Zeroth-Order (Gradient-Free) Optimization

• Zeroth-order (gradient-free) optimization approximates the full gradient via a random gradient estimate.

Summary of Our Work

We investigate the convergence of ZO stochastic projected gradient descent (ZO-SPGD) for *constrained* convex/nonconvex optimization. Our work is motivated by the ZO proximal gradient algorithm proposed in [1]. However, the ZO gradient estimator considered in [1] is different from our work: we construct the gradient estimate through random direction samples drawn from a bounded uniform distribution rather than a Gaussian distribution in [1]. This analysis leads to different statistics of our random gradient estimator. We establish the following convergence results.

- ZO-SPGD has a $O(\frac{d}{bq\sqrt{T}} + \frac{1}{\sqrt{T}})$ convergence rate to minimize convex (but possibly *non-smooth*) loss functions.
- For constrained *nonconvex* optimization, ZO-SPGD yields a $O(\frac{1}{\sqrt{T}})$ convergence rate up to an *additional error correction* term of order $O(\frac{d+q}{bq})$.

Problem Statement

Consider a constrained finite-sum problem of the form	
$\underset{\mathbf{x}\in\mathcal{C}}{\text{minimize }} f(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{x}),$	(1)
	_

where $\mathbf{x} \in \mathbb{R}^d$ is the optimization variable, $\mathcal{C} \in \mathbb{R}^d$ is a closed convex set, and $\{f_i(\mathbf{x})\}$ are *n* component functions (not necessarily convex).

We consider the problem setting in which A1 and/or A2 are satisfied.

A1: Functions $\{f_i\}$ are L_1 -Lipschitz continuous for a finite positive constant L_1 .

A2: Functions $\{f_i\}$ are differentiable and have L_2 -Lipschitz continuous gradients, where L_2 is a finite positive constant.

A1 allows $\{f_i\}$ to be non-differentiable and implies that subgradients of $\{f_i\}$ are bounded. When A2 holds, $\{f_i\}$ are restricted to differentiable functions and it implies that

$$f_i(\mathbf{x}) - f_i(\mathbf{y}) \le \nabla f_i(\mathbf{y})\mathbf{x} - \mathbf{y} + (L_2/2) \|\mathbf{x} - \mathbf{y}\|^2.$$

Zeroth-Order Stochastic Projected Gradient Descent for Nonconvex Optimization

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Random Gradient Estimation

Given an *arbitrary* function f (not necessarily in a finite-sum form), a twopoint based <u>average random</u> gradient <u>estimator</u> $\hat{\nabla} f(\mathbf{x})$ is defined by

$$\hat{\nabla}f(\mathbf{x}) = \frac{d}{q} \sum_{j=1}^{q} \frac{f(\mathbf{x} + \mu \mathbf{u}_j) - f(\mathbf{x} - \mu \mathbf{u}_j)}{2\mu} \mathbf{u}_j, \qquad \text{(Avg-RandGradEst)}$$

where d is the number of optimization variables, $\mu > 0$ is a smoothing parameter, and $\{\mathbf{u}_j\}$ are i.i.d. random directions drawn from a uniform distribution over a unit sphere.

Lemma 1: Statistics of random gradient estimate

Define $f_{\mu} = \mathbb{E}_{\mathbf{v} \in U_{b}}[f(\mathbf{x} + \mu \mathbf{v})]$, where U_{b} denotes a uniform distribution with respect to the unit Euclidean ball. Then Avg-RandGradEst yields the following results:

a) For any
$$\mathbf{x} \in \mathbb{R}^{d}$$

$$\mathbb{E}\left[\hat{\nabla}f(\mathbf{x})\right] = \mathbb{E}_{\mathbf{u}}\left[(d/\mu)f(\mathbf{x}+\mu\mathbf{u})\mathbf{u}\right] = \nabla f_{\mu}(\mathbf{x}), \qquad (2)$$

where **u** is a vector picked uniformly at random from the Euclidean unit sphere. Moreover, under assumptions **A1**, the smoothing function f_{μ} is L_1 -Lipschitz continuous. Under **A2**, f_{μ} has L_2 -Lipschitz continuous gradient. b) Suppose that assumption **A1** holds, for any $\mathbf{x} \in \mathbb{R}^d$

$$\mathbb{E}\left[\|\hat{\nabla}f(\mathbf{x})\|^{2}\right] \leq \frac{(c_{1}d + 4q)L_{1}^{2}}{4q},$$
(3)

and under assumption A2, for any $\mathbf{x} \in \mathbb{R}^d$

$$\mathbb{E}\left[\|\hat{\nabla}f(\mathbf{x})\|^{2}\right] \leq 2\left(1+\frac{d}{q}\right)\|\nabla f(\mathbf{x})\|_{2}^{2} + \left(1+\frac{1}{q}\right)\frac{\mu^{2}L_{2}^{2}d^{2}}{2},\tag{4}$$

where the expectation is taken with respect to random direction vectors $\{\mathbf{u}_j\}$ in Avg-RandGradEst, and c_1 is a numerical constant in (3).

Lemma 1 uncovers important properties of Avg-RandGradEst.

- The use of multiple (q > 1) random direction vectors $\{\mathbf{u}_j\}$ does not reduce the bias of $\hat{\nabla} f$ (with respect to ∇f). That is because $\hat{\nabla} f$ is unbiased with respect to ∇f_{μ} , and the distance between ∇f and ∇f_{μ} is fixed: As $\mu \to 0$, we obtain $\nabla f_{\mu}(\mathbf{x}) \to \nabla f(\mathbf{x})$. However, if μ is too small, then the function difference could be dominated by the system noise and fails to represent the function differential.
- The variance of the random gradient estimator is reduced as q increases. In particular, a large q mitigates the dimension (d) dependency on the second-order moment of Avg-RandGradEst.

Algorithm

- 1: Input: Total number of iterations T, step sizes $\{\eta_k\}_{k=0}^{T-1}$, mini-batch size b, initial iterate $\mathbf{x}_0 \in \mathcal{C}$,
- 2: for $k = 0, 1, \dots, T 1$ do
- 3: choose a mini-batch \mathcal{I}_k with b i.i.d. samples from [n]
- 4: compute a gradient estimate $\hat{\mathbf{g}}_k = \frac{1}{b} \sum_{i \in \mathcal{I}_k} \hat{\nabla} f_i(\mathbf{x}_k)$
- 5: project onto $\pi_{\mathcal{C}}$

$$\mathbf{x}_{k+1} = \Pi_{\mathcal{C}} \left[\mathbf{x}_k - \eta_k \hat{\mathbf{g}}_k \right] \tag{5}$$

6: **end for**

7: output: \mathbf{x}_R averaged/sampled from $\{\mathbf{x}_k\}_{k=0}^{T-1}$

Convergence Analysis: Convex Case

Theorem 1: Convergence rate of ZO-SPGD for convex optimization

Suppose that assumption **A1** holds and f in problem (1) is convex. Given $\eta_k = \eta$, $\|\mathbf{x}_0 - \mathbf{x}^*\| \leq R$, and $\mathbf{x}_R = \frac{1}{T} \sum_{k=0}^{T-1} \mathbf{x}_k$ in Algorithm 1, then $\mathbb{E}[f(\mathbf{x}_R) - f(\mathbf{x}^*)] \leq \frac{R^2}{\eta T} + \frac{(c_1 d + 4q)L_1^2}{4bq} \eta + L_1^2 \eta + 2L_1 \mu.$

In Theorem 1, let $\eta = \frac{1}{\sqrt{T}}$ and $\mu = \frac{1}{\sqrt{T}}$ (milder conditions than many other works), we obtain the convergence rate $O(\frac{d}{bq\sqrt{T}} + \frac{1}{\sqrt{T}})$. We can also conclude that the use of multiple minibatch samples (b) and random direction vectors (q) improves the convergence rate of ZO-SPGD.

Convergence Analysis: Nonconvex Case

For constrained non-convex problems, the convergence of an algorithm at point \mathbf{x}_k can be measured by 'gradient mapping' [2, 1],

$$P_{\mathcal{C}}(\mathbf{x}_k, \nabla f(\mathbf{x}_k), \eta) = (1/\eta) \left[\mathbf{x}_k - \Pi_{\mathcal{C}} \left(\mathbf{x}_k - \eta \nabla f(\mathbf{x}_k) \right) \right].$$
(6)

Interpretation: projected gradient, which offers a feasible update from the previous point \mathbf{x}_k ,

$$\Pi_{\mathcal{C}}(\mathbf{x}_{k} - \eta \nabla f(\mathbf{x}_{k})) = \mathbf{x}_{k} - \eta P_{\mathcal{C}}(\mathbf{x}_{k}, \nabla f(\mathbf{x}_{k}), \eta).$$

bound $\mathbb{E}[\|P_{\mathcal{C}}(\mathbf{x}_{k}, \nabla f(\mathbf{x}_{k}), \eta)\|_{2}^{2}]$

Our goal is to bound $\mathbb{E}[\|P_{\mathcal{C}}(\mathbf{x}_k, \nabla f(\mathbf{x}_k), \eta)\|_2^2].$

Proposition 1: Relationship between the variance of a gradient estimator and the convergence rate

If assumption **A2** holds and $\eta_k \in (0, 1/L_2)$, then the outputs $\{\mathbf{x}_k\}_{k=0}^{T-1}$ of Algorithm 1 satisfies

$$\sum_{k=0}^{T-1} \left(\left(2\eta_k - L_2 \eta_k^2 \right) \mathbb{E} \left[\| P_{\mathcal{C}}(\mathbf{x}_k, \hat{\mathbf{g}}_k, \eta_k) \|^2 \right] \right)$$

$$\leq \sum_{k=0}^{T-1} \left(2\eta_k \mathbb{E} \left[\| \hat{\mathbf{g}}_k - \mathbb{E}[\hat{\mathbf{g}}_k | \mathbf{x}_k]] \|^2 \right] \right) + 2\mu^2 L_2 + c_2 d_2$$

where \mathbb{E} is taken with respect to all the randomness (e.g., minibatch and random directions), $P_{\mathcal{C}}$ is the gradient mapping given by (6), and $c_2 = 2(f(\mathbf{x}_0) - f(\mathbf{x}^*))$.

Theorem 2: Convergence rate of ZO-SPGD for nonconvex optimization

Suppose that A1-A2 hold, and $\eta_k \in (0, 2/L_2)$. By randomly selecting \mathbf{x}_R from $\{\mathbf{x}_k\}_{k=0}^{T-1}$ with probability

$$P(R = k) = \frac{2\eta_k - L_2\eta_k^2}{\sum_{k=0}^{T-1} (2\eta_k - L_2\eta_k^2)},$$

the convergence rate of Algorithm 1 is given by

T 1

$$\mathbb{E}\left[\|P_{\mathcal{C}}(\mathbf{x}_{R}, \nabla f(\mathbf{g}_{R}), \eta_{R})\|^{2} \right]$$

$$\leq \frac{3(c_{1}d + 4q)L_{1}^{2}(\sum_{k=0}^{T-1} \eta_{k})}{2bq\sum_{k=0}^{T-1}(2\eta_{k} - L_{2}\eta_{k}^{2})} + \frac{6\mu^{2}L_{2} + 3c_{2}}{\sum_{k=0}^{T-1}(2\eta_{k} - L_{2}\eta_{k}^{2})} + \frac{3\mu^{2}L_{2}^{2}d^{2}}{4} + \frac{3(c_{1}d + 4q)L_{1}^{2}}{4bq}$$

$$(7)$$

Several insights can be drawn from Theorem 2.

- The first term in the convergence rate (7) is bounded by by $O(\frac{d+q}{bq})$ up to a constant factor.
- If we choose the constant stepsize $\eta = \frac{c_{\eta}}{\sqrt{T}} \in (0, 1/L_2)$ for some constant c_{η} and $\mu = \frac{1}{d^{1/2}(bq)^{1/2}}$, then Theorem 1 implies the convergence rate $O(\frac{1}{\sqrt{T}} + \frac{d+q}{bq})$.

References

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