Minimization by Incremental Stochastic Surrogate Optimization for Large Scale Nonconvex Problems

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Stochastic Approximation

- Objective: Find a stationary point of smooth Lyapunov function $V(\eta)$.
- SA scheme (Robbins and Monro, 1951) is a stochastic process:

$$\eta_{n+1} = \eta_n - \gamma_{n+1} H_{\eta_n}(X_{n+1}), \quad n \in \mathbb{N}$$
(1)

where $\eta_n \in \mathcal{H} \subseteq \mathbb{R}^d$ is the *n*th state, $\gamma_n > 0$ is the step size.

• The drift term $H_{\eta_n}(X_{n+1})$ depends on an i.i.d. random element X_{n+1} and

$$h(\boldsymbol{\eta}_n) = \mathbb{E}\big[H_{\boldsymbol{\eta}_n}(X_{n+1})|\mathcal{F}_n\big] = \nabla V(\boldsymbol{\eta}_n),$$

where $\mathcal{F}_n = \sigma(\eta_0, \{X_m\}_{m \le n})$. In this case, SA is better known as the SGD method.

Biased SA Scheme

 The mean field is biased ← gradient is sometimes difficult to compute... We have $h(\eta) \neq \nabla V(\eta)$ and for some $c_0 \geq 0$, $c_1 > 0$,

$$c_0 + c_1 \langle \nabla V(\boldsymbol{\eta}) | h(\boldsymbol{\eta}) \rangle \ge \|h(\boldsymbol{\eta})\|^2$$
, $\forall \boldsymbol{\eta} \in \mathcal{H}$

• The **drift term** $\{H_{\eta_n}(X_{n+1})\}_{n\geq 1}$ is **not i.i.d.**. For example, in reinforcement learning, η_n controls the policy in a MDP & $H_{\eta_n}(X_{n+1})$ is computed from the MDP's state.

The random elements $\{X_n\}_{n\geq 1}$ form a state-dependent Markov chain:

$$\mathbb{E}[H_{\boldsymbol{\eta}_n}(X_{n+1})|\mathcal{F}_n] = P_{\boldsymbol{\eta}_n}H_{\boldsymbol{\eta}_n}(X_n) = \int H_{\boldsymbol{\eta}_n}(x)P_{\boldsymbol{\eta}_n}(X_n,dx),$$

where $P_{m{\eta}_n}:\mathsf{X} imes\mathcal{X} o\mathbb{R}_+$ is Markov kernel with a unique stationary distribution $\pi_{m{\eta}_n}$.

- In the latter case, the mean field is given by $h(\eta) = \int H_{\eta}(x)\pi_{\eta}(\mathrm{d}x)$.
- Stopping criterion: fix any $n \ge 1$, we stop the SA at a random iteration N with

$$\mathbb{P}(N = \ell) = (\sum_{k=0}^{n} \gamma_{k+1})^{-1} \gamma_{\ell+1}$$
, with $N \in \{1, ..., n\}$.

Prior Work

• We focus on the **non-asymptotic convergence** analysis of SA scheme, where the relevant results are rare. Define:

$$e_{n+1} := H_{\eta_n}(X_{n+1}) - h(\eta_n)$$
 (2)

Case 1: When $\{e_n\}_{n\geq 1}$ is Martingale difference — $\mathbb{E}[e_{n+1}|\mathcal{F}_n]=0$

• Asymptotic analysis: (Robbins and Monro, 1951); Non-asymptotic analysis: (Ghadimi and Lan, 2013).

Case 2: When $\{e_n\}_{n\geq 1}$ is state-controlled Markov noise

$$\mathbb{E}[\boldsymbol{e}_{n+1}|\mathcal{F}_n] = P_{\boldsymbol{\eta}_n}H_{\boldsymbol{\eta}_n}(X_n) - h(\boldsymbol{\eta}_n) \neq 0.$$

• Asymptotic analysis: (Tadić and Doucet, 2017); Non-asymptotic analysis: (Sun et al., 2018), (Duchi et al., 2012), (Bhandari et al., 2018)

Analysis For Martingale Difference Noise (Case 1)

Assumption: $\mathbb{E}\left[e_{n+1} \mid \mathcal{F}_n\right] = \mathbf{0}$, $\mathbb{E}\left[\|e_{n+1}\|^2 \mid \mathcal{F}_n\right] \leq \sigma_0^2 + \sigma_1^2 \|h(\boldsymbol{\eta}_n)\|^2$. (e.g., when \boldsymbol{X}_n is i.i.d. similar to the SGD setting).

Theorem 1. Let $\gamma_{n+1} \leq (2c_1L(1+\sigma_1^2))^{-1}$ and $V_{0,n} := \mathbb{E}[V(\eta_0) - V(\eta_{n+1})]$,

$$\mathbb{E}[\|h(\boldsymbol{\eta}_N)\|^2] \leq \frac{2c_1(V_{0,n} + \sigma_0^2 L \sum_{k=0}^n \gamma_{k+1}^2)}{\sum_{k=0}^n \gamma_{k+1}} + 2c_0,$$

Set $\gamma_k = (2c_1L(1+\sigma_1^2)\sqrt{k})^{-1} \Longrightarrow \mathbb{E}[\|h(\eta_N)\|^2] = \mathcal{O}(c_0 + \log n/\sqrt{n})$. Remark: if $h(\eta) = 0$ $\nabla V(\eta)$ (with $c_0 = d_0 = 0$), it recovers (Ghadimi and Lan, 2013, Theorem 2.1).

Analysis For State-dependent Markov Noise (Case 2)

Assumptions: we need a few regularity conditions in this case,

1. There exists a Borel measurable function $\hat{H}:\mathcal{H} imes \mathsf{X} o \mathcal{H}$,

$$\hat{H}_{\eta}(x) - P_{\eta}\hat{H}_{\eta}(x) = H_{\eta}(x) - h(\eta), \ \forall \ \eta \in \mathcal{H}, x \in X.$$

⇒ existence of solution to the *Poisson equation*.

2. For all $\eta \in \mathcal{H}$ and $x \in X$, $\|\hat{H}_{\eta}(x)\| \le L_{PH}^{(0)}$, $\|P_{\eta}\hat{H}_{\eta}(x)\| \le L_{PH}^{(0)}$, and

$$\sup_{\mathbf{x} \in \mathbf{X}} \|P_{\boldsymbol{\eta}} \hat{H}_{\boldsymbol{\eta}}(\mathbf{x}) - P_{\boldsymbol{\eta}'} \hat{H}_{\boldsymbol{\eta}'}(\mathbf{x})\| \le L_{PH}^{(1)} \|\boldsymbol{\eta} - \boldsymbol{\eta}'\|, \ \forall \ (\boldsymbol{\eta}, \boldsymbol{\eta}') \in \mathcal{H}^2.$$

- \implies smoothness of $\hat{H}_{\eta}(x)$, satisfied if P_{η} , $H_{\eta}(X)$ are smooth w.r.t. η .
- 3. It holds that $\sup_{\eta \in \mathcal{H}, x \in X} \|H_{\eta}(x) h(\eta)\| \leq \sigma$.
- \Longrightarrow requires the noise is *uniformly bounded* for all $x \in X$.

Example: assumptions 1 & 2 are satisfied if the Markov kernel P_{n_n} is geometrically ergodic + smooth, and the drift term is smooth w.r.t. η .

Theorem 2. Suppose that the step sizes are decreasing and $\gamma_1 \leq 0.5(c_1(L+C_h))^{-1}$ (+other conditions). Let $V_{0,n}:=\mathbb{E}[V(\boldsymbol{\eta}_0)-V(\boldsymbol{\eta}_{n+1})]$,

$$\mathbb{E}[\|h(\boldsymbol{\eta}_N)\|^2] \leq \frac{2c_1(V_{0,n} + C_{0,n} + (\sigma^2 L + C_{\gamma}) \sum_{k=0}^n \gamma_{k+1}^2)}{\sum_{k=0}^n \gamma_{k+1}} + 2c_0.$$

- Set $\gamma_k = (2c_1L(1+C_h)\sqrt{k})^{-1} \Longrightarrow \mathbb{E}[\|h(\boldsymbol{\eta}_N)\|^2] = \mathcal{O}(c_0 + \log n/\sqrt{n})$ (same as Case 1).
- ullet Proof idea: challenge is that e_{n+1} is not zero-mean \Longrightarrow bound the sum of $\mathbb{E}[\langle \nabla V(\eta_n) | e_{n+1} \rangle]$ w/ Poisson equation + a novel decomposition (cf. Lemma 2).

Regularized Online EM Algorithm

• Special Case of GMM: we fit the data $\{Y_n\}_{n\geq 1}$, $Y_n\sim \pi$ into the parametric model with $\boldsymbol{\theta} = (\{\omega_m\}_{m=1}^{M-1}, \{\mu_m\}_{m=1}^{M})$

$$g(y; \boldsymbol{\theta}) \propto \left(1 - \sum_{m=1}^{M-1} \omega_m\right) \exp\left(-\frac{(y - \mu_M)^2}{2}\right) + \sum_{m=1}^{M-1} \omega_m \exp\left(-\frac{(y - \mu_m)^2}{2}\right)$$
,

• Data arrives in a streaming fashion, Cappé and Moulines (2009) does:

E-step:
$$\hat{s}_{n+1} = \hat{s}_n + \gamma_{n+1} \{ \overline{s}(Y_{n+1}; \hat{\theta}_n) - \hat{s}_n \}$$
,
M-step: $\hat{\theta}_{n+1} = \overline{\theta}(\hat{s}_{n+1})$.

ullet The **E-step** is a biased SA step on s with the drift term & mean field

$$H_{\hat{m{s}}_n}(Y_{n+1}) = \hat{m{s}}_n - \overline{m{s}}(Y_{n+1}; \overline{m{ heta}}(\hat{m{s}}_n)), \quad h(\hat{m{s}}_n) = \hat{m{s}}_n - \mathbb{E}_{\pi}igl[\overline{m{s}}(Y_{n+1}; \overline{m{ heta}}(\hat{m{s}}_n))igr]$$

Analysis of the ro-EM Algorithm (Application of Case 1)

Consider the KL divergence as a function of sufficient statistics s:

$$V(s) := \mathsf{KL}(\pi|g(\cdot; \overline{\boldsymbol{\theta}}(s))) + \mathsf{R}(\overline{\boldsymbol{\theta}}(s)) = \mathbb{E}_{\pi}\big[\log\big(\pi(Y)/g(Y; \overline{\boldsymbol{\theta}}(s))\big)\big] + \mathsf{R}(\overline{\boldsymbol{\theta}}(s)).$$

Corollary 1. Set $\gamma_k = (2c_1L(1+\sigma_1^2)\sqrt{k})^{-1}$. Ro-EM method for GMM finds \hat{s}_N such that

$$\mathbb{E}[\|\nabla V(\hat{\boldsymbol{s}}_N)\|^2] = \mathcal{O}(\log n/\sqrt{n})$$

The expectation is taken w.r.t. N and the observation law π .

- First explicit non-asymptotic rate given for online EM method.
- Consider a slightly modified/regularized M-step update for satisfaction of the technical conditions.

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(Online) Policy Gradient Method

- Consider a Markov Decision Process (MDP) (S, A, R, P):
- -S, A is the finite set of state/action.
- -R: $S \times A \rightarrow [0, R_{max}]$ is a reward function; P is the transition model.
- ullet A **policy** is parameterized by $oldsymbol{\eta} \in \mathbb{R}^d$ as (e.g., soft-max):

$$\Pi_{\eta}(a';s') = \text{probability of taking action } a' \text{ in state } s'$$

 \bullet Update η in an online fashion (Tadić and Doucet, 2017) using observed stateaction pair:

$$G_{n+1} = \lambda G_n + \nabla \log \Pi_{\boldsymbol{\eta}_n}(A_{n+1}; S_{n+1})$$
,
 $\boldsymbol{\eta}_{n+1} = \boldsymbol{\eta}_n + \gamma_{n+1}G_{n+1}\operatorname{R}(S_{n+1}, A_{n+1})$

where $\lambda \in (0,1)$ is a parameter for the variance-bias trade-off.

 \bullet The η -update is an biased SA step with the drift term:

$$H_{n_n}(X_{n+1}) = G_{n+1} R(S_{n+1}, A_{n+1})$$

Analysis of Policy Gradient Method (Application of Case 2)

Let $v_n(s, a)$ be the invariant distribution of $\{(S_t, A_t)\}_{t>1}$, we consider:

$$J(oldsymbol{\eta}) := \sum_{s \in \mathsf{S}, a \in \mathsf{A}} v_{oldsymbol{\eta}}(s, a) \, \mathsf{R}(s, a)$$
 .

Corollary 2. Set $\gamma_k = (2c_1L(1+C_h)\sqrt{k})^{-1}$. For any $n \in \mathbb{N}$, the policy gradient algorithm (3) finds a policy that

$$\mathbb{E}\big[\|\nabla J(\boldsymbol{\eta}_N)\|^2\big] = \mathcal{O}\Big((1-\lambda)^2\Gamma^2 + c(\lambda)\log n/\sqrt{n}\Big),$$

where $c(\lambda) = \mathcal{O}(\frac{1}{1-\lambda})$. Expectation is taken w.r.t. N and (A_n, S_n) .

- It shows the *first convergence rate* for the online PG method.
- Our result shows the *variance-bias trade-off* with $\lambda \in (0, 1)$.
- ullet Setting $\lambda \to 1$ reduces the bias, but decreases the convergence speed.

Conclusion

- Theorem 1 & 2 show the non-asymptotic convergence rate of biased SA scheme with smooth (possibly non-convex) Lyapunov function.
- ullet With appropriate step size, in *n* iterations the SA scheme finds $\mathbb{E}[\|h(\eta_N)\|^2] = 0$ $\mathcal{O}(c_0 + \log n/\sqrt{n})$, where c_0 is the bias and $h(\cdot)$ is the mean field.
- Applications to online EM and online policy gradient.

References

Jalaj Bhandari, Daniel Russo, and Raghav Singal. A finite time analysis of temporal difference learning with linear function approximation. In Conference On Learning Theory, pages 1691–1692, 2018.

Olivier Cappé and Eric Moulines. On-line Expectation Maximization algorithm for latent data models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 71(3):593–613, 2009.

John C Duchi, Alekh Agarwal, Mikael Johansson, and Michael I Jordan. Ergodic mirror descent. SIAM Journal on Optimization, 22(4):1549–1578, 2012.

Saeed Ghadimi and Guanghui Lan. Stochastic first-and zeroth-order methods for nonconvex stochastic programming. SIAM Journal on Optimization, 23(4):2341–2368, 2013.

Herbert Robbins and Sutton Monro. A stochastic approximation method. The Annals of Mathematical Statistics, 22(3):400-407, 1951.

Tao Sun, Yuejiao Sun, and Wotao Yin. On Markov chain gradient descent. In Advances in Neural Information Processing Systems 31, pages 9918–9927. Curran Associates, Inc., 2018.

Vladislav B Tadić and Arnaud Doucet. Asymptotic bias of stochastic gradient search. The Annals of Applied Probability, 27(6):3255-3304, 2017.