A weak tail-bound probabilistic condition for function estimation in stochastic derivative-free optimization (with improved sample sizing)

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12th US–Mexico Workshop on Optimization and its Applications

Steve's "60th" Birthday

January 11, 2023

Problem formulation

$$\min_{x\in\mathbb{R}^n} f(x)$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is

- locally Lipschitz continuous
- possibly non-smooth and with $\inf f = f^*$
- given by a stochastic oracle

$$F(x,\xi) \simeq f(x)$$

with oracle given by sampling over ξ.

Some notation

- Probability space $(\mathbb{P}, \Omega, \mathcal{F})$
- w outcome of the sample space Ω
- Our algorithms generate random processes:
  - g_k direction realization (shorthand for $G_k(w)$)
  - δ_k stepsize realization (shorthand for $\Delta_k(w)$)
  - f_k estimate realization for $f(x_k)$ (shorthand for $F_k(w)$)
  - same for $f_k^g \simeq f(x_k + \delta_k g_k)$
- $\mathcal{F}_{k-1}$ is the $\sigma-$algebra of events up to the choice of g_k
- The acceptance criterion is $f_k - f_k^g \geq \theta \delta_k^q$, for $\theta > 0, q > 1$

Tail-bound probabilistic condition

Assumption (Tail bound)

For some $\varepsilon_q > 0$ *(independent of* k*):*

$$\mathbb{P}\left(|F_k - F_k^g - (f(X_k) - f(X_k + \Delta_k G_k))| \geq \alpha \Delta_k^q \;|\mathcal{F}_{k-1}\right) \;\leq\; \frac{\varepsilon_q}{\alpha^{q/(q-1)}}$$

a.s. for every $\alpha > 0$.

- power law tail bound on error with exponent $q/(q-1)$

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a.s. for every $\alpha > 0$.

- power law tail bound on error with exponent $q/(q-1)$
- satisfied, since if r-moment of noise is finite (r ≥ 2), then:

$$\mathbb{E}(|A_k|^r) \;\leq\; C_r \; p_k^{-\frac{r}{2}}$$

when $A_k = F_k - F_k^g - (f(X_k) - f(X_k + \Delta_k G_k))$ considers averaging p_k i.i.d. samples in F_k,F_k^g (and that estimator is unbiased)

Sample bound for bounded moment – (i)

Assumption (Bounded moment)

For some $r > 1$, $\qquad \mathbb{E}_\xi[|F(x,\xi) - f(x)|^r] \;\leq\; M_r \;<\; +\infty$

Sample bound for bounded moment – (i)

Assumption (Bounded moment)

For some $r > 1, \qquad \mathbb{E}_\xi[|F(x,\xi) - f(x)|^r] \;\leq\; M_r \;<\; +\infty$

Theorem

Assume the estimator for A_k *is unbiased (true if* $f(x) = \mathbb{E}_\xi[F(x,\xi)]$*).*

When $r = r(q) = \frac{q}{q-1}$, $q \in (1,2]$, *the tail bound can be satisfied by averaging*

$$O\left(\Delta_k^{-2q}\right) \qquad \textit{i.i.d. samples}$$

- for $q = 1.5$ $(r = 3)$ only $O(\Delta_k^{-3})$ samples needed

  for $q = 2$ $(r = 2)$ the known bound is $O(\Delta_k^{-4})$

Sample bound for bounded moment – (ii)

Use of r-th moment and q,r being conjugates:

$$\mathbb{P}(|A| \geq \alpha\Delta^{\frac{r}{r-1}})$$

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$$\leq \; \frac{\mathbb{E}[|A|^r]}{\alpha^r\Delta^{r^2/(r-1)}}$$

Sample bound for bounded moment – (ii)

Use of r-th moment and q,r being conjugates:

$$\mathbb{P}(|A| \geq \alpha\Delta^{\frac{r}{r-1}}) = \mathbb{P}(|A|^r \geq \alpha^r\Delta^{\frac{r^2}{r-1}})$$
$$\leq \frac{\mathbb{E}[|A|^r]}{\alpha^r\Delta^{r^2/(r-1)}} \leq \frac{2^r C_r M_r p^{-\frac{r}{2}}}{\alpha^r\Delta^{r^2/(r-1)}}$$

Sample bound for bounded moment – (ii)

Use of r-th moment and q,r being conjugates:

$$\begin{aligned} \mathbb{P}(|A| \geq \alpha \Delta^{\frac{r}{r-1}}) \ &= \ \mathbb{P}(|A|^r \geq \alpha^r \Delta^{\frac{r^2}{r-1}}) \\ \leq \ \frac{\mathbb{E}[|A|^r]}{\alpha^r \Delta^{r^2/(r-1)}} \ &\leq \ \frac{2^r C_r M_r p^{-\frac{r}{2}}}{\alpha^r \Delta^{r^2/(r-1)}} = \frac{\varepsilon_q}{\alpha^r} \end{aligned}$$

for $p = O(\Delta^{\frac{-2r}{r-1}}) = O(\Delta^{-2q})$.

Correlated errors

Suppose we have access to the random number generator (we can fix ξ and sample $F(\cdot, \xi)$), and the errors are correlated in the form:

Assumption (Correlated error)

Let $\bar{F}(x, \xi) = F(x, \xi) - f(x)$. *For some* $r > 1$*:*

$$\mathbb{E}_\xi[|\bar{F}(x, \xi) - \bar{F}(y, \xi)|^r] \leq D_r \|x - y\|^r$$

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- ensured, for every r, when $F(x,\xi)$ is a Gaussian process with exponentiated quadratic kernel $K(x,y) = \sigma^2 \text{exp}\left(-\frac{\|x-y\|^2}{2l^2}\right)$

  in which case $\text{Var}_\xi[F(x,\xi)]$ is constant and

$$\text{Cov}_\xi(F(x,\xi), F(y,\xi)) \;\geq\; \mathcal{O}\left(1 - \|x-y\|^2\right)$$

Sample bound for correlated errors

Theorem

Assume the estimator for A_k is unbiased (true if $f(x) = \mathbb{E}_\xi[F(x,\xi)]$).

When $r = \frac{q}{q-1}$, $q \in (1,2]$, the tail bound can be satisfied by averaging:

$$O(\Delta_k^{2-2q}) \qquad \textit{i.i.d. samples}$$

- for $q = 1.5$ $(r = 3)$ only $O(\Delta_k^{-1})$ samples needed

  for $q = 2$ $(r = 2)$ one gets $O(\Delta_k^{-2})$

Numerical experiments – setup

- tested the direct-search algorithm for $q \in \{1.5, 2\}$, for which $r(q) \in \{3, 2\}$
- algorithms tested on a set of 96 well known non-smooth problems
- added Gaussian noise $N(0, 10^{-2})$ in the general case, $N(0, \delta_k 10^{-2})$ in the correlated one
- for the moment bound case, number of samples was: $\lceil \delta_k^{-4} \rceil$ $(q = 2)$ and $\lceil \delta_k^{-3} \rceil$ $(q = 1.5)$
- for the correlated errors case, number of samples was: $\lceil \delta_k^{-2} \rceil$ $(q = 2)$ and $\lceil \delta_k^{-1} \rceil$ $(q = 1.5)$
- data and performance profiles

Numerical experiments – bounded moment

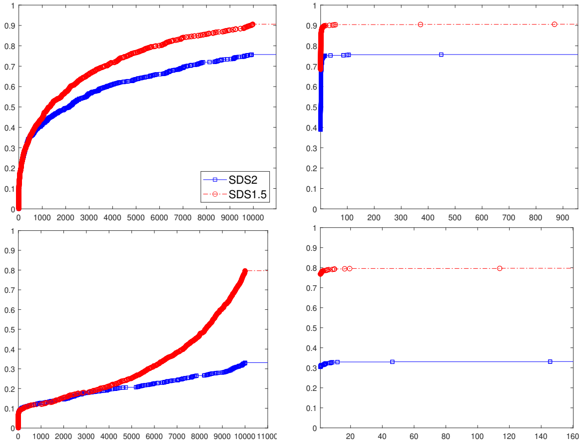

Figure: From left to right, data and performance profiles. From top to bottom, tolerance 10^{-2} and 10^{-4}

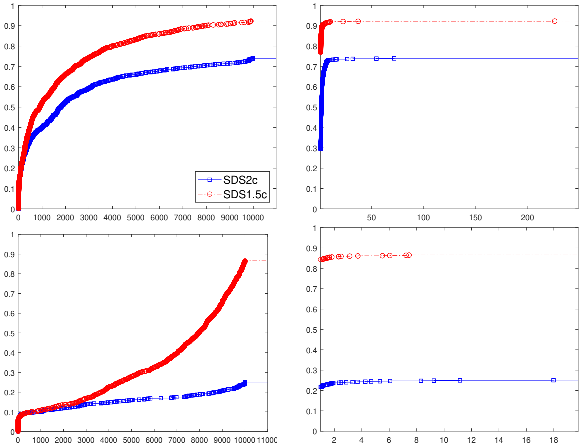

Figure: From left to right, data and performance profiles. From top to bottom, tolerance 10^{-2} and 10^{-4}

Is there an optimal q in (1,2]?

Sample bound for bounded moment – (iv)

When $F(x, \varepsilon) - f(x) \sim N(0, \sigma)$, the tail bound condition is satisfied using

$$p = B(q) := \left\lceil \frac{4\sigma^2 M_{r(q)}^{2/r(q)}}{\varepsilon_q^{2/r(q)}} \Delta^{-2q} \right\rceil$$

where $r(q) = \frac{q}{q-1}$ and $M_{r(q)}$ is the $r(q)$-th moment of a standard normal distribution.

The continuous version of $B(q)$ has always a minimum in $(1, 2]$.

Comparison with other assumptions – 1

k_f-variance conditions [Audet et al., 2021]

$$\mathbb{E}[|F_k^g - f(X_k + \Delta_k G_k)|^2 \mid \mathcal{F}_{k-1}] \le k_f^2 \Delta_k^4$$
$$\mathbb{E}[|F_k - f(X_k)|^2 \mid \mathcal{F}_{k-1}] \le k_f^2 \Delta_k^4$$

Proposition

Then tail bound condition is satisfied for $\varepsilon_q = 4k_f^2$ *and* $q = 2$.

- follows from Markov's inequality

Comparison with other assumptions – 2

β-probabilistically accurate function estimate [Chen et al. 2018]

$$\mathbb{P}(\{|F_k - f(X_k)| \le \tau_f \Delta_k^2\} \cap \{|F_k^g - f(X_k + \Delta_k G_k)| \le \tau_f \Delta_k^2\}| \mathcal{F}_{k-1}) \ge \beta$$

Proposition

If satisfied for all β in a chosen interval (and τ_f depending on β and accuracy parameter ε), then tail bound is satisfied with ε_q depending on ε.

- follows from the inclusion

$$\begin{aligned}&\{|F_k - F_k^g - (f(X_k) - f(X_k + \Delta_k G_k))| < \alpha \Delta_k^2\}\\ &\supset \{|F_k - f(X_k)| \le \tau_f \Delta_k^2\} \cap \{|F_k^g - f(X_k + \Delta_k G_k)| \le \tau_f \Delta_k^2\}\end{aligned}$$

for any $\tau_f < \frac{\alpha}{2}$.

Algorithm Stochastic direct search

Initialization. Choose a point x_0, $\delta_0, \theta > 0$, $\tau \in (0,1)$, $\bar{\tau} \in [1, 1+\tau]$.
For $k = 0, 1 \ldots$
  Select a direction g_k in the unitary sphere.
  Compute estimates f_k and f_k^g for f in x_k and $x_k + \delta_k g_k$.
  If $f_k - f_k^g \geq \theta \delta_k^q$, **Then** set $x_{k+1} = x_k + \delta_k g_k$, $\delta_{k+1} = \bar{\tau}\delta_k$.
  Else set $x_{k+1} = x_k$, $\delta_{k+1} = (1-\tau)\delta_k$.
  End if
End for

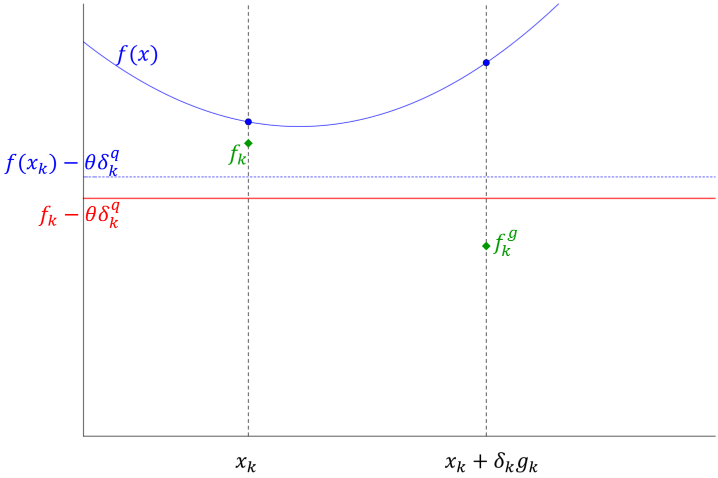

Figure: A bad successful step

Tail-bound probabilistic condition (again)

Assumption (Tail bound)

For some $\varepsilon_q > 0$ *(independent of* k*):*

$$\mathbb{P}\left(|F_k - F_k^g - (f(X_k) - f(X_k + \Delta_k G_k))| \geq \alpha \Delta_k^q \,|\mathcal{F}_{k-1}\right) \;\leq\; \frac{\varepsilon_q}{\alpha^{q/(q-1)}}$$

a.s. for every $\alpha > 0$.

Convergence of stepsizes

Lemma

Under the tail bound condition, if $\theta > \theta^{ds}(q, \tau, \varepsilon_q)$, then a.s.

$$\sum \Delta_k^q \; < \; +\infty$$

- let $\Phi_k = f(X_k) - f^* + C_1 \Delta_k^q$
- the lemma follows from Robbins-Siegmund once we get to

$$\mathbb{E}[\Phi_k - \Phi_{k+1} | \mathcal{F}_{k-1}] \; \geq \; C_2 \Delta_k^q$$

- for a certain ρ_k, the above LHS is $\geq$ than

$$\left(C_3 - \rho_k \underbrace{(\mathbb{P} \text{ in tail bound with } \alpha = \rho_k)}_{\leq C_4(1/\rho_k)} \right) \Delta_k^q$$

Tail-bound probabilistic condition (again)

Assumption (Tail bound)

For some $\varepsilon_q > 0$ (independent of k):

$$\mathbb{P}\left(|F_k - F_k^g - (f(X_k) - f(X_k + \Delta_k G_k))| \geq \alpha \Delta_k^q \,|\mathcal{F}_{k-1}\right) \;\leq\; \frac{\varepsilon_q}{\alpha^{q/(q-1)}}$$

a.s. for every $\alpha > 0$.

An intermediate result

Lemma

Let K be the set of indices of unsuccessful iterations. Then under the tail bound assumption and $\theta > \theta^{ds}$ we have a.s.

$$\liminf_{k \in K,\, k \to \infty} \frac{f(X_k + \Delta_k G_k) - f(X_k)}{\Delta_k} \;\geq\; 0$$

- need to prove $|F_k - F_k^g - (f(X_k) - f(X_k + \Delta_k G_k))| / \Delta_k \to 0$
- apply the tail bound assumption with $\alpha = \frac{\Delta_k^{1-q}}{m}$

$$\mathbb{P}(|F_k - F_k^g - (f(X_k) - f(X_k + \Delta_k G_k))| \geq \frac{\Delta_k}{m} \mid \mathcal{F}_{k-1}) \leq m^{r(q)} \Delta_k^q \varepsilon_q$$

- conclusion from Borel-Cantelli's First Lemma for every m

Convergence to Clarke stationary points

Theorem

Let the tail bound assumption hold, $\theta > \theta^{ds}$, and f Lipschitz continuous around any limit point.

If $L \subset K$ is such that $\{G_k\}_{k\in L}$ is dense in the unit sphere and

$$\lim_{k\in L,\, k\to\infty} X_k \;=\; X^*$$

then X^* is Clarke stationary (a.s.).

- follows from last lemma and $\limsup \geq \liminf$ (and $\Delta_k \longrightarrow 0$)

A simple stochastic trust-region scheme

Algorithm `Stochastic DFO Trust-Region Algorithm`

Initialization. Select $x_0 \in \mathbb{R}^n$, $\theta > 0$, $\tau \in (0,1)$, $\bar{\tau} \in [1, 1+\tau]$, $\delta_0 > 0$, $q > 1$.

For $k = 0, 1 \ldots$

  Select a direction $g_k \neq 0$ and build a symmetric matrix B_k.

  Compute
$$s_k \in \operatorname{argmin}_{\|s\| \leq \delta_k} g_k^\top s + \frac{1}{2} s^\top B_k s.$$

  Compute estimates $f_k \simeq f(x_k)$ and $f_k^s \simeq f(x_k + s_k)$.

  If
$$\frac{f_k - f_k^s}{\theta \|s_k\|^q} \geq 1$$

  Then set $x_{k+1} = x_k + s_k$, $\delta_{k+1} = \bar{\tau}\delta_k$.

  Else set $x_{k+1} = x_k$, $\delta_{k+1} = (1-\tau)\delta_k$.

End For

How to adapt the tail bound to TR

Assumption (Trust-region tail bound)

For some $\varepsilon_q > 0$ (independent of k):

$$\mathbb{P}\left(|F_k - F_k^g - (f(X_k) - f(X_k + S_k))| \geq \alpha \|S_k\|^q \;|\mathcal{F}_{k-1}\right) \;\leq\; \frac{\varepsilon_q}{\alpha^{q/(q-1)}}$$

a.s. every $\alpha > 0$.

- S_k, $\|S_k\|$, F_k^s replace $\Delta_k G_k$, Δ_k, F_k^g
- same improved sampling bounds of direct-search case

Convergence to Clarke stationary points – 1

Under the tail bound condition

$$\sum \|S_k\|^q < +\infty$$

for a different lower bound $\theta > \theta^{tr}(q, \tau, \varepsilon_q, \rho)$.

Assumption (Hessian bound 1)

There exists $\rho \in (0, 1]$ such that, for every k,

$$\|B_k\| \leq \frac{1}{\rho} \frac{\|G_k\|}{\Delta_k}$$

- when $\|G_k\| = 1$, Hessian is "unbounded" by $1/\Delta_k$
- it implies $\|S_k\| \geq \rho\Delta_k$, which then gives $\sum \Delta_k^q < +\infty$

Convergence to Clarke stationary points – 2

Assumption (Hessian bound 2)

There exists a sequence $\{a_k\} \downarrow 0$ *and such that, for every* k*,*

$$\|B_k\| \leq a_k \frac{\|G_k\|}{\Delta_k}$$

Lemma (asymptotic alignment)

If S_k *solves the trust-region subproblem,*

$$\lim_{k\to\infty} \frac{G_k}{\|G_k\|} + \frac{S_k}{\|S_k\|} = 0$$

a.s. (it holds for every realization, actually).

- for k large, S_k becomes aligned with $-G_k$

Convergence to Clarke stationary points – 3

Theorem

Let the tail bound assumption hold, $\theta > \theta^{tr}$, f Lipschitz continuous around any limit point, and Hessian bound 2.

If $L \subset K$ is such that $\{G_k\}_{k \in L}$ is dense in the unit sphere and

$$\lim_{k \in L,\, k \to \infty} X_k = X^*$$

then X^* is Clarke stationary (a.s.).

- corollary of analogous DS result for $\left\{ \frac{S_k}{\|S_k\|} \right\}$ + asymptotic alignment

Conclusions and extensions

Conclusions

- introduced a tail bound condition tailored to acceptance criterion
- proved improved bounds on the corresponding number of samples
- proved convergence of a direct-search and a trust-region schemes

Extensions

- more general random trust-region models (e.g. piecewise linear)
- composition of smooth function with known non-smooth function
- numerical experiments for trust-region method