# Stochastic Bilevel Optimization

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#### 1 Problem

We now have the bilevel problem

$$\min_{\lambda \in \mathcal{D} \subset \mathbb{P}^r} \mathcal{L}(\lambda) \triangleq C(\hat{x}(\lambda), \lambda) \tag{1}$$

$$\min_{\lambda \in \mathcal{D} \subset \mathbb{R}^r} \mathcal{L}(\lambda) \triangleq C(\hat{x}(\lambda), \lambda) \tag{1}$$
s.t.  $\hat{x}(\lambda) = \operatorname*{arg\,min}_{x \in \mathbb{R}^n} F(x, \lambda)$ .

We will denote the sampled terms as follows:

$$\mathbb{E}_{\zeta}[\tilde{F}(x_k, \lambda_k; \zeta)] = F(x_k, \lambda_k)$$

$$\mathbb{E}_{\xi}[\tilde{C}(x_k, \lambda_k, \xi)] = C(x_k, \lambda_k)$$

#### Algorithm 2

### Algorithm 1 Stochastic HOAG

- 1: At iteration k = 1, 2, ..., given random samples  $\xi_i, \zeta_j$ , stepsize  $\nu_k$ , perform the following:
  - 1. Solve the inner optimization problem up to tolerance  $\varepsilon_k$ . That is, find  $x_k$  such that

$$\mathbb{E}\left[\|\hat{x}\left(\lambda_{k}\right) - x_{k}\|\right] \leq \varepsilon_{k}$$

2.

$$v_Q = \eta \sum_{q=-1}^{Q-1} \prod_{j=Q-q}^{Q} \left( I - \eta \nabla_{xx}^2 \tilde{F}(x_k, \lambda_k; \zeta_j) \right) \nabla_x \tilde{C}(x_k, \lambda_k, \xi_0), \tag{3}$$

3. Compute approximate stochastic gradient  $\widehat{\nabla} \mathcal{L}(\lambda_k)$  as

$$\widehat{\nabla} \mathcal{L}(\lambda_k) = \nabla_{\lambda} \widetilde{C}(x_k, \lambda_k, \xi_1) - \nabla_{x_k}^2 \widetilde{F}(x_k, \lambda_k, \xi_2)^{\top} v_Q$$

4. Update hyperparameters:

$$\lambda_{k+1} = \lambda_k - \nu_k \widehat{\nabla} \mathcal{L}(\lambda_k).$$

#### 3 Stochastic HOAG

In the following section we adapt the convergence proof of HOAG to the case when all terms are sampled using a single sample.

**Assumption 3.1** (Convexity). The lower-level function  $F(x,\lambda)$  is  $\mu$  strongly-convex w.r.t. x and the total objective function  $\mathcal{L}(\lambda) = C(\lambda, \hat{x}(\lambda))$  is nonconvex w.r.t.  $\lambda$ . For the stochastic setting, the same assumptions hold for  $F(x, \lambda; \zeta)$  and  $\mathcal{L}(\lambda, \zeta)$ , respectively.

**Assumption 3.2** (Smoothness). Let  $z = (x, \lambda) \in \mathbb{R}^n \times \mathcal{D}$ . The loss function C(z) and F(z) satisfy - The function C(z) is M-Lipschitz, i.e., for any z, z',

$$|C(z) - C(z')| \le M ||z - z'||.$$

-  $\nabla C(z)$  and  $\nabla F(z)$  are L-Lipschitz, i.e., for any z, z',

$$\|\nabla C(z) - \nabla C(z')\| \le L \|z - z'\|,$$
  
 $\|\nabla F(z) - \nabla F(z')\| \le L \|z - z'\|.$ 

For the stochastic case, the same assumptions hold for  $F(z;\xi)$  and  $G(z;\zeta)$  for any given  $\xi$  and  $\zeta$ .

**Assumption 3.3** (Partial Lipschitz Smoothness). Let  $z = (x, \lambda) \in \mathbb{R}^n \times \mathcal{D}$ . Suppose the derivatives  $\nabla_{x\lambda} F(z)$  and  $\nabla_x^2 F(z)$  are  $\tau$  - and  $\rho$  - Lipschitz, i.e., - For any  $z, z', \|\nabla_{x\lambda} F(z) - \nabla_{x\lambda} F(z')\| \le \tau \|z - z'\|$ . For any  $z, z', \|\nabla_x^2 F(z) - \nabla_y^2 F(z')\| \le \rho \|z - z'\|$ . For the stochastic case, the same assumptions hold for  $\nabla_{x\lambda} F(z; \zeta)$  and  $\nabla_x^2 F(z; \zeta)$  for any  $\zeta$ .

**Assumption 3.4** (Bounded Gradient). Assume that the partial gradient  $\nabla^2_{x\lambda} F$  is bounded in norm, i.e.  $\|\nabla^2_{x\lambda} F\| \leq K$ .

**Assumption 3.5** (Lower bound on objective.). The sequence of iterates  $\{\lambda_k\}$  is contained in an open set over which  $\mathcal{L}$  is bounded below by a scalar  $\mathcal{L}_{inf}$ .

#### 3.1 Preliminary Results

Let us list some useful definitions. We have

$$\nabla \mathcal{L}(\lambda_k) = \nabla_{\lambda} C(\hat{x}(\lambda_k), \lambda_k) - \nabla_{x\lambda}^2 F(\hat{x}(\lambda_k), \lambda_k)^{\top} \left[ \nabla_{xx} F(\hat{x}(\lambda_k), \lambda_k) \right]^{-1} \nabla_x C(\hat{x}(\lambda_k), \lambda_k)$$

$$\tilde{\nabla} \mathcal{L}(\lambda_k) = \nabla_{\lambda} C(x_k, \lambda_k) - \nabla_{x\lambda}^2 F(x_k, \lambda_k)^{\top} \left[ \nabla_{xx} F(x_k, \lambda_k) \right]^{-1} \nabla_x C(x_k, \lambda_k)$$

$$\hat{\nabla} \mathcal{L}(\lambda_k) = \nabla_{\lambda} \tilde{C}(x_k, \lambda_k, \xi_1) - \nabla_{x\lambda}^2 \tilde{F}(x_k, \lambda_k, \xi_2)^{\top} v_Q$$

**Definition 3.6** (Jensen's Inequality). Theorem 1 (Jensen's Inequality) Let  $\varphi$  be a convex function on  $\mathbb{R}$  and let  $X \in L_1$  be integrable. Then

$$\varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)]$$

**Lemma 3.7** (Neumann Series). For non-singular  $A \in \mathbb{R}^{n \times n}$ ,

$$A^{-1} = \sum_{i=0}^{\infty} (I - A)^{i}, \quad A \succ 0, ||A|| < 1.$$
 (4)

Firstly, we will present an immediate consequence of the assumptions in the previous section.

**Proposition 3.8** (Bounded variance of  $\nabla \tilde{C}$ ,  $\nabla \tilde{F}$ ,  $\nabla^2_{x\lambda} \tilde{F}$ ,  $\nabla^2_{xx} \tilde{F}$ . Lemma 1 in [2]). Suppose, Assumption 3.2 holds. Then for any  $z = (x, \lambda), \zeta$ ,

$$\begin{split} & \mathbb{E}_{\zeta} \|\nabla \tilde{C}(z,\zeta) - \nabla C(z)\|^2 \leq M^2 \\ & \mathbb{E}_{\zeta} \|\nabla_{x\lambda}^2 \tilde{F}(z,\zeta) - \nabla_{x\lambda}^2 F(z)\|^2 \leq L^2 \\ & \mathbb{E}_{\zeta} \|\nabla_{xx}^2 \tilde{F}(z,\zeta) - \nabla_{xx}^2 F(z)\|^2 \leq L^2 \end{split}$$

Note that

$$v_Q = \eta \sum_{q=-1}^{Q-1} \prod_{j=Q-q}^{Q} \left( I - \eta \nabla_{xx}^2 \tilde{F}(x_k, \lambda_k; \zeta_j) \right) \nabla_x \tilde{C}(x_k, \lambda_k, \xi_0), \tag{5}$$

where we assume  $\prod_{j=Q+1}^Q(\cdot)=I.$  From this we easily get

$$\mathbb{E}[v_Q] = \eta \sum_{i=0}^{Q} \left[ I - \eta \nabla_{xx}^2 F(x_k, \lambda_k) \right]^i \nabla_x C(x_k, \lambda_k).$$

Denote by  $\mathbb{E}[v_{\infty}]$ :

$$\mathbb{E}[v_{\infty}] = \left[\nabla_x^2 F(x_k, \lambda_k)\right]^{-1} \nabla_x C(x_k, \lambda_k)$$

**Proposition 3.9** (Bound on  $||\mathbb{E}v_Q||$ ). Suppose Assumptions 3.1, 3.2 hold. Then

$$\|\mathbb{E}v_Q\| \le \frac{M}{\mu} (1 - (1 - \eta\mu)^{Q+1})$$

**Proposition 3.10** (Bound on  $Var(v_Q)$ ). Suppose Assumptions 3.1, 3.2 and 3.4 hold. Denote the condition number as  $\kappa = \frac{L}{u}$ . Choose  $\eta$ , such that  $\eta \mu < 1$ . Then we have that

$$Var(v_Q) = \mathbb{E}||v_Q - \mathbb{E}(v_Q)||^2 \le 2\eta^3 M^2 L\kappa + \frac{2\eta M^2}{\mu}.$$

**Proposition 3.11** (Bound on  $Var(\widehat{\nabla}\mathcal{L})$ ). Suppose Assumptions 3.1, 3.2 and 3.4 hold. Choose  $\eta$ , such that  $\eta\mu < 1$ . Denote the condition number as  $\kappa = \frac{L}{\mu}$ . Then the variance of the approximate hypergradient satisfies

$$\operatorname{Var}(\widehat{\nabla}\mathcal{L}(\lambda_k)) = \mathbb{E}\|\widehat{\nabla}\mathcal{L}(\lambda_k) - \mathbb{E}\widehat{\nabla}\mathcal{L}(\lambda_k)\|^2 \le$$

$$\operatorname{Var}(v_Q)(L^2 + K^2) + L^2\|\mathbb{E}v_Q\|^2 + M^2 \le$$

$$\left(2\eta^3 M^2 L\kappa + \frac{2\eta M^2}{\mu}\right) \left(L^2 + K^2\right) + \kappa^2 M^2 + M^2.$$

In particular, we have that if  $Var(v_Q)$  is bounded, then so is  $Var(\widehat{\nabla}\mathcal{L}(\lambda_k))$ .

**Proposition 3.12** (Bound on  $\|\mathbb{E}_{\lambda_k}\widehat{\nabla}\mathcal{L}(\lambda_k) - \nabla\mathcal{L}(\lambda_k)\|$ . Lemma 7 of [2].). Let

$$T_4 = \sqrt{2} \left( L + \frac{L^2}{\mu} + \frac{M\tau}{\mu} + \frac{LM\rho}{\mu^2} \right), \quad T_5 = \sqrt{2} \frac{LM(1 - \eta\mu)^Q}{\mu}.$$
 (6)

Then we have that

$$\|\mathbb{E}_{\lambda_k}\widehat{\nabla}\mathcal{L}(\lambda_k) - \nabla\mathcal{L}(\lambda_k)\|_2 \le T_4\epsilon_k + T_5.$$

#### 3.2 Convergence Proof

**Theorem 3.13** (Global Convergence (SGD step)). In Algorithm 2, assume that the stepsize  $\nu_k$  is chosen such that

$$\sum_{k=1}^{\infty} \nu_k = \infty, \quad \sum_{k=1}^{\infty} \nu_k^2 < \infty.$$

Assume also, that  $\lambda_k \in \mathcal{D}$  for all k > 0. If the sequence  $\epsilon_k$  obeys

$$\sum_{i=1}^{\infty} \epsilon_i < \infty, \quad \epsilon_k > 0 \quad \forall k \ge 0,$$

then we have

$$\liminf_{k \to \infty} \mathbb{E}\left[\left\|\nabla \mathcal{L}(\lambda_k)\right\|_2^2\right] = 0.$$

*Proof.* An equivalent condition to  $\mathcal{L}(\lambda)$  having Lipschitz continuous gradient is that for any  $\alpha, \beta \in \mathcal{D}$ :

$$\mathcal{L}(\beta) \le \mathcal{L}(\alpha) + \nabla \mathcal{L}(\alpha)^{\top} (\beta - \alpha) + \frac{L}{2} \|\beta - \alpha\|^{2}.$$
 (7)

Substituting for  $\alpha = \lambda_k, \beta = \lambda_{k+1} = \lambda_k - \nu_k \widehat{\nabla} \mathcal{L}(\lambda_k),$ 

$$\mathcal{L}(\lambda_{k+1}) \leq \mathcal{L}(\lambda_k) + \nabla \mathcal{L}(\lambda_k)^{\top} \left( -\nu_k \widehat{\nabla} \mathcal{L}(\lambda_k) \right) + \frac{L}{2} \left\| -\nu_k \widehat{\nabla} \mathcal{L}(\lambda_k) \right\|^2.$$

Taking expectation, conditioning on  $\lambda_k$ ,

$$\mathbb{E}_{\lambda_k} \left[ \mathcal{L}(\lambda_{k+1}) \right] \leq \mathcal{L}(\lambda_k) - \nu_k \nabla \mathcal{L}(\lambda_k)^\top \mathbb{E}_{\lambda_k} \left[ \widehat{\nabla} \mathcal{L}(\lambda_k) \right] + \frac{L\nu_k^2}{2} \mathbb{E}_{\lambda_k} \left[ \left\| \widehat{\nabla} \mathcal{L}(\lambda_k) \right\|^2 \right].$$

$$= \mathcal{L}(\lambda_k) - \nu_k \left( \nabla \mathcal{L}(\lambda_k) - \mathbb{E}_{\lambda_k} \left[ \widehat{\nabla} \mathcal{L}(\lambda_k) \right] \right)^{\top} \mathbb{E}_{\lambda_k} \left[ \widehat{\nabla} \mathcal{L}(\lambda_k) \right] - \nu_k \left\| \mathbb{E}_{\lambda_k} \left[ \widehat{\nabla} \mathcal{L}(\lambda_k) \right] \right\|^2 + \frac{L\nu_k^2}{2} \mathbb{E}_{\lambda_k} \left[ \left\| \widehat{\nabla} \mathcal{L}(\lambda_k) \right\|^2 \right]$$

$$\leq \mathcal{L}(\lambda_{k}) + \nu_{k} \left\| \nabla \mathcal{L}(\lambda_{k}) - \mathbb{E}_{\lambda_{k}} \left[ \widehat{\nabla} \mathcal{L}(\lambda_{k}) \right] \right\| \left\| \mathbb{E}_{\lambda_{k}} \left[ \widehat{\nabla} \mathcal{L}(\lambda_{k}) \right] \right\| - \nu_{k} \left\| \mathbb{E}_{\lambda_{k}} \left[ \widehat{\nabla} \mathcal{L}(\lambda_{k}) \right] \right\|^{2} + \frac{L\nu_{k}^{2}}{2} \mathbb{E}_{\lambda_{k}} \left[ \left\| \widehat{\nabla} \mathcal{L}(\lambda_{k}) \right\|^{2} \right]$$

$$= \mathcal{L}(\lambda_k) + \nu_k \left\| \nabla \mathcal{L}(\lambda_k) - \mathbb{E}_{\lambda_k} \left[ \widehat{\nabla} \mathcal{L}(\lambda_k) \right] \right\| \left\| \mathbb{E}_{\lambda_k} \left[ \widehat{\nabla} \mathcal{L}(\lambda_k) \right] \right\| + \frac{L\nu_k^2}{2} \operatorname{Var}(\widehat{\nabla} \mathcal{L}(\lambda_k)) - \left( \nu_k - \frac{L\nu_k^2}{2} \right) \| \mathbb{E}_{\lambda_k} \widehat{\nabla} \mathcal{L}(\lambda_k) \|^2,$$
(8)

Let  $T_{45} = T_4 \epsilon_k + T_5$ , where  $T_4, T_5$  are as in (6) of Proposition 3.12. From Proposition 3.12 and by assumption on  $\epsilon_k$ , we have that

$$\|\mathbb{E}_{\lambda_k}\widehat{\nabla}\mathcal{L}(\lambda_k) - \nabla\mathcal{L}(\lambda_k)\|_2 \le T_{45}.$$
(9)

By reverse triangle inequality, we have that

$$\left| \| \mathbb{E}_{\lambda_k} \widehat{\nabla} \mathcal{L}(\lambda_k) \|_2 - \| \nabla \mathcal{L}(\lambda_k) \|_2 \right| \le T_{45}.$$

Hence,

$$\|\mathbb{E}_{\lambda_k}\widehat{\nabla}\mathcal{L}(\lambda_k)\|_2 \le T_{45} + \|\nabla\mathcal{L}(\lambda_k)\|_2$$

Note, that from this we have

$$\|\mathbb{E}_{\lambda_k}\widehat{\nabla}\mathcal{L}(\lambda_k)\|_2 \le T_{45} + 1 + \|\nabla\mathcal{L}(\lambda_k)\|_2^2 \tag{10}$$

Furthermore,

$$\|\mathbb{E}_{\lambda_k} \widehat{\nabla} \mathcal{L}(\lambda_k)\|_2^2 \le T_{45}^2 + 2T_{45} \|\nabla \mathcal{L}(\lambda_k)\|_2 + \|\nabla \mathcal{L}(\lambda_k)\|_2^2 \le T_{45}^2 + 2T_{45} \left(1 + \|\nabla \mathcal{L}(\lambda_k)\|_2^2\right) + \|\nabla \mathcal{L}(\lambda_k)\|_2^2$$

$$= T_{45}^2 + 2T_{45} + (2T_{45} + 1) \|\nabla \mathcal{L}(\lambda_k)\|_2^2. \tag{11}$$

Finally, by proposition 3.11, we have that

$$\operatorname{Var}\left(\widehat{\nabla}\mathcal{L}(\lambda_k)\right) \le T_2 = \left(2\eta^3 M^2 L\kappa + \frac{2\eta M^2}{\mu}\right) \left(L^2 + K^2\right) + \kappa^2 M^2 + M^2. \tag{12}$$

Set  $M_1 = T_{45}^2 + 2T_{45}$ ,  $M_2 = 2T_{45} + 1$ . Substituting (9),(10), (11) and (12) into (8), and rearranging, we get

$$\left(\nu_{k} - \frac{L\nu_{k}^{2}}{2}\right)\left(M_{1} + M_{2}\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2}\right) - \nu_{k}\left(\left(T_{4}\epsilon + T_{5}\right)\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2} + T_{5}^{2} + T_{5}\right) \leq \mathcal{L}(\lambda_{k}) - \mathbb{E}_{\lambda_{k}}\left[\mathcal{L}(\lambda_{k+1})\right] + \left(\frac{L\nu_{k}^{2}}{2}\right)\left(M_{1} + M_{2}\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2}\right) - \nu_{k}\left(\left(T_{4}\epsilon + T_{5}\right)\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2} + T_{5}^{2} + T_{5}\right) \leq \mathcal{L}(\lambda_{k}) - \mathbb{E}_{\lambda_{k}}\left[\mathcal{L}(\lambda_{k+1})\right] + \left(\frac{L\nu_{k}^{2}}{2}\right)\left(M_{1} + M_{2}\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2}\right) - \nu_{k}\left(\left(T_{4}\epsilon + T_{5}\right)\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2} + T_{5}^{2} + T_{5}\right) \leq \mathcal{L}(\lambda_{k}) - \mathbb{E}_{\lambda_{k}}\left[\mathcal{L}(\lambda_{k+1})\right] + \left(\frac{L\nu_{k}^{2}}{2}\right)\left(M_{1} + M_{2}\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2}\right) - \nu_{k}\left(\left(T_{4}\epsilon + T_{5}\right)\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2} + T_{5}^{2} + T_{5}\right) \leq \mathcal{L}(\lambda_{k}) - \mathbb{E}_{\lambda_{k}}\left[\mathcal{L}(\lambda_{k+1})\right] + \left(\frac{L\nu_{k}^{2}}{2}\right)\left(M_{1} + M_{2}\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2}\right) - \nu_{k}\left(\left(T_{4}\epsilon + T_{5}\right)\|\nabla\mathcal{L}(\lambda_{k})\|_{2}^{2} + T_{5}^{2} + T_{5}^{2}\right) \leq \mathcal{L}(\lambda_{k}) - \mathbb{E}_{\lambda_{k}}\left[\mathcal{L}(\lambda_{k+1})\right] + \mathcal{L}(\lambda_{k}) + \mathcal{L}(\lambda_{k})$$

$$+\nu_k \epsilon_k \left(\underbrace{T_4^2 T_\epsilon + 2T_4 T_5 + T_4}_{\triangleq T_c}\right) + \frac{T_2 \nu_k^2}{2L} \tag{13}$$

Now, let us inspect the left-hand-side of (13). Expanding  $M_1, M_2$  and collecting like terms, we get

$$\left(\nu_k - \frac{L\nu_k^2}{2}\right)(M_1 + M_2 \|\nabla \mathcal{L}(\lambda_k)\|_2^2) - \nu_k((T_4\epsilon + T_5) \|\nabla \mathcal{L}(\lambda_k)\|_2^2 + T_5^2 + T_5) =$$

$$= \left(\underbrace{\nu_{k}(\underbrace{2T_{45}+1-T_{5}}) - \frac{M_{2}L\nu_{k}^{2}}{2} - T_{4}\nu_{k}\epsilon_{k}}_{\triangleq \gamma_{k}}\right) \|\nabla \mathcal{L}(\lambda_{k})\|_{2}^{2} + \nu_{k}\epsilon_{k}(T_{4}\epsilon + 2T_{4}T_{5} + 2T_{4}) + \nu_{k}T_{5} \geq$$

$$\geq \gamma_k \|\nabla \mathcal{L}(\lambda_k)\|_2^2 + \nu_k \epsilon_k (T_4 \epsilon + 2T_4 T_5 + 2T_4).$$

We can now rewrite the inequality (13) as

$$\gamma_k \|\nabla \mathcal{L}(\lambda_k)\|_2^2 \le \mathcal{L}(\lambda_k) - \mathbb{E}_{\lambda_k} \left[ \mathcal{L}(\lambda_{k+1}) \right] + \frac{T_2 \nu_k^2}{2L} + \nu_k \epsilon_k \left( \underbrace{T_6 - T_4 \epsilon - 2T_4 T_5 - 2T_4}_{\triangleq T_7} \right) \tag{14}$$

Note that, by Cauchy-Schwarz,  $\sum_{k=1}^{\infty} \nu_k \epsilon_k \leq \sqrt{\sum_{k=1}^{\infty} \nu_k^2} \sqrt{\sum_{k=1}^{\infty} \epsilon_k^2} < \infty$ . As such,  $\gamma_k$  is summable. Summing (14) for k=1 to  $\infty$ , we get

$$\sum_{k=1}^{\infty} \gamma_k \|\nabla \mathcal{L}(\lambda_k)\|_2^2 \leq \sum_{k=1}^{\infty} \left(\mathcal{L}(\lambda_k) - \mathbb{E}_{\lambda_k} \left[\mathcal{L}(\lambda_{k+1})\right]\right) + \frac{T_2}{2L} \sum_{k=1}^{\infty} \nu_k^2 + T_7 \sum_{k=1}^{\infty} \nu_k \epsilon_k.$$

Taking total expectation and telescoping, we get

$$\sum_{k=1}^{\infty} \gamma_k \mathbb{E} \|\nabla \mathcal{L}(\lambda_k)\|_2^2 \le \mathcal{L}(\lambda_1) - \mathcal{L}_{inf} + \frac{T_2}{2L} \sum_{k=1}^{\infty} \nu_k^2 + T_7 \sum_{k=1}^{\infty} \nu_k \epsilon_k.$$
(15)

and so the right-hand side of the inequality (15) is finite. From this, we immediately get that

$$\sum_{k=1}^{\infty} \gamma_k \mathbb{E} \|\nabla \mathcal{L}(\lambda_k)\|_2^2 < \infty. \tag{16}$$

Furthermore, from (16), we get that

$$\liminf_{k\to\infty} \mathbb{E} \|\nabla \mathcal{L}(\lambda_k)\|_2^2 = 0.$$

### 4 Discussion

## References

- [1] Bottou, L., Curtis, F., & Nocedal, J. (2016). Optimization Methods for Large-Scale Machine Learning.
- [2] Ji, K. Yang, J. & Liang. Y. Bilevel optimization: Nonasymptotic analysis and faster algorithms. *International Conference on Machine Learning (ICML)*, 2021.
- [3] Pedregosa, F. Hyperparameter optimization with approximate gradient. *Proceedings of The 33rd International Conference on Machine Learning*, *PMLR* 48:737-746, 2016. Available from https://proceedings.mlr.press/v48/pedregosa16.html.

## Appendix

Proof of proposition 3.9.

$$\mathbb{E}v_{Q} = \|\eta \sum_{i=0}^{Q} (I - \eta \mu \nabla_{xx}^{2} F)^{i} \nabla_{x} C\| \leq \eta \|\sum_{i=0}^{Q} (I - \eta \mu \nabla_{xx}^{2} F)^{i}\| \|\nabla_{x} C\| \leq \eta M \sum_{i=0}^{Q} (1 - \eta \mu)^{i} = \eta M \frac{1 - (1 - \eta \mu)^{Q+1}}{\eta \mu}$$
$$= \frac{M}{\mu} \left( 1 - (1 - \eta \mu)^{Q+1} \right).$$

Proof of Proposition 3.10. Denote

$$A_{j} = I - \eta \nabla_{xx}^{2} \tilde{F}(x_{k}, \lambda_{k}, \xi_{j});$$

$$\tilde{B} = \nabla_{x} \tilde{C}(x_{k}, \lambda_{k}, \zeta);$$

$$A = \mathbb{E}A_{j} = I - \eta \nabla_{xx}^{2} F(x_{k}, \lambda_{k});$$

$$B = \mathbb{E}B = \nabla_{x} C(x_{k}, \lambda_{k});$$

Then

$$\operatorname{Var}(v_{Q}) = \mathbb{E} \|v_{Q} - \mathbb{E} v_{Q}\|^{2}$$

$$= \mathbb{E} \left\| \eta \sum_{q=-1}^{Q-1} \prod_{j=Q-q}^{Q} A_{j} \tilde{B} - \eta \sum_{i=0}^{Q} A^{i} B \right\|^{2}$$

$$\leq 2\mathbb{E} \left\| \eta \sum_{q=-1}^{Q-1} \prod_{j=Q-q}^{Q} A_{j} \tilde{B} - \eta \sum_{i=0}^{Q} A^{i} \tilde{B} \right\|^{2} + 2\mathbb{E} \left\| \eta \sum_{i=0}^{Q} A^{i} \tilde{B} - \eta \sum_{i=0}^{Q} A^{i} B \right\|^{2}$$

$$= 2\mathbb{E} \left\| \eta \sum_{q=-1}^{Q-1} \left( \prod_{j=Q-q}^{Q} A_{j} - A^{q+1} \right) \tilde{B} \right\|^{2} + 2\mathbb{E} \left\| \eta \sum_{j=Q}^{Q} A^{i} (\tilde{B} - B) \right\|^{2}.$$

Now, note that  $\mathbb{E}\left(\prod_{j=Q-q}^{Q}A_{j}-A^{q+1}\right)=0$ , and that each  $A_{i}$  is independently sampled. Expanding the first term, we get

$$2\mathbb{E} \left\| \eta \sum_{q=-1}^{Q-1} \left( \prod_{j=Q-q}^{Q} A_j - A^{q+1} \right) \tilde{B} \right\|^2 + 2\mathbb{E} \left\| \eta \sum_{i=0}^{Q} A^i (\tilde{B} - B) \right\|^2.$$

$$\leq 2\eta^2 \sum_{q=-1}^{Q-1} \mathbb{E} \left\| \left( \prod_{j=Q-q}^{Q} A_j - A^{q+1} \right) \tilde{B} \right\|^2 + 2\eta^2 \left\| \sum_{i=0}^{Q} A^i \right\|^2 \mathbb{E} \|\tilde{B} - B\|^2$$

$$\leq 2\eta^2 \sum_{q=-1}^{Q-1} \mathbb{E} \left\| \prod_{j=Q-q}^{Q} A_j - A^{q+1} \right\|^2 \mathbb{E} \left\| \tilde{B} \right\|^2 + 2\eta^2 \sum_{i=0}^{Q} \|A\|^{2i} \mathbb{E} \|\tilde{B} - B\|^2$$

$$= 2\eta^2 \sum_{q=0}^{Q} \mathbb{E} \left\| \prod_{j=Q-q+1}^{Q} A_j - A^q \right\|^2 \mathbb{E} \left\| \tilde{B} \right\|^2 + 2\eta^2 \frac{1 - \|A\|^{2Q}}{1 - \|A\|^2} \mathbb{E} \|\tilde{B} - B\|^2$$

We will now bound  $\mathbb{E}M_i$  for  $M_i = \left\| \prod_{j=Q-q+1}^Q A_j - A^q \right\|^2$ . Note, that  $M_0 = 0$ . As in the proof of proposition 3 in [2], we write

$$\prod_{j=Q-q+1}^{Q} \left( I - \eta \nabla_{xx}^2 \tilde{F}_j \right) = \prod_{j=Q-q+2}^{Q} \left( I - \eta \nabla_{xx}^2 \tilde{F}_j \right) - \eta \nabla_x^2 \tilde{F}_j \prod_{j=Q-q+2}^{Q} \left( I - \eta \nabla_{xx}^2 \tilde{F}_j \right)$$

Then, we have

$$\mathbb{E}M_{i} = \mathbb{E} \left\| \prod_{j=Q-i+1}^{Q} \left( I - \eta \nabla_{xx}^{2} \tilde{F}\left(x_{k}, \lambda_{k}; \zeta_{j}\right) \right) - \left[ I - \eta \nabla_{xx}^{2} F\left(x_{k}, \lambda_{k}\right) \right]^{i} \right\|^{2}$$

$$= \mathbb{E} \left\| \prod_{j=Q-i+2}^{Q} \left( I - \eta \nabla_{xx}^{2} \tilde{F}_{j} \right) - \eta \nabla_{x}^{2} \tilde{F}_{j} \prod_{j=Q-i+2}^{Q} \left( I - \eta \nabla_{xx}^{2} \tilde{F}_{j} \right) - \left[ I - \eta \nabla_{xx}^{2} F\left(x_{k}, \lambda_{k}\right) \right]^{i} \right\|^{2}$$

Add and subtract  $\eta \nabla_x^2 F \prod_{j=Q+2-i} (I - \eta \nabla_x^2 \tilde{F}_j)$ :

$$\mathbb{E}\left\|\left(\underbrace{\left(I-\eta\nabla_{x}^{2}F\right)\prod_{j=Q-i+2}^{Q}\left(I-\eta\nabla_{xx}^{2}\tilde{F}_{j}\right)-\left[I-\eta\nabla_{xx}^{2}F\left(x_{k},\lambda_{k}\right)\right]^{i}}_{c}\right)+\left(\underbrace{\left(\eta\nabla_{x}^{2}F-\eta\nabla_{x}^{2}\tilde{F}_{j}\right)\prod_{j=Q-i+2}^{Q}\left(I-\eta\nabla_{xx}^{2}\tilde{F}_{j}\right)}_{d}\right)\right\|^{2}$$

$$= \mathbb{E} \|c\|^2 + \mathbb{E} \|d\|^2 + \underbrace{2\mathbb{E} \langle c, d \rangle}_{=0 \text{ as } \mathbb{E} (\eta \nabla_x^2 F - \eta \nabla_x^2 \tilde{F}_j) = 0}$$

Using convexity assumptions and Proposition 3.8, we get the bound

$$\mathbb{E}M_i \le (1 - \eta\mu)^2 \mathbb{E}M_{i-1} + \eta^2 (1 - \eta\mu)^{2q-2} L^2.$$

Telescoping, we get

$$\mathbb{E}M_i \le (1 - \eta\mu)^{2k} \mathbb{E}M_{i-k} + \eta^2 L^2 (1 - \eta\mu)^{2i-2} \sum_{i=1}^k (1 - \eta\mu)^{j-1}$$

Setting i = q, k = q,

$$\mathbb{E}M_q \le (1 - \eta\mu)^{2q - 2} \mathbb{E}M_0 + \eta^2 L^2 (1 - \eta\mu)^{2q - 2} \sum_{j=1}^q (1 - \eta\mu)^{j-1}$$

Note that  $\mathbb{E}(M_0) = 0$ . Thus, we finally get

$$\mathbb{E}M_{q} \leq \eta^{2} L^{2} (1 - \eta \mu)^{2q - 2} \sum_{j=0}^{q} (1 - \eta \mu)^{j} = \eta^{2} L^{2} (1 - \eta \mu)^{2q - 2} \frac{1 - (1 - \eta \mu)^{q + 1}}{1 - (1 - \eta \mu)} = \frac{\eta L^{2}}{\mu} \left( (1 - \eta \mu)^{2q - 2} - (1 - \eta \mu)^{3q - 1} \right)$$

$$\tag{17}$$

Hence.

$$\mathbb{E} \left\| \prod_{j=Q-q+1}^{Q} A_j - A^q \right\|^2 \le \eta^2 L^2 (1 - \eta \mu)^{2q-2} \frac{1 - (1 - \eta \mu)^{q+1}}{1 - (1 - \eta \mu)} = \frac{\eta L^2}{\mu} \left( (1 - \eta \mu)^{2q-2} - (1 - \eta \mu)^{3q-1} \right)$$

Hence, using the continuity and convexity assumptions, we get

$$\operatorname{Var}(v_Q) \leq 2\eta^2 \sum_{q=0}^{Q} \mathbb{E} \left\| \prod_{j=Q-q+1}^{Q} A_j - A^q \right\|^2 \mathbb{E} \left\| \tilde{B} \right\|^2 + 2\eta^2 \frac{1 - \|A\|^{2Q}}{1 - \|A\|^2} \mathbb{E} \|\tilde{B} - B\|^2$$

$$\leq 2\eta^2 M^2 \left( \sum_{q=0}^{Q} \frac{\eta L^2}{\mu} \left( (1 - \eta \mu)^{2q-2} - (1 - \eta \mu)^{3q-1} \right) + \frac{1 - (1 - \eta \mu)^{2Q}}{1 - (1 - \eta \mu)^2} \right)$$

$$= \frac{2\eta^3 M^2 L^2}{\mu} \left( \frac{1 - (1 - \eta \mu)^{2Q+2}}{1 - (1 - \eta \mu)^2} - (1 - \eta \mu)^2 \frac{1 - (1 - \eta \mu)^{3Q+3}}{1 - (1 - \eta \mu)^3} \right) + 2\eta^2 M^2 \frac{1 - (1 - \eta \mu)^{2Q}}{1 - (1 - \eta \mu)^2}$$

$$\leq \frac{2\eta^3 M^2 L^2}{\mu} \left( \frac{1}{1 - (1 - \eta \mu)^2} \right) + 2\eta^2 M^2 \frac{1}{1 - (1 - \eta \mu)^2} \leq \frac{2\eta^3 M^2 L^2 + 2\eta M^2}{2\mu - \eta \mu^2}$$

Furthermore, since  $\eta \mu < 1$ , we have that

$$\frac{2\eta^3 M^2 L^2 + 2\eta M^2}{2\mu - \eta \mu^2} \le \frac{2\eta^3 M^2 L^2 + 2\eta M^2}{2\mu - \mu} = 2\eta^3 M^2 L\kappa + \frac{2\eta M^2}{\mu}$$

Proof of Proposition 3.11.

$$\operatorname{Var}(\widehat{\nabla}\mathcal{L}(\lambda_{k})) = \mathbb{E}\|\widehat{\nabla}\mathcal{L}(\lambda_{k}) - \mathbb{E}\widehat{\nabla}\mathcal{L}(\lambda_{k})\|^{2} =$$

$$\mathbb{E}\|\nabla_{\lambda}\widetilde{C}(x_{k},\lambda_{k},\xi_{1}) - \nabla_{x_{\lambda}}^{2}\widetilde{F}(x_{k},\lambda_{k},\xi_{2})^{\top}v_{Q} - \left(\nabla_{\lambda}C(x_{k},\lambda_{k}) - \nabla_{x_{\lambda}}^{2}F(x_{k},\lambda_{k})^{\top}\mathbb{E}v_{Q}\right)\|^{2}$$

$$= \mathbb{E}\|\nabla_{\lambda}\widetilde{C}(x_{k},\lambda_{k},\xi_{1}) - \nabla_{\lambda}C(x_{k},\lambda_{k})\|^{2} + \mathbb{E}\|\nabla_{x_{\lambda}}^{2}F(x_{k},\lambda_{k})^{\top}\mathbb{E}v_{Q} - \nabla_{x_{\lambda}}^{2}\widetilde{F}(x_{k},\lambda_{k},\xi_{2})^{\top}v_{Q}\|^{2} -$$

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$$-2\mathbb{E}\left[\left(\underbrace{\nabla_{\lambda}\tilde{C}(x_{k},\lambda_{k},\xi_{1}) - \nabla_{\lambda}C(x_{k},\lambda_{k})}_{\mathbf{0} \text{ in expectation}}\right)^{\top}\left(\nabla_{x\lambda}^{2}F(x_{k},\lambda_{k})^{\top}\mathbb{E}v_{Q} - \nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})^{\top}v_{Q}\right)\right]$$

$$= \mathbb{E}\|\nabla_{\lambda}\tilde{C}(x_{k},\lambda_{k},\xi_{1}) - \nabla_{\lambda}C(x_{k},\lambda_{k})\|^{2} + \mathbb{E}\|\nabla_{x\lambda}^{2}F(x_{k},\lambda_{k})^{\top}\mathbb{E}v_{Q} - \nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})^{\top}v_{Q}\|^{2}$$

$$= \operatorname{Var}\left(\nabla_{\lambda}\tilde{C}(x_{k}, \lambda_{k}, \xi_{1})\right) + \operatorname{Var}\left(\nabla_{x_{\lambda}}^{2}\tilde{F}(x_{k}, \lambda_{k}, \xi_{2})^{\top}v_{Q}\right)$$
(18)

$$= \operatorname{Var}\left(\nabla_{\lambda}\tilde{C}(x_{k},\lambda_{k},\xi_{1})\right) + \operatorname{Var}\left(\nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})\right)\operatorname{Var}\left(v_{Q}\right) + \operatorname{Var}\left(\nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})\right) \|\mathbb{E}[v_{Q}]\|^{2} + \left(\operatorname{Var}\left(\nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})\right) + \operatorname{Var}\left(\nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})\right) + \operatorname{Var}\left(\nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k}$$

$$+\operatorname{Var}(v_Q)\left\|\mathbb{E}\left[\nabla^2_{x\lambda}\tilde{F}(x_k,\lambda_k,\xi_2)\right]\right\|^2,\tag{19}$$

where we get from (18) to (19) using the the identity  $Var[XY] = Var[X]Var[Y] + Var[X]\mathbb{E}[Y]^2 + Var[Y]\mathbb{E}[X]^2$  for independent X, Y. Now, by Proposition 3.8, and Assumption 3.4, we have

$$\operatorname{Var}\left(\nabla_{\lambda}\tilde{C}(x_{k},\lambda_{k},\xi_{1})\right) \leq M^{2}, \quad \operatorname{Var}\left(\nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})\right) \leq L^{2}, \quad \left\|\mathbb{E}\left[\nabla_{x\lambda}^{2}\tilde{F}(x_{k},\lambda_{k},\xi_{2})\right]\right\|^{2} \leq K^{2}.$$

By Proposition 3.9, we also obtain

$$\|\mathbb{E}[v_Q]\|^2 \le \frac{M^2}{\mu^2} (1 - (1 - \eta\mu)^{Q+1})^2 \le \frac{M^2}{\mu^2}.$$

Finally, from Proposition 3.10, we have

$$\operatorname{Var}(v_Q) \le 2\eta^3 M^2 L \kappa + \frac{2\eta M^2}{\mu}.$$

Thus, we can bound (19) by

$$\left(2\eta^3M^2L\kappa+\frac{2\eta M^2}{\mu}\right)\left(L^2+K^2\right)+\kappa^2M^2+M^2,$$

and we are done.