Stochastic Extragradient with Flip-Flop Anchoring: Provable Improvements

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Minimax Problems

We consider unconstrained minimax problems with a *finite-sum* structure:

$$\min_{\boldsymbol{x}} \max_{\boldsymbol{y}} f(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{n} \sum_{i=1}^{n} f_i(\boldsymbol{x}, \boldsymbol{y}).$$

Very versatile, and has many ML applications:

- Generative Adversarial Networks
- Consistency Trajectory Models
- Sharpness-aware Minimization
- Computing Optimal Transport Maps

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$$\min_{\boldsymbol{x}} \max_{\boldsymbol{y}} f(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{n} \sum_{i=1}^{n} f_i(\boldsymbol{x}, \boldsymbol{y}).$$

Denote both min. and max. variables at once by $m{z}\coloneqq(m{x},m{y}).$

The saddle gradient

$$oldsymbol{F}(oldsymbol{z}) = egin{bmatrix}
abla_{oldsymbol{x}} f(oldsymbol{x},oldsymbol{y}) \
-
abla_{oldsymbol{y}} f(oldsymbol{x},oldsymbol{y}) \end{bmatrix}$$

is more natural than ∇f in minimax problems.

The Extragradient Method

The gradient descent-ascent (GDA) method

$$oldsymbol{z}_{k+1} = oldsymbol{z}_k - \eta_k oldsymbol{F}(oldsymbol{z}_k)$$
 or $oldsymbol{x}_{k+1} = oldsymbol{x}_k - \eta_k
abla_{oldsymbol{x}} f(oldsymbol{x}_k, oldsymbol{y}_k)$
 $oldsymbol{y}_{k+1} = oldsymbol{y}_k + \eta_k
abla_{oldsymbol{y}} f(oldsymbol{x}_k, oldsymbol{y}_k)$

already does not work for simple convex-concave problems.

The extragradient (EG) method (Korpelevich, 1976)

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on the other hand, works on convex-concave problems.

Stochastic Extragradient?

Unlike GDA vs EG, the stochastic EG (SEG)

$$oldsymbol{z}_{k+1} = oldsymbol{z}_k - \eta_k oldsymbol{F}_{i(k)}(oldsymbol{z}_k - \eta_k oldsymbol{F}_{i(k)}(oldsymbol{z}_k))$$

does not show a clear advantage in convex-concave problems over GDA.

Even if we additionally assume each f_i are also convex-concave, convergence rates typically look something like:

$$\min_{k=0,1,\dots,K} \|\boldsymbol{F}\boldsymbol{z}_k\|^2 \leq \mathcal{O}\left(\frac{1}{\operatorname{poly}(K)}\right) + (\mathsf{abs. const.})$$

* The constant term can be decreased only with strong additional assumptions, such as for example, increasing the batch size every iteration.

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For minimization problems...

With-replacement stochastic gradient descent (SGD) works well.

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \eta_k \nabla f_{i(k)}(\boldsymbol{x}_k), \qquad i(k) \sim \mathrm{Unif}(\{1, \dots, n\})$$

In practice, *shuffling based* SGD is used.

Random reshuffling (RR): in the *k*th epoch, a permutation $\tau_k : \{1, \ldots, n\} \rightarrow \{1, \ldots, n\}$ is chosen randomly, and

$$\begin{aligned} \boldsymbol{x}_{i}^{k} &= \boldsymbol{x}_{i-1}^{k} - \eta_{k} \nabla f_{\tau_{k}(i)}(\boldsymbol{x}_{i-1}^{k}), \qquad i = 1, \dots, n, \\ \boldsymbol{x}_{0}^{k+1} \leftarrow \boldsymbol{x}_{n}^{k}. \end{aligned}$$

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For minimization problems...

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$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \eta_k \nabla f_{i(k)}(\boldsymbol{x}_k), \qquad i(k) \sim \mathrm{Unif}(\{1, \dots, n\})$$

In practice, *shuffling based* SGD is used.

Flip-flop sampling (FF) (Rajput et al., 2022) goes one step even further in search for a better sampling scheme: in the *k*th epoch, a permutation $\tau_k : \{1, \ldots, n\} \rightarrow \{1, \ldots, n\}$ is chosen randomly, and

$$\begin{aligned} \boldsymbol{x}_{i}^{k} &= \boldsymbol{x}_{i-1}^{k} - \eta_{k} \nabla f_{\tau_{k}(i)}(\boldsymbol{x}_{i-1}^{k}), & i = 1, \dots, n, \\ \boldsymbol{x}_{i}^{k} &= \boldsymbol{x}_{i-1}^{k} - \eta_{k} \nabla f_{\tau_{k}(2n+1-i)}(\boldsymbol{x}_{i-1}^{k}), & i = n+1, \dots, 2n, \\ \boldsymbol{x}_{0}^{k+1} &\leftarrow \boldsymbol{x}_{2n}^{k}. \end{aligned}$$

For minimization problems...

With-replacement stochastic gradient descent (SGD) works well.

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \eta_k \nabla f_{i(k)}(\boldsymbol{x}_k), \qquad i(k) \sim \mathrm{Unif}(\{1, \dots, n\})$$

In practice, *shuffling based* SGD is used.

In terms of convergence rates,

• RR is in general faster than with-replacement SGD.

(Ahn et al., 2020; Mishchenko et al., 2020)

• If all f_i are quadratic functions then FF is even faster, thanks to the stochastic error term being smaller. (Rajput et al., 2022)

Our contributions

- Stochastic EG indeed does not work on convex-concave problems. Shuffling does not resolve the problem.
 - An explicit counterexample with divergent iterates
- On top of FF, adding a simple *anchoring* step

$$\boldsymbol{z}_0^{k+1} \leftarrow \frac{\boldsymbol{z}_{2n}^k + \boldsymbol{z}_0^k}{2}$$

reduces the stochastic error by an order of magnitude (w.r.t. stepsize), finally allowing a convergence rate of $\tilde{O}(1/k^{1/3})$.

- The reduced error also benefits the convergence on strongly-convexstrongly-concave problems, enjoying a rate of $\tilde{O}(1/nk^4)$.
 - Without anchoring (*i.e.*, with-replacement sampling or RR only), the convergence rate is at best $\Omega(1/nk^3)$.

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Algorithm

Stochastic Extragradient with Flip-Flop Anchoring (SEG-FFA)

$$\begin{array}{lll} \text{For each } k=0,1,\ldots: & \text{ $$\#$ epoch level outer loop$}\\ \tau_k\sim \text{Unif}(\mathfrak{S}_n) & \text{ $$\#$ sample random permutation$}\\ \text{For each } i=1,\ldots,n: & \text{ $$\#$ flip$}\\ z_i^k=z_{i-1}^k-\eta_k F_{\tau_k(i)}\left(z_{i-1}^k-\frac{\eta_k}{2}F_{\tau_k(i)}(z_{i-1}^k)\right) \\ \text{For each } i=n+1,\ldots,2n: & \text{ $$\#$ flop$}\\ z_i^k=z_{i-1}^k-\eta_k F_{\tau_k(2n+1-i)}\left(z_{i-1}^k-\frac{\eta_k}{2}F_{\tau_k(2n+1-i)}(z_{i-1}^k)\right) \\ z_0^{k+1}\leftarrow \frac{z_{2n}^k+z_0^k}{2} & \text{ $$\#$ anchoring$} \end{array}$$

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Thank you for your attention.

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References I

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