Stochastic Methods in Variational Inequalities: Ergodicity, Bias and Refinements



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Motivation

• Probably, any interesting ML problem can be categorized in one of the following classical frameworks:



Motivation

• In this work, we aim to answer a question in the intersection of these three worlds:





Our Task

For a problem Π & a method Alg : *Does* Alg *produce an unbiased estimator for the solution of our problem ?* $\Pr[Alg(\Pi, Z_n) \xrightarrow[n \to \infty]{} SOL(\Pi, Z)] = 1$

Variational Inequality Problem (VIP)

• Variational Inequality Problem:

Find $x^* \in \mathscr{X} \subseteq \mathbb{R}^d$ s.t. $\langle V(x^*), x - x^* \rangle \ge 0$, for all $x \in \mathscr{X}$ where $V : \mathscr{X} \to \mathbb{R}^d$ is some operator.

- Example 1: Loss minimization
 - $V = \nabla f$: the gradient of some loss function $f: \mathbb{R}^d \to \mathbb{R}$
 - VIP: find a stationary point of f, i.e., $\nabla f(x^*) = 0$
- Example 2: Fixed point problem
 - V(x) = F(x) x for some function F
 - VIP: solves the fixed-point equation $F(x^*) x^* = 0$.
- Example 3: Saddle-point problem
 - $L: \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \to \mathbb{R}, \ L(x_1, x_2):$ cost for player choosing x_1 , payoff for player x_2
 - $V = (\nabla_{x_1}L, -\nabla_{x_2}L)$, VIP finds saddle point of L: min max $L(x_1, x_2)$



 x_2

Stochastic Methods for VIP

• Variational Inequality Problem:

Find $x^* \in \mathscr{X} \subseteq \mathbb{R}^d$ s.t. $\langle V(x^*), x - x^* \rangle \ge 0$, for all $x \in \mathscr{X}$ where $V : \mathscr{X} \to \mathbb{R}^d$ is some operator.

- Typically, the exact function V is unknown, corrupted, biased
- The optimizer has access to **stochastic** estimate of *V*: given an input *x*, $\hat{V}(x) = V(x) + U(x)$, where $U(\cdot)$ is any kind of noise/sample/uncertainty

Goal: Use stochastic estimates to find x*

The New York Times

Opinion

OP-ED CONTRIBUTOR

When an Algorithm Helps Send You to Prison





Stochastic Methods for VIP: SGDA and SEG

• Stochastic Gradient Descent Ascent (SGDA) [Nemirovski et al '09]:

$$x_{t+1} = x_t - \gamma_t \Big(V(x_t) + U_t(x_t) \Big)$$

- $\gamma_t > 0$: stepsize
- For loss minimization problems: SGDA reduces to SGD
- Stochastic Extra Gradient (SEG) [Korpelevich '76]: at each iteration t

$$\begin{aligned} x_{t+1/2} &= x_t - \gamma_t \Big(V(x_t) + U_{t+1/2}(x_t) \Big), & \text{\%Ex} \\ x_{t+1} &= x_t - \eta_t \Big(V(x_{t+1/2}) + U_t(x_{t+1/2}) \Big) & \text{\%up} \\ \bullet & \gamma_t > 0, \ \eta_t > 0: \text{ stepsizes} \end{aligned}$$

tra look-ahead step

date

Classical asymptotic convergence results with diminishing stepsizes

SGDA:
$$\sum_{t} \gamma_{t} = \infty$$
, and $\sum_{t} \gamma_{t}^{2} < \infty$
SEG: $\sum_{t} \gamma_{t} \eta_{t} = \infty$, $\sum_{t} \gamma_{t}^{2} \eta_{t} < \infty$ and $\sum_{t} \eta_{t}^{2} < \infty$ [Hsieh '20]
Standard Example: $\gamma_{t} = 1/\sqrt{t}$ For Simplicity $\mathscr{X} = \mathbb{R}^{4}$



- Using constant stepsizes:
 - Might be non-convergent
 - But faster converges to the neighborhood
- Goal: A fine-grained characterization of *distributional* behaviors of SEG/SGDA with constant stepsize



Recent Non-asymptotic Results (Incomplete List)

- SGDA/SEG and variants: constant or diminishing stepsizes
 - Upper-bound on <u>mean-squared error (MSE)</u> $\mathbb{E} \|x_t x^*\|^2$ or

<u>vector-field amplitude</u> $\mathbb{E} \left\| V(x_t) \right\|^2$ or other metrics ...

[Gorbuno-Berard-Gidel-Loizou, '22] [Gorbunov-Loizou-Gidel '22] [Hsie-Iutzeler-Malick-Mertikopoulos, '20] [Beznosikov-Gorbunov-Berard-Loizou, '23]...

- Special case of VI: Constant stepsize SGD and Stochastic approximation
 - Study $\{x_t\}$ from the lens of Markov chain
 - Distributional convergence, characterization of stationary distribution
 - SGD for strongly convex objectives: [Dieuleveut-Durmus-Bach '20]
 - SGD for non-smooth non-convex functions: [Yu-Balasubramania-Volgushev-Erdogdu, '21]
 - Linear stochastic approximation with Markovian data: [Huo-Chen-Xie, '23]

Today Question...What is the distribution of x_t ?

This Talk: Weak Quasi Strongly Monotone Operator V

• The operator V is λ -weak μ -quasi strongly monotone with $\lambda \ge 0, \ \mu > 0$

$$\langle V(x), x - x^* \rangle \ge \mu \|x - x^*\|^2 - \lambda, \quad \forall x \in \mathbb{R}^d.$$

- (Quasi-)strong monotonicity
 - Resemble the notion of (quasi-)strong convexity in optimization literature
- μ -quasi strongly monotone: relaxation of μ -strong monotone:

$$\langle V(x) - V(x'), x - x' \rangle \ge \mu \|x - x'\|^2, \quad \forall x, x' \in \mathbb{R}^d.$$

- λ -weak
 - Resemble the notion of weak convex optimization
- Assume the operator *V* is at most *L*-linear growth, i.e., $||V(x)|| \le L(1 + ||x||), \quad \forall x \in \mathbb{R}^d.$



For Simplicity $\mathscr{X} = \mathbb{R}^d$

Our Analytical Approach: the Lens of Markov Chain

• Stochastic Gradient Descent Ascent (SGDA):

$$x_{t+1} = x_t - \gamma \Big(V(x_t) + U_t(x_t) \Big)$$

• Stochastic Extra Gradient (SEG) [Korpelevich '76]: at iteration t

$$\begin{aligned} x_{t+1/2} &= x_t - \gamma \Big(V(x_t) + U_{t+1/2}(x_t) \Big), & \text{\%Extra look-ahead step} \\ x_{t+1} &= x_t - \eta \Big(V(x_{t+1/2}) + U_t(x_{t+1/2}) \Big) & \text{\%update} \end{aligned}$$

- Assumptions on noise:
 - Zero-mean: $\|\mathbb{E}[U_t(x_t) | \mathcal{F}_t]\| \le b_{\text{bias}};$
 - Bounded variance: $\mathbb{E}[\|U_t(x_t)\|^2 | \mathcal{F}_t] \le \sigma_{\text{variance}}^2 + \rho^2 d(x_t, \mathcal{X}^*)$
- Key observations: with constant stepsizes,
 - the iterates $\{x_t\}_{t>0}$ of SGDA/SEG forms a **homogeneous Markov chain in** \mathbb{R}^d .

Roadmap for Understanding Distributional Properties

• For a homogeneous Markov chain $\{x_t\}_{t>0}$ in **continuous** state space \mathbb{R}^d :



[Meyn-Tweedie, '09]

First Result: Convergence up to Constant Factors

Theorem 1

Under previous assumptions, for SGDA with γ satisfies $\gamma < \frac{\mu}{L^2}$, then for any initial point $x_0 \in \mathbb{R}^d$, $\mathbb{E}[\|x_t - x^*\|^2] \le (1 - c_1)^t \|x_0 - x^*\|^2 + c_2$, with $c_1 \ge \mu \gamma$, $c_2 \le \frac{\lambda + \gamma \sigma^2}{\mu}$.

- Similar guarantee for SEG
- Byproduct of the proof: Geometric Lyapunov drift condition

$$\mathbb{E}\Big[W(x_{t+1}) - W(x_t) \mid \mathcal{F}_t\Big] \le -\beta W(x_t) + b\mathbb{I}_C(x)$$

where W(x): = $||x - x^*||^2 + 1$, and C is bounded set.

Main Results: Harris Positive Recurrence of Markov Chain

Theorem 2

Under previous assumptions, the iterates $\{x_t\}_{t\geq 0}$ of SGDA/SEG is a Harris positive recurrent Markov chain.

- 1. It admits a unique stationary distribution π_{γ} ;
- 2. For each test function $\phi : \mathbb{R}^d \to \mathbb{R}$ with $\|\phi(x)\| \le L_{\phi}(1 + \|x\|)$,

$$\left|\mathbb{E}[\phi(x_t)] - \mathbb{E}_{\pi_{\gamma}}[\phi(x)]\right| \le c\rho^t,$$

where $\rho \in (0,1)$;

Main Results: LLN and CLT of Averaged Iterates

Theorem 3

Under previous assumptions, for any function ϕ with $\pi_{\gamma}(|\phi|) < \infty$,

1. (LLN)
$$\frac{1}{T} \sum_{t=0}^{T-1} \phi(x_t) \to \mathbb{E}_{\pi_{\gamma}}[\phi(x)]$$
, a.s.;

2. **(CLT)**
$$\frac{1}{\sqrt{T}} \sum_{t=0}^{T-1} \left[\phi(x_t) - \mathbb{E}_{\pi_{\gamma}}[\phi(x)] \right] \xrightarrow{d} N(0, Var_{\pi_{\gamma}}(\phi)).$$

- Implication: Statistical inference
 - CLT results can be used for constructing confidence intervals.
- But how far $\mathbb{E}_{\pi_{\gamma}}[x]$ is away from x^* ?

Main Results: Bias Characterization w.r.t. step-size



- Implication: Richardson-Romberg (RR) extrapolation for bias reduction
 - Run SGDA with two stepsizes γ and 2γ in parallel
 - Let $\{\bar{x}_t^{(\gamma)}\}, \{\bar{x}_t^{(2\gamma)}\}\)$ be the averaging iterates
 - Richardson-Romberg (RR)-extrapolated iterate:

$$\hat{x}_{t} := 2\bar{x}_{t}^{(\alpha)} - \bar{x}_{t}^{(2\alpha)}$$

$$\rightarrow 2\mathbb{E}_{\pi_{\gamma}}[x] - \mathbb{E}_{\pi_{2\gamma}}[x] \quad \text{(LLN)}$$

$$= x^{*} + O(\gamma^{2})$$

Bias reduced from $\gamma \Delta(x^*) + O(\gamma^2)$ to $O(\gamma^2)$

Numerical Result: Normality and Bias



• SEG/SGDA for min-max game with $\min_{x_1} \max_{x_2} L(x_1, x_2)=0$

Numerical Results: RR for Bias Reduction in Zero-sum Games



• SGDA for min-max problems

Summary

- Stochastic VIP: Constant Stepsize + Ergodicity + Bias Reduction
 - Constant stepsize: <u>fast convergence</u> with exponential decay rate of optimization error
 - Polyak-Ruppert average: <u>LLN and Asymptotic normality</u>
 - RR Extrapolation: reduce bias
- Extensions:
 - Beyond martingale noise: Markovian noise (Goal Multi-agent RL)
 - Statistical inference: variance estimation and CI construction
 - Constant stepsize with RR extrapolation

