{\delta}(\xi'_{k}, y_{k+1})\psi_{\theta_{k}}(s_{k}, a_{k})|y_{k+1}]\|^{2}$$

$$\leq 2 \|\nabla F(\theta_{k}) - \mathbb{E}[\hat{\delta}(\xi'_{k}, y^{*}(\theta_{k}))\psi_{\theta_{k}}(s_{k}, a_{k})|y_{k+1}]\|^{2}$$

$$+ 2 \|\mathbb{E}[(\hat{\delta}(\xi'_{k}, y^{*}(\theta_{k})) - \hat{\delta}(\xi'_{k}, y_{k+1}))\psi_{\theta_{k}}(s_{k}, a_{k})|y_{k+1}]\|^{2}$$

$$\leq 4 \|\nabla F(\theta_{k}) - \mathbb{E}[\delta(\xi'_{k}, \theta_{k})\psi_{\theta_{k}}(s_{k}, a_{k})|y_{k+1}]\|^{2}$$

$$+ 4 \|\mathbb{E}[\delta(\xi'_{k}, \theta_{k})\psi_{\theta_{k}}(s_{k}, a_{k})|y_{k+1}] - \mathbb{E}[\hat{\delta}(\xi'_{k}, y^{*}(\theta_{k}))\psi_{\theta_{k}}(s_{k}, a_{k})|y_{k+1}]\|^{2}$$

$$+ 2 \|\mathbb{E}[(\hat{\delta}(\xi'_{k}, y^{*}(\theta_{k})) - \hat{\delta}(\xi'_{k}, y_{k+1}))\psi_{\theta_{k}}(s_{k}, a_{k})|y_{k+1}]\|^{2}. (103)$$

Then we bound I_1 as

$$I_{1} = \|\nabla F(\theta_{k}) - \mathbb{E}[\delta(\xi'_{k}, \theta_{k})\psi_{\theta_{k}}(s_{k}, a_{k})|\theta_{k}, y_{k+1}]\|^{2}$$

$$= \left\|\nabla F(\theta_{k}) - \mathbb{E}_{\substack{s_{k} \sim d_{\theta_{k}} \\ a_{k} \sim \pi_{\theta_{k}}, s'_{k} \sim \mathcal{P}}} \left[\left(r(s_{k}, a_{k}, s'_{k}) + \gamma V_{\pi_{\theta_{k}}}(s'_{k}) - V_{\pi_{\theta_{k}}}(s_{k}) \right) \psi_{\theta_{k}}(s_{k}, a_{k}) \middle| \theta_{k}, y_{k+1} \right] \right\|^{2}$$

$$= \left\|\nabla F(\theta_{k}) - \mathbb{E}_{\substack{s_{k} \sim d_{\theta_{k}} \\ a_{k} \sim \pi_{\theta_{k}}}} \left[A_{\pi_{\theta_{k}}}(s_{k}, a_{k}) \psi_{\theta_{k}}(s_{k}, a_{k}) \middle| \theta_{k}, y_{k+1} \right] \right\|^{2} = 0$$

where the last equality follows from the policy gradient theorem.

Then we bound I_2 as

$$\begin{split} I_2 &= \left\| \mathbb{E}[\delta(\xi_k', \theta_k) \psi_{\theta_k}(s_k, a_k) | \theta_k, y_{k+1}] - \mathbb{E}[\hat{\delta}(\xi_k', y^*(\theta_k)) \psi_{\theta_k}(s_k, a_k) | \theta_k, y_{k+1}] \right\|^2 \\ &= \left\| \mathbb{E}\left[\left(\delta(\xi_k', \theta_k) - \hat{\delta}(\xi_k', y^*(\theta_k)) \right) \psi_{\theta_k}(s_k, a_k) | \theta_k, y_{k+1} \right] \right\|^2 \\ &= \left\| \mathbb{E}\left[\left| \delta(\xi_k', \theta_k) - \hat{\delta}(\xi_k', y^*(\theta_k)) \right| \|\psi_{\theta_k}(s_k, a_k) \| | \theta_k, y_{k+1} \right] \right\|^2 \\ &= C_{\psi}^2 \left\| \mathbb{E}\left[\left| \delta(\xi_k', \theta_k) - \hat{\delta}(\xi_k', y^*(\theta_k)) \right| | \theta_k, y_{k+1} \right] \right\|^2 \\ &\leq C_{\psi}^2 \left(\gamma \mathbb{E}\left| \phi(s_k')^\top y^*(\theta_k) - V_{\pi_{\theta_k}}(s_k') \right| + \mathbb{E}\left| V_{\pi_{\theta_k}}(s_k) - \phi(s_k)^\top y^*(\theta_k) \right| \right) \\ &\leq C_{\psi}^2 \left(\gamma \sqrt{\mathbb{E}\left| \phi(s_k')^\top y^*(\theta_k) - V_{\pi_{\theta_k}}(s_k') \right|^2} + \sqrt{\mathbb{E}\left| V_{\pi_{\theta_k}}(s_k) - \phi(s_k)^\top y^*(\theta_k) \right|^2} \right) \\ &\leq C_{\psi}^2 (1 + \gamma) \epsilon_{app}. \end{split}$$

Then we bound I_3 as

$$I_{3} = \left\| \mathbb{E}[(\hat{\delta}(\xi'_{k}, y^{*}(\theta_{k})) - \hat{\delta}(\xi'_{k}, y_{k+1}))\psi_{\theta_{k}}(s_{k}, a_{k})|\theta_{k}, y_{k+1}] \right\|^{2}$$

$$\leq C_{\psi}^{2} \mathbb{E}\left[\|\hat{\delta}(\xi'_{k}, y^{*}(\theta_{k})) - \hat{\delta}(\xi'_{k}, y_{k+1})\|^{2}|\theta_{k}, y_{k+1}] \right]$$

$$= C_{\psi}^{2} \mathbb{E}\left[\|\gamma\phi(s'_{k})^{\top}y^{*}(\theta_{k}) - \phi(s_{k})^{\top}y^{*}(\theta_{k}) - \gamma\phi(s'_{k})^{\top}y_{k+1} + \phi(s_{k})^{\top}y_{k+1}\|^{2}|\theta_{k}, y_{k+1}] \right]$$

$$\leq C_{\psi}^{2} (1 + \gamma) \|y^{*}(\theta_{k}) - y_{k+1}\|^{2}.$$

Then (103) can be rewritten as

$$\left\|\nabla F(\theta_k) - \bar{h}_f(\theta_k, y_{k+1})\right\|^2 \le 4C_{\psi}^2 (1+\gamma)\epsilon_{app} + 2C_{\psi}^2 (1+\gamma)\|y^*(\theta_k) - y_{k+1}\|^2$$

plugging which into (102) leads to

$$\mathbb{E}[F(\theta_{k+1})] \geq F(\theta_{k}) + \frac{\alpha_{k}}{2} \mathbb{E} \|\nabla F(\theta_{k})\|^{2} + \left(\frac{\alpha_{k}}{2} - \frac{L_{F}\alpha_{k}^{2}}{2}\right) \mathbb{E} \|\bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} - \frac{\alpha_{k}}{2} \mathbb{E} \|\nabla F(\theta_{k}) - \bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} - \frac{L_{F}C_{f}^{2}\alpha_{k}^{2}}{2}$$

$$\geq F(\theta_{k}) + \frac{\alpha_{k}}{2} \mathbb{E} \|\nabla F(\theta_{k})\|^{2} + \left(\frac{\alpha_{k}}{2} - \frac{L_{F}\alpha_{k}^{2}}{2}\right) \mathbb{E} \|\bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} - \frac{L_{F}C_{f}^{2}\alpha_{k}^{2}}{2} - 2\alpha_{k}C_{\psi}^{2}(1 + \gamma)\epsilon_{app} - \alpha_{k}C_{\psi}^{2}(1 + \gamma)\|y^{*}(\theta_{k}) - y_{k+1}\|^{2}.$$

$$(104)$$

Consider the difference of the Lyapunov function $\mathbb{V}^k := -F(\theta_k) + \|y_k - y^*(\theta_k)\|_2^2$, given by

$$\mathbb{E}[\mathbb{V}^{k+1}] - \mathbb{E}[\mathbb{V}^{k}] = -\mathbb{E}[F(\theta_{k+1})] + \mathbb{E}\|y_{k+1} - y^{*}(\theta_{k+1})\|_{2}^{2} + \mathbb{E}[F(\theta_{k})] - \mathbb{E}\|y_{k} - y^{*}(\theta_{k})\|_{2}^{2} \\
\leq -\frac{\alpha_{k}}{2}\mathbb{E}\|\nabla F(\theta_{k})\|^{2} - \left(\frac{\alpha_{k}}{2} - \frac{L_{F}\alpha_{k}^{2}}{2}\right)\mathbb{E}\|\bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} + \frac{L_{F}C_{f}^{2}\alpha_{k}^{2}}{2} + 2\alpha_{k}C_{\psi}^{2}(1+\gamma)\epsilon_{app} \\
+ \alpha_{k}C_{\psi}^{2}(1+\gamma)\|y^{*}(\theta_{k}) - y_{k+1}\|^{2} + \mathbb{E}\|y_{k+1} - y^{*}(\theta_{k+1})\|_{2}^{2} - \mathbb{E}\|y_{k} - y^{*}(\theta_{k})\|_{2}^{2} \\
\leq -\frac{\alpha_{k}}{2}\mathbb{E}\|\nabla F(\theta_{k})\|^{2} - \left(\frac{\alpha_{k}}{2} - \frac{\alpha_{k}}{4} - \frac{L_{F}\alpha_{k}^{2}}{2}\right)\mathbb{E}\|\bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} + \frac{L_{F}C_{f}^{2}\alpha_{k}^{2}}{2} \\
+ \left(1 + \alpha_{k}L_{y,2}^{2} + \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{4} + \alpha_{k}C_{\psi}^{2}(1+\gamma)\right)\mathbb{E}\left[\|y_{k+1} - y^{*}(\theta_{k})\|_{2}^{2}\right] \\
- \mathbb{E}\|y_{k} - y^{*}(\theta_{k})\|_{2}^{2} + \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{4} + L_{y}^{2}C_{f}^{2}\alpha_{k}^{2} + 2\alpha_{k}C_{\psi}^{2}(1+\gamma)\epsilon_{app}. \quad (105)$$

Applying (95) to bound $\mathbb{E}\left[\left\|y_{k+1}-y^*(\theta_k)\right\|_2^2\right]$, we have

$$\mathbb{E}[\mathbb{V}^{k+1}] - \mathbb{E}[\mathbb{V}^{k}] \\
\leq -\frac{\alpha_{k}}{2} \mathbb{E} \|\nabla F(\theta_{k})\|^{2} - \left(\frac{\alpha_{k}}{2} - \frac{\alpha_{k}}{4} - \frac{L_{F}\alpha_{k}^{2}}{2}\right) \mathbb{E} \|\bar{h}_{f}(\theta_{k}, y_{k+1})\|^{2} + \frac{L_{F}C_{f}^{2}\alpha_{k}^{2}}{2} + 2\alpha_{k}C_{\psi}^{2}(1+\gamma)\epsilon_{app} \\
+ \left[\left(1 + \alpha_{k}L_{y,2}^{2} + \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{4} + \alpha_{k}C_{\psi}^{2}(1+\gamma)\right)(1 - 2\lambda\beta_{k}) - 1\right] \mathbb{E} \|y_{k} - y^{*}(\theta_{k})\|_{2}^{2} \\
+ \left(1 + \alpha_{k}L_{y,2}^{2} + \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{4} + \alpha_{k}C_{\psi}^{2}(1+\gamma)\right)C_{g}^{2}\beta_{k}^{2} + \frac{\alpha_{k}^{2}C_{f}^{2}L_{y,2}^{2}}{4} + L_{y}^{2}C_{f}^{2}\alpha_{k}^{2}. \tag{106}$$

Similar to the steps (54)-(56), if we select

$$\alpha_k = \min\left\{\frac{1}{2L_F}, \frac{\alpha}{\sqrt{K}}\right\}, \qquad \beta_k = \frac{4L_{y,2}^2 + 8C_{\psi}^2 + C_f^2 L_{y,2}^2 / 2L_F}{8\lambda}\alpha_k.$$
 (107)

which ensures that

$$\frac{\alpha_k}{4} - \frac{L_F \alpha_k^2}{2} \ge 0 \tag{108a}$$

(106)

$$\left(1 + \alpha_k L_{y,2}^2 + \alpha_k C_{\psi}^2 (1+\gamma) + \frac{\alpha_k^2 C_f^2 L_{y,2}^2}{4}\right) (1 - 2\lambda \beta_k) \le 1$$
(108b)

we can simplify (106) as

$$\mathbb{E}[\mathbb{V}^{k+1}] - \mathbb{E}[\mathbb{V}^k] \le -\frac{\alpha_k}{2} \mathbb{E} \|\nabla F(\theta_k)\|^2 + \frac{L_F C_f^2 \alpha_k^2}{2} + 2\alpha_k C_{\psi}^2 (1+\gamma) \epsilon_{app} + \frac{\alpha_k^2 C_f^2 L_{y,2}^2}{4} + \left(1 + \alpha_k L_{y,2}^2 + \frac{\alpha_k^2 C_f^2 L_{y,2}^2}{4} + \alpha_k C_{\psi}^2 (1+\gamma)\right) C_g^2 \beta_k^2 + L_y^2 C_f^2 \alpha_k^2.$$
(109)

After telescoping, we have

$$\frac{1}{K} \sum_{k=1}^{K} \mathbb{E} \left\| \nabla F(\theta_k) \right\|^2 \leq \frac{2\mathbb{V}^1}{\alpha_k K} + L_F C_f^2 \alpha_k + 4C_{\psi}^2 (1+\gamma) \epsilon_{app} + \frac{\alpha_k C_f^2 L_{y,2}^2}{2} + 2L_y^2 C_f^2 \alpha_k + 2\left(1 + \alpha_k L_{y,2}^2 + \frac{\alpha_k^2 C_f^2 L_{y,2}^2}{4} + \alpha_k C_{\psi}^2 (1+\gamma)\right) \frac{C_g^2 \beta_k^2}{\alpha_k} \tag{110}$$

which, together with $\alpha_k = \mathcal{O}(1/\sqrt{K}), \beta_k = \mathcal{O}(1/\sqrt{K})$, completes the proof.