ECE 8101: Nonconvex Optimization for Machine Learning

Lecture Note 4-1: Zeroth-Order Methods with Random Directions of Gradient Estimations

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Outline

In this lecture:

- Overview of Zeroth-Order Methods and Their Applications
- Representative Techniques for Random Directions of Gradient Estimations
- Convergence Results

Overview of Zeroth-Order Methods

- Zeroth-order (gradient free) method: Use only function values
  - Reinforcement learning [Malik et al., AISTATS'20]
  - Blackbox adversarial attacks on DNN [Papernot et al., CCS'17]
  - Or problems with structure making gradients difficult or infeasible to obtain
- Two major classes of zeroth-order methods
  - Methods that do not have any connections to gradient
    - Random search algorithm [Schumer and Steiglitz, TAC'68]
    - Nelder-Mead algorithm [Nelder and Mead, Comp J. '65]
    - Model-based methods [Conn et al., SIAM'09]
    - Stochastic three points methods (STP) [Bergou et al., SIAM J. Opt. '20]
    - STP with momentum [Gorbunov et al., ICLR'20]
  - Methods that rely on gradient estimations
    - More modern approach, the focus of this course

Reinforcement Learning

Model-based RL

MDP: $P(s_{t+1}, s_t, a_t)$ $r(s_t, a_t)$

Policy iteration $\pi_\theta(s,a)$

Value iteration $V(s)$

Dynamic Prog. &

Bellman Optimality Principle.

Opt. Ctrl: HJB

CT, DT, Linear/Nonlinear.

$\underline{x}(t+1) = f(\underline{x}(t), \underline{u}(t)) + n$

$\dot{\underline{x}} = f(\underline{x}, \underline{u}) + n.$

Actor-Critic.

$Q(s,a) = V(s) + A(s,a)$

DQN

Deep Policy Netw.

Deep RL

Model-free RL

Gradient-free

TD (temporal diff).

Bellman: $V(s) = \mathbb{E}[r_t + \gamma V(s_{t+1})]$

TD(0): $r_t + V(s_{t+1}) - V(s_t)$

$\vdots$

TD(n): – – – –

TD(λ): $R_\Sigma^\lambda - V(s_t)$

TD learning on Q-fn: $Q(s_t, a_t)$

Off-Policy (Q-learning)

exp. vs. exploit

On-Policy (SASAR).

Gradient-based Approach.

$\theta^{new} = \underline{\theta}^{old} + s\nabla_{\underline{\theta}} R_{\Sigma,\theta}$

Surrogate Obj: TRPO, PPO ...

Ex: Discrete-time Linear-Quadratic Regulator (LQR)

$(\underline{s}_t, \underline{a}_t)$: $\underline{s}_t \in \mathbb{R}^m$, $\underline{a}_t \in \mathbb{R}^k$

$$\begin{cases} c_t = \underline{s}_t^T \underline{\underline{Q}}\, \underline{s}_t + \underline{a}_t^T \underline{\underline{R}}\, \underline{a}_t \\ \underline{s}_{t+1} = \underline{\underline{A}}\, \underline{s}_t + \underline{\underline{B}}\, \underline{a}_t + \underline{v} \end{cases}$$

$(\underline{\underline{Q}}, \underline{\underline{R}} > 0)$, Q: $m\times m$, R: $k\times k$.

$(\underline{\underline{A}}, \underline{\underline{B}})$, A: $m\times m$, B: $m\times k$

$\Sigma^{-\frac{1}{2}}\underline{s}_{t+1} = \Sigma^{-\frac{1}{2}}\underline{\underline{A}}\,\underline{s}_t + \Sigma^{-\frac{1}{2}}\underline{\underline{B}}\,\underline{a}_t + \Sigma^{-\frac{1}{2}}\underline{v}$: s'_{t+1}, $\underline{\underline{A}}'$, $\underline{\underline{B}}'$, $\underline{v}'$

w.l.o.g. assume $\underline{v}$ a r. vec. $\underline{v} \sim D$ s.t. $\mathbb{E}[\underline{v}] = \underline{0}$ $\mathbb{E}[\underline{v}\underline{v}^T] = \underline{\underline{I}}$

$\mathbb{E}[\underline{v}\underline{v}^T] = \underline{\underline{\Sigma}}$ $\quad \underline{\underline{\Sigma}}^{-\frac{1}{2}}\underline{v}\underline{v}^T\underline{\underline{\Sigma}}^{-\frac{1}{2}} = \underline{\underline{I}}$

By classical opt. ctrl theory: $\underline{a}_t = -\underline{\underline{K}}^* \underline{s}_t$, where $\underline{\underline{K}}^*$ can be found by the dt-Riccati eqn. (assuming $\underline{\underline{A}}, \underline{\underline{B}}, \underline{\underline{Q}}, \underline{\underline{R}}$)

If we don't know $\underline{\underline{A}}, \underline{\underline{B}}, \underline{\underline{R}}, \underline{\underline{Q}}$, we can search over lin. policies:

1. Rand initialization: $C_{init}(\underline{\underline{K}}, \underline{s}_0) \leftarrow$ cost of executing a lin. policy $\underline{\underline{K}}$ from $\underline{s}_0$.

$$C_{init}(\underline{\underline{K}}, \underline{s}_0) = \sum_{t=0}^{\infty} (\underline{s}_t^T \underline{\underline{Q}}\, \underline{s}_t + \underline{a}_t^T \underline{\underline{R}}\, \underline{a}_t + \cancel{\underline{w}_t}) \gamma^t$$

ZO-opt.

Goal: $\min_{\underline{\underline{K}} \text{ "contrl'ble"}} C_{init,\gamma}(\underline{\underline{K}}) = \mathbb{E}_{s_0 \sim D_0}\left[C_{init,\gamma}(\underline{\underline{K}}, \underline{s}_0) \right]$

We don't know $\underline{\underline{A}}, \underline{\underline{B}}, \underline{\underline{Q}}, \underline{\underline{R}}$. Can only observe a noisy fn evaluation of $C_{init}(\underline{\underline{K}}, \underline{s}_0)$.

spectral radius.

A policy $\underline{\underline{K}}$ is said to be ctrl'ble for $(\underline{\underline{A}}, \underline{\underline{B}})$ if $\rho(\underline{\underline{A}} - \underline{\underline{K}}\,\underline{\underline{B}}) < 1$

$\{\underline{\underline{K}} : \rho(\underline{\underline{A}} - \underline{\underline{K}}\,\underline{\underline{B}}) < 1\}$

Note: 1°. LQR is locally Lipschitz

$$|C_{init,\gamma}(\underline{\underline{K}}', \underline{s}_0) - C_{init,\gamma}(\underline{\underline{K}}, \underline{s}_0)| \le \lambda \, \|\underline{\underline{K}}' - \underline{\underline{K}}\|_F$$

2°. LQR has locally Lipschitz cont. grad.

$$\|\nabla C_{init,\gamma}(\underline{\underline{K}}') - \nabla C_{init,\gamma}(\underline{\underline{K}})\|_F \le \phi \, \|\underline{\underline{K}}' - \underline{\underline{K}}\|_F.$$

3°. $C_{init,\gamma}(\underline{\underline{K}})$ is nonconvex: $\{K : \rho(\underline{\underline{A}} - \underline{\underline{K}}\,\underline{\underline{B}}) < 1\}$ is nonconvex.

4°. LQR is PL.

Basic Idea of (Deterministic) Gradient Estimation

- Gradient estimation with finite-difference directional derivative estimation:

$$\text{(Forward version): } \mathbf{g}(\mathbf{x}) = \sum_{i=1}^{d} \frac{f(\mathbf{x}+\mu\mathbf{e}_i) - f(\mathbf{x})}{\mu}\mathbf{e}_i,$$

d+1

2d.

$$\text{(Centered version): } \mathbf{g}(\mathbf{x}) = \sum_{i=1}^{d} \frac{f(\mathbf{x}+\mu\mathbf{e}_i) - f(\mathbf{x}-\mu\mathbf{e}_i)}{2\mu}\mathbf{e}_i,$$

symmetric

antithetic

where $\mathbf{e}_i$ is the i-th natural basis vector of $\mathbb{R}^d$ and μ is the sampling radius

cont. diff.

- For the gradient estimation above, it can be shown that for $f \in \boxed{C_L^{1,1}}$ (i.e., continuously differentiable with Lipschitz-continuous gradient)

Nesterov notation.

$$\|\mathbf{g}(\mathbf{x}) - \nabla f(\mathbf{x})\|_2 \leq \mu L\sqrt{d}$$

- Natural idea: Replace actual gradient with gradient estimation in any first-order optimization scheme (deterministic ZO methods)
  - Pro: Use Lipschitz-like bound above to characterize convergence performance
  - Con: Suffer from problem dimensionality for large d ($O(d)$ ZO-oracle calls)

Randomized Gradient Estimation

- Two-point random gradient estimator

2-pt.

$$\hat{\nabla} f(\mathbf{x}) = (d/\mu)[f(\underline{\mathbf{x} + \mu\mathbf{u}}) - f(\underline{\mathbf{x}})]\mathbf{u},$$

where $\mathbf{u}$ is an i.i.d. random direction

- $(q+1)$-point random gradient estimator

q+1 points.

$$\hat{\nabla} f(\mathbf{x}) = (d/(\mu q)) \sum_{i=1}^{q} [f(\mathbf{x} + \mu\mathbf{u}_i) - f(\mathbf{x})]\underline{\mathbf{u}}_i,$$

which is also referred to as average random gradient estimator

- Benefits:
  - Make every iteration simpler
  - Easy convergence proof
  - For problems limited to only several (or even one) ZO oracle queries

Formalization of Stochastic Zeroth-Order Methods

- Consider the problem of the following form:

$$\min_{\mathbf{x} \in Q \subseteq \mathbb{R}^d} f(\mathbf{x})$$

$= \mathbb{R}^d$

- A stochastic ZO method generates $\{\mathbf{x}_k\}$ as follows:

$$\mathbf{x}_{k+1} = \mathcal{A}\left(\hat{f}, \mathbf{X}, P, \{\mathbf{x}_i\}_{i=0}^{k}, \{\mathbf{u}_i\}_{i=0}^{k}\right)$$

  - $\hat{f}$: ZO-oracle (could be noisy, i.e., $\hat{f}$ is not necessarily equal to f; e.g., $\hat{f}(\mathbf{x}) = f(\mathbf{x}) + \epsilon(\mathbf{x})$ or $\hat{f}(\mathbf{x}, \mathbf{u}) = f(\mathbf{x}) + \epsilon(\mathbf{x}, \mathbf{u})$ with $\mathbb{E}_{\mathbf{u}}[\hat{f}(\mathbf{x}, \mathbf{u})] = f(\mathbf{x})$)
  - $\{\mathbf{x}_i\}_{i=0}^{k}$: history of $\mathbf{x}$-variables
  - $\{\mathbf{u}_i\}_{i=0}^{k}$: random sampling directions
  - P: parameters (dimension d of $\mathbf{x}$, L-Lipschitz constant, etc.)

- This lecture: Focus on non-convex objective function

Random Directions Gradient Estimations

- Consider the following ZO scheme using gradient approximation:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - s_k \mathbf{g}(\mathbf{x}_k, \mathbf{u}_k),$$

where $\mathbf{g}(\mathbf{x}_k, \mathbf{u}_k)$ follows the two-point random gradient estimator:

$$\mathbf{g}(\mathbf{x}_k, \mathbf{u}_k) = \frac{\hat{f}(\mathbf{x}_k + \mu \mathbf{u}_k) - \hat{f}(\mathbf{x}_k)}{\mu} \mathbf{u}_k$$

- It makes sense to use centrally symmetric distributions for $\mathbf{u}_k$:
  - Uniformly distributed over unit Euclidean sphere [Flaxman et al. SODA'05], [Gorbunov et al. SIOPT'18], [Dvurechensky et al., E. J. OR'21]:

$$\mathbf{u}_k \sim \mathcal{U}\{S^{d-1}\}, \text{ where } S^{d-1} = \{\mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\|_2 = 1\}$$

  - Gaussian smoothing [Nesterov and Spokoiny, Math Prog.'06]:

$$\mathbf{u}_k \sim \mathcal{N}(0, \mathbf{I}_d)$$

Gaussian Smoothing [Nesterov and Spokoiny, FCM'17]

- Gaussian smoothing approximation:

$$f_\mu(\mathbf{x}) = \frac{1}{\kappa}\int_{\mathbb{R}^d} f(\mathbf{x}+\mu\mathbf{u})e^{-\frac{1}{2}\|\mathbf{u}\|_2^2}d\mathbf{u},$$

where $\kappa = \int_{\mathbb{R}^d} e^{-\frac{1}{2}\|\mathbf{u}\|_2^2}d\mathbf{u} = (2\pi)^{d/2}$.

- Good properties:
  - Convexity preservation: If f is convex, so is f_μ
  - Differentiability
  - If $f \in C_{L_0}^{0,0}$ (or $f \in C_{L_1}^{1,1}$), the same holds for f_μ with $L_0(f_\mu) \le L_0(f)$ (or $L_1(f_\mu) \le L_1(f)$)
  - $|f_\mu(\mathbf{x}) - f(\mathbf{x})| \le \mu L_0\sqrt{d}$ if $f \in C_{L_0}^{0,0}$

Gaussian Smoothing [Nesterov and Spokoiny, FCM'17]

- Consider the following algorithm:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - s_k \mathbf{g}(\mathbf{x}_k, \mathbf{u}_k), \text{ and } \mathbf{u}_k \sim \mathcal{N}(0, \mathbf{I}_d).$$

- For nonconvex $f \in C^{1,1}_{L_1}$, we have (let $U = \{\mathbf{u}_k\}_{k=0}^{K-1}$):

$$\frac{1}{K}\sum_{k=0}^{K-1} \mathbb{E}_U[\|\nabla f_\mu(\mathbf{x}_k)\|_2^2] \le 8(d+4)L_1 \left[\underbrace{\frac{f_\mu(\mathbf{x}_0) - f^*}{K}}_{=O(\frac{1}{K})} + \underbrace{\frac{3\mu^2(d+4)}{32} L_1}_{\text{Const. "error ball"}} \right]$$

- Using the facts that $\|f_\mu(\mathbf{x}) - \nabla f(\mathbf{x})\|_2 \le \frac{\mu L_1}{2}(d+3)^{\frac{3}{2}}$ and $\|\nabla f(\mathbf{x})\|_2^2 \le 2\|\nabla f_\mu(\mathbf{x}) - \nabla f(\mathbf{x})\|_2^2 + 2\|\nabla f_\mu(\mathbf{x})\|_2^2$, we obtain:

$$\frac{1}{K}\sum_{k=0}^{K-1} \mathbb{E}_U[\|\nabla f(\mathbf{x}_k)\|_2^2] \le 2\frac{\mu^2 L_1^2}{4}(d+3)^3 \quad O(d^3)$$

$$+ 16(d+4)L_1 \left[\underbrace{\frac{f_\mu(\mathbf{x}_0) - f^*}{K}}_{O(\frac{1}{K}) \text{ conv. rate.}} + \frac{3\mu^2(d+4)}{32} L_1 \right]$$

Gaussian Smoothing [Nesterov and Spokoiny, FCM'17]

- Choosing $\mu = O(\epsilon/[d^3 L_1])$ ensures $\frac{1}{K}\sum_{k=0}^{K-1} \mathbb{E}_U[\|\nabla f(\mathbf{x}_k)\|_2^2] \le \epsilon^2$, which implies the following sample complexity:

radius O(ε) "SPIDER"

$$K = O(d\epsilon^{-2}).$$

similar to GD
But dep. on dim.

- For $f \in C_{L_0}^{0,0}$, we have (let $S_K = \sum_{k=0}^{K-1} s_k$):

$$\frac{1}{S_K}\sum_{k=0}^{K-1} s_k \mathbb{E}_U[\|\nabla f_\mu(\mathbf{x}_k)\|_2^2] \le \frac{1}{S_K}\left[(f_\mu(\mathbf{x}_0) - f^*) + \frac{1}{\mu} d^{\frac{1}{2}} (d+4)^2 L_0^3 \sum_{k=0}^{K-1} s_k^2\right]$$

- Consider a bounded domain Q with $\mathrm{diam}(Q) \le R$. To ensure $\frac{1}{K}\sum_{k=0}^{K-1} \mathbb{E}_U[\|\nabla f_\mu(\mathbf{x}_k)\|_2^2] \le \epsilon^2$ and $|f_\mu(\mathbf{x}) - f(\mathbf{x})| \le \delta$, we have the following sample complexity:

Not $\|\nabla f(x)\|$

$$K = O\left(\frac{d(d+4)^2 L_0^5 R}{\epsilon^4 \delta}\right). \quad O(d^3 \epsilon^{-4})$$

- If $s_k \to 0$ and $\mu \to 0$, convergence of $\mathbb{E}_U[\|\nabla f(\mathbf{x}_k)\|_2]$ can also be proved.

Extensions of Gaussian Smoothing to Noisy $\hat{f}$

Consider the following:

- Noisy $\hat{f}$: $|\hat{f}(\mathbf{x}) - f(\mathbf{x})| \leq \delta$ RL: a "rollout". any stoch. obj.
- Hölder continuous gradient (intermediate smoothness)

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \leq L_\nu \|\mathbf{x} - \mathbf{y}\|_2^\nu, \text{ for some } \nu \in [0, 1],$$

which implies the following generalized descent lemma:

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{L_\nu}{1+\nu} \|\mathbf{y} - \mathbf{x}\|^{1+\nu}$$

over all randomness of Gaussian smoothing.

- To ensure $\frac{1}{K}\sum_{k=0}^{K-1} \mathbb{E}_U[\|\nabla f(\mathbf{x}_k)\|_2^2] \leq \epsilon^2$, we have the following sample complexity [Shibaev et al., Opt. Lett. '21]:

as $\nu\uparrow$, sample complexity$\downarrow$

$$K = O\left(\frac{d^{2+\frac{1-\nu}{2\nu}}}{\epsilon^{\frac{2}{\nu}}}\right) \text{ if } \underline{\delta = O\left(\frac{\epsilon^{\frac{3+\nu}{2\nu}}}{d^{\frac{3+7\nu}{4\nu}}}\right)}.$$

as $\nu\uparrow$, $\delta\downarrow$ dep. on d more sensitive.

Extensions of Gaussian Smoothing to Noisy $\hat{f}$

- Special case of $\nu = 1$ (i.e., $f \in C^{1,1}_{L_1}$): Sample complexity is improved to

$$K = O(d\epsilon^{-2}),$$

similar to GD.
dep. on d.

which is d times better ~~than~~ same as [Nesterov and Spokoiny, FCM'17]

- If $|\hat{f}(\mathbf{x}) - f(\mathbf{x})| \leq \epsilon_f$, where f is convex and 1-Lipschitz and $\epsilon_f \sim \max\{\epsilon^2/\sqrt{d}, \epsilon/d\}$, then [Risteski and Li, NeurIPS'16] showed that there exists an algorithm that finds ϵ-optimal solution (i.e., $\hat{f}(\mathbf{x}) - \hat{f}^* \leq \epsilon$) with sample complexity $\underline{\text{Poly}(d, \epsilon^{-1})}$. Also, the dependence $\epsilon_f(\epsilon)$ is optimal

LB – matching.

opt. gap.

much better than non-convex.

Randomized Stochastic Gradient-Free Methods

$\frac{1}{T}\sum_{i=0}^{T-1} \|\nabla f(x_i)\|^2 \le \cdots$ $O(\frac{1}{\sqrt{T}})$ if $s_k = \frac{1}{\sqrt{T}}, \forall k.$

Gaussian smoothing is extended to [Ghadimi and Lan, SIAM J. Opt. '13] [Ghadimi et al., Math Prog. '16] (unconstrained case, i.e., $Q = \mathbb{R}^d$):

- noisy/inexact ZO-oracle takes specific form. unbiased.
  $\hat{f} = F(\mathbf{x}, \xi)$ such that $\mathbb{E}_\xi[F(\mathbf{x}, \xi)] = f(\mathbf{x})$, where ξ is a random variable whose distribution P is supported on $\Xi \subseteq \mathbb{R}^d$
- $F(\cdot, \xi)$ has L_1-Lipschitz continuous gradient
- Consider the following randomized stochastic gradient-free method (RSGF):

$$\mathbf{x}_{k+1} = \mathbf{x}_k - s_k G(\mathbf{x}_k, \xi_k, \mathbf{u}_k),$$

$$G(\mathbf{x}_k, \xi_k, \mathbf{u}_k) = \frac{\hat{f}(\mathbf{x}_k + \mu \mathbf{u}_k, \xi_k) - \hat{f}(\mathbf{x}_k, \xi_k)}{\mu} \mathbf{u}_k$$

- It follows from $\mathbb{E}_\xi[F(\mathbf{x}, \xi)] = f(\mathbf{x})$ that $\mathbb{E}_{\xi,\mathbf{u}}[G(\mathbf{x}, \xi, \mathbf{u})] = \nabla f_\mu(\mathbf{x})$
- Similar to FO-SGD in [Ghadimi and Lan, SIAM J. Opt. '13], RSGF chooses $\mathbf{x}_R$ from $\{\mathbf{x}_k\}_{k=1}^K$ where R is a r.v. with p.m.f. P_R supported on $\{1, \ldots, K\}$

rand. termination index.

Randomized Stochastic Gradient-Free Methods

const. (init gap).

- For $f \in C^{1,1}_{L_1}$, smoothing parameter μ, $D_f = (2(f(\mathbf{x}_1) - f^*)/L)^{\frac{1}{2}}$, and $\mathbb{E}_\xi[\|\nabla \hat{f}(\mathbf{x}, \xi) - \nabla f(\mathbf{x})\|_2^2] \leq \sigma^2$ and p.m.f. of R being:

$$P_R(k) = \frac{s_k - 2L(d+4)s_k^2}{\sum_{i=1}^K (s_i - 2L(d+4)s_i^2)},$$

it then holds that:

$$\frac{1}{L_1}\mathbb{E}[\|\nabla f(\mathbf{x}_R)\|_2^2] \leq \frac{1}{\sum_{k=1}^K [s_k - 2L_1(d+4)s_k^2]}\Bigg[D_f^2 + 2\mu^2(d+4)\times \left(1 + L_1(d+4)^2 \sum_{k=1}^K (\frac{s_k}{4} + Ls_k^2)\right) + 2(d+4)\sigma^2 \sum_{k=1}^K s_k^2\Bigg],$$

where the expectation is taken w.r.t. R and $\{\xi_k\}$.

Randomized Stochastic Gradient-Free Methods

- Choose constant step-size $s_k = \frac{1}{\sqrt{d+4}} \min\{\frac{1}{4L\sqrt{d+4}}, \frac{\tilde{D}}{\sigma\sqrt{K}}\}$ for some $\tilde{D} > 0$ (some estimation of D_f):

$O(\frac{1}{\sqrt{d}})$ $(O(\frac{1}{d}))$.

$$\frac{1}{L_1}\mathbb{E}[\|\nabla f(\mathbf{x}_R)\|_2^2] \leq \frac{12(d+4)L_1 D_f^2}{K} + \frac{2\sigma\sqrt{d+4}}{\sqrt{K}}\left(\tilde{D} + \frac{D_f^2}{\tilde{D}}\right)$$

$O(\frac{d}{K})$ $O(\sqrt{\frac{d}{K}})$

- To ensure $\Pr\{\|\nabla f(\mathbf{x}_R)\|_2^2 \leq \cancel{\epsilon}\ \epsilon^2\} \geq 1 - \delta$ (i.e., (ϵ, δ)-solution), the zeroth-order oracle sample complexity is: w.h.p.

$$O\left(\frac{dL_1^2 D_f^2}{\delta\epsilon} + \frac{dL_1^2}{\delta^2}\left(\tilde{D} + \frac{D_f^2}{\tilde{D}}\right)\frac{\sigma^2}{\epsilon^2}\right)$$

ϵ^4

$O(\delta^{-2})$

$O(d\epsilon^{-4})$ similar to SGD.

$O(\log(\frac{1}{\delta}))$

Randomized Stochastic Gradient-Free Methods

Two-phase randomized stochastic gradient-free method (2-RSGF) [Ghadimi and Lan, SIAM J. Opt. '13]

- Run RSGF $S = \log(1/\delta)$ times as a subroutine producing a list $\{\bar{\mathbf{x}}_k\}_{k=1}^S$
- Output point $\bar{\mathbf{x}}^*$ is chosen in such a way that:

$$\|\mathbf{g}(\bar{\mathbf{x}}^*)\|_2 = \min_{s=1,\ldots,S} \|\mathbf{g}(\bar{\mathbf{x}}_s)\|_2, \text{ where } \mathbf{g}(\bar{\mathbf{x}}_s) = \frac{1}{T}\sum_{k=1}^{T} G_\mu(\bar{\mathbf{x}}_s, \xi_k, \mathbf{u}_k),$$

  where $G_\mu(\bar{\mathbf{x}}_s, \xi_k, \mathbf{u}_k)$ is defined as in RSGF
- The zeroth-order oracle sample complexity for achieving (ϵ, δ)-solution:

poly log dep. on $\frac{1}{\delta}$ $\quad$ $O(d\epsilon^{-2})$

$$O\left(\frac{dL_1^2 D_f^2 \log(1/\delta)}{\epsilon} + dL_1^2\left(\tilde{D} + \frac{D_f^2}{\tilde{D}}\right)^2 \frac{\sigma^2}{\epsilon^2}\log(1/\delta) + \frac{d\log^2(1/\delta)}{\delta}\left(1 + \frac{\sigma^2}{\epsilon}\right)\right)$$

- A more general problem $\min_{\mathbf{x}\in Q\subseteq\mathbb{R}^d} \Psi(\mathbf{x}) = f(\mathbf{x}) + \underline{h(\mathbf{x})}$ is also solved in [Ghadimi et al., Math Prog.'16]

  non-smooth.
  - $f \in C_L^{1,1}$: nonconvex; $h(\mathbf{x})$ is simple convex and possibly non-smooth

RSGF Based on Uniform Sampling over Unit Sphere

- Consider the problem $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}) \triangleq \mathbb{E}_\xi[F(\mathbf{x},\xi)] = \mathbb{E}_\xi[\hat{f}(\mathbf{x},\xi)]$
  - $f(\mathbf{x})$ is L-Lipschitz and μ-smooth $\nabla f(\mathbf{x})$ is μ-Lipschitz : μ happens to be sampling radius.
  - $|F(\mathbf{x},\xi)| \le \Omega$ and F's variance is bounded by V_f
- Stochastic gradient estimation based on uniform sampling over unit sphere:

$$\mathbf{g}(\mathbf{x}_k,\xi_k,\mathbf{u}_k) = n\frac{\hat{f}(\mathbf{x}_k+\mu\mathbf{u}_k,\xi_k) - \hat{f}(\mathbf{x}_k-\mu\mathbf{u}_k,\xi_k)}{2\mu},$$

where $\mathbf{u}_k \sim \mathcal{U}(S^{n-1})$. The update process is $\mathbf{x}_{k+1} = \mathbf{x}_k - s\mathbf{g}(\mathbf{x}_k,\xi_k,\mathbf{u}_k)$

- After K steps, we have [Sener and Koltun, ICML'20]:

$$\frac{1}{K}\sum_{k=1}^{K}\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|_2^2] = O\left(\frac{n}{K^{1/2}} + \underbrace{\frac{n^{2/3}}{K^{1/3}}}_{\text{dominant term.}}\right)$$

RSGF Based on Uniform Sampling over Unit Sphere

[Nguyen & Mondelli; NeurIPS '19]

- Consider the case for a given ξ, $F(\mathbf{x}, \xi) = g(r(\mathbf{x}, \theta^*), \Psi^*)$, where $g(\cdot, \Psi)$ and $r(\cdot, \theta)$ are parameterized function classes "pyramid structure"
  - $r(\cdot, \theta^*) : \mathbb{R}^n \to \mathbb{R}^d$, where $d \ll n$ CNN. "conv, dropout".
  - $F(\cdot, \xi) : \mathbb{R}^n \to \mathbb{R}$ is actually defined on a d-dimensional manifold $\mathcal{M}$ for all ξ

- Thus, if one knows the manifold (i.e., θ^*) and g and r are smooth, we have from chain rule: $\nabla f(\mathbf{x}) = J(\mathbf{x}, \theta^*)\nabla_r g(r, \Psi)$, where $J(\mathbf{x}, \theta^*) = \frac{\partial r(\mathbf{x}, \theta^*)}{\partial \mathbf{x}}$. Jacobian
  This leads to [Sener and Koltun, ICML'20]:

$$G(\mathbf{x}_k, \xi_k, \mathbf{u}_k) = d\frac{\hat{f}(\mathbf{x}_k + \mu J_q \mathbf{u}_k, \xi_k) - \hat{f}(\mathbf{x}_k - \mu J_q \mathbf{u}_k, \xi_k)}{2\mu}\mathbf{u}_k,$$

  where J_q is the orthonomalized $J(\mathbf{x}_k, \theta^*)$ and $\mathbf{u}_k \sim \mathcal{U}(S^{d-1})$. It follows that

$$\frac{1}{K}\sum_{k=1}^{K}\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|_2^2] = O\left(\frac{n^{1/2}}{K} + \frac{n^{1/2} + d + dn^{1/2}}{K^{1/2}} + \frac{d^{2/3} + n^{1/2}d^{2/3}}{K^{1/3}}\right).$$

$O(K^{-\frac{1}{3}})$.

  which is much better than the previous bound for $d \leq n^{1/2}$.

Which Gradient Estimation Works Better?

- Gradient estimations with random directions are worse than finite differences in terms of # of samples required to ensure the norm condition:

$$\|\mathbf{g}(\mathbf{x}) - \nabla f(\mathbf{x})\|_2 \leq \theta \|\nabla f(\mathbf{x})\|_2, \text{ for some } \theta \in [0,1)$$

- Gradient estimation methods are studied in [Berahas et al., FCM'21]: Compare the # of calls r (i.e., "batch size") to ensure norm condition

deterministic

  - FFD (Forward Finite Differences): $\sum_{i=1}^{d} \frac{\hat{f}(\mathbf{x}+\mu \mathbf{e}_i) - \hat{f}(\mathbf{x})}{\mu} \mathbf{e}_i$
  - CFD (Centered Finite Differences): $\sum_{i=1}^{d} \frac{\hat{f}(\mathbf{x}+\mu \mathbf{e}_i) - \hat{f}(\mathbf{x}-\mu \mathbf{e}_i)}{2\mu} \mathbf{e}_i$
  - LI (Linear Interpolation): $\sum_{i=1}^{d} \frac{\hat{f}(\mathbf{x}+\mu \mathbf{u}_i) - \hat{f}(\mathbf{x})}{\mu} \mathbf{u}_i$, $\mathbf{u}_i = [\mathbf{Q}]_i$ any non-singular matrix in $\mathbb{R}^d$.

randomized
(r+1)-pt.

  - GSG (Gaussian Smoothed Gradients): $\frac{1}{r} \sum_{i=1}^{r} \frac{\hat{f}(\mathbf{x}+\mu \mathbf{u}_i) - \hat{f}(\mathbf{x})}{\mu} \mathbf{u}_i$, $\mathbf{u}_i \sim \mathcal{N}(0, \mathbf{I}_d)$
  - cGSG (Centered GSG): $\frac{1}{r} \sum_{i=1}^{r} \frac{\hat{f}(\mathbf{x}+\mu \mathbf{u}_i) - \hat{f}(\mathbf{x}-\mu \mathbf{u}_i)}{2\mu} \mathbf{u}_i$, $\mathbf{u}_i \sim \mathcal{N}(0, \mathbf{I}_d)$
  - SSG (Sphere Smoothed Gradients): $\frac{d}{r} \sum_{i=1}^{r} \frac{\hat{f}(\mathbf{x}+\mu \mathbf{u}_i) - \hat{f}(\mathbf{x})}{\mu} \mathbf{u}_i$, $\mathbf{u}_i \sim \mathcal{U}(S^{d-1})$
  - cSSG (Centered SSG): $\frac{d}{r} \sum_{i=1}^{r} \frac{\hat{f}(\mathbf{x}+\mu \mathbf{u}_i) - \hat{f}(\mathbf{x}-\mu \mathbf{u}_i)}{2\mu} \mathbf{u}_i$, $\mathbf{u}_i \sim \mathcal{U}(S^{d-1})$

Which Gradient Estimation Works Better?

- Consider an unconstrained problem $\min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x})$ [Berahas et al., FCM'21]:
  - Noisy ZO oracle: $\hat{f}(\mathbf{x}) = f(\mathbf{x}) + \epsilon(\mathbf{x})$
  - Noise ϵ is bounded uniformly: $|\epsilon(\mathbf{x})| \leq \epsilon_f$ (noise not neccessarily random)
  - $f(\mathbf{x}) \in C_L^{1,1}$ or $f(\mathbf{x}) \in C_M^{2,2}$ (twice continuously differentiable with M-Lipschitz Hessian)

Method	Number of calls r	$\|\nabla f(\mathbf{x})\|_2$	
FFD	d	$\frac{2\sqrt{dL\epsilon_f}}{\theta}$	
CFD	d	$\frac{2\sqrt{d}\sqrt[3]{M\epsilon_f^2}}{\sqrt[3]{6}\theta}$	$O(\sqrt{d})$
LI	d	$\frac{2\|Q^{-1}\|\sqrt{dL\epsilon_f}}{\theta}$	
GSG	$\frac{12d}{\sigma\theta^2} + \frac{d+20}{16\delta}$ $O(d)$	$\frac{6d\sqrt{L\epsilon_f}}{\theta}$	$O(d)$
cGSG	$\frac{12d}{\sigma\theta^2} + \frac{d+30}{144\delta}$	$\frac{12\sqrt[3]{d^{7/2}M\epsilon_f^2}}{\theta}$	
SSG	$[\frac{8d}{\theta^2} + \frac{8d}{3\theta} + \frac{11d+104}{24}]\log\frac{d+1}{\delta}$	$\frac{4d\sqrt{L\epsilon_f}}{\theta}$	$O(d^{7/6})$.
cSSG	$[\frac{8d}{\theta^2} + \frac{8d}{3\theta} + \frac{9d+192}{27}]\log\frac{d+1}{\delta}$ $\tilde{O}(d)$	$\frac{4\sqrt[3]{d^{7/2}M\epsilon_f^2}}{\theta}$	

- LI is essentially FFD with directions given as columns of a nonsingular matrix $\mathbf{Q}$
- For GSG, cGSG, SSG, and cSSG, results are w.p. $1-\delta$

Next Class

Variance-Reduced Zeroth-Order Methods