Quadratic Regularization Methods with Finite-Difference Gradient Approximations

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Outline

- Introduction and Motivation
- New Methods
- Preliminary Numerical Results

Problem Definition

We are interested in the unconstrained optimization problem

$$\text{Minimize } f(x), \quad x \in \mathbb{R}^n, \tag{1}$$

where

- $f : \mathbb{R}^n \to \mathbb{R}$ is nonconvex and has a lower bound $f_{low} \in \mathbb{R}$.
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Derivative-Free Optimization: We want to (approximately) solve (1) relying only on evaluations of $f(\cdot)$.

Worst-Case Evaluation Complexity Bounds

Practical Goal: Given $\epsilon > 0$, generate $\bar{x}$ such that

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Question: In the worst-case, how many function evaluations an specific method performs to generate $\bar{x}$ satisfying (2)?

Worst-Case Evaluation Complexity Bounds

Deterministic DFO Methods: $\mathcal{O}\left(n^2\epsilon^{-2}\right)$ function evaluations

- Direct Search Methods: Vicente (2013); Konecny & Richtárik (2014).
- Derivative-free trust-region methods: Garmanjani, Júdice & Vicente (2016)

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Randomized Methods: Random steps, directions, subspaces...

- Nesterov & Spokoiny (2011): $\mathcal{O}\left(n\epsilon^{-2}\right)$.
- Gratton, Royer, Vicente & Zhang (2015): $\mathcal{O}\left(mn\epsilon^{-2}\right)$.
- Bergou, Gorbunov & Richtárik (2020): $\mathcal{O}\left(n\epsilon^{-2}\right)$.
- Kimiaei & Neumaier (2021): $\mathcal{O}\left(mn\epsilon^{-2}\right)$.
- Cartis & Roberts (2021): $\mathcal{O}\left(r\epsilon^{-2}\right)$.

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Remark: Complexity bounds to generate x_k such that

$$E\left[\|\nabla f(x_k)\|\right] \leq \epsilon \quad \text{or} \quad P\left(\|\nabla f(x_k)\| \leq \epsilon\right) \geq 1 - e^{-c\epsilon^{-2}}.$$

This Work

Question: Is it possible to design deterministic DFO methods with worst-case evaluation complexity of $\mathcal{O}\left(n\epsilon^{-2}\right)$?

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Generic First-Order Method with Line Search (Template)

Step 0 Given $x_1 \in \mathbb{R}^n$ and $\sigma_1 > 0$, set $k := 1$.

Step 1 Set $i := 0$.

Step 1.1 Compute $\nabla f(x_k)$.

Step 1.2 Set

$$x_{k,i}^{+} = x_k - \left(\frac{1}{2^i \sigma_k}\right) \nabla f(x_k).$$

Step 1.3 If $x_{k,i}^{+}$ satisfies a certain Line search condition, set $i_k := i$ and go to Step 2. Otherwise, set $i := i + 1$ and go to Step 1.2.

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Choice of h_i

Recently, Kohler and Lucchi (2017) and Wang *et al.* (2019) considered adaptations of the Cubic Regularization of the Newton's Method where $\nabla^2 f(x_k)$ is replaced by a matriz B_k such that

$$\|\nabla^2 f(x_k) - B_k\| \leq \kappa_B \|x_k - x_{k-1}\|. \tag{3}$$

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Our choice:

$$h_i = \frac{2\kappa_g}{\sqrt{n}\,(2^i \sigma_k)} \|x_k - x_{k-1}\|.$$

If $2^i \sigma_k \geq L$, then (4) holds.

Derivative-Free Method

Step 0 Given $x_0, x_1 \in \mathbb{R}^n$ $(x_0 \neq x_1)$, $\kappa_g > 0$, and $\sigma_1 > 0$, set $k := 1$.

Step 1 Set $i := 0$.

Step 1.1 For

$$h_i = \frac{2\kappa_g \|x_k - x_{k-1}\|}{\sqrt{n}\,(2^i \sigma_k)}$$

compute $g_{k,i} \in \mathbb{R}^n$ with

$$[g_{k,i}]_j = \frac{f(x_k + h_i e_j) - f(x_k)}{h_i}, \quad i = 1, \ldots, n.$$

Step 1.2 Set

$$x_{k,i}^+ = x_k - \left(\frac{1}{2^i \sigma_k}\right) g_{k,i}.$$

Step 1.3 If $x_{k,i}^+$ satisfies a certain Line search condition, set $i_k := i$ and go to Step 2. Otherwise, set $i := i + 1$ and go to Step 1.1.

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Derivative-Free Method

Lemma: Let

$$x_{k,i}^{+} = x_k - \left(\frac{1}{2^i \sigma_k}\right) g_{k,i}.$$

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Lemma: Let

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If

$$2^i \sigma_k \geq 2\,(L + \kappa_g)$$

then

$$f(x_k) - f(x_{k,i}^{+}) \geq \frac{2^i \sigma_k}{4} \|x_{k,i}^{+} - x_k\|^2 - \frac{\kappa_g}{2} \|x_k - x_{k-1}\|^2.$$

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set $i_k := i$ and go to Step 2. Otherwise, set $i := i + 1$ and go to Step 1.1.

Step 2 Set $x_{k+1} = x_{k,i}^+$, $\sigma_{k+1} = \frac{1}{2}\left(2^{i_k} \sigma_k\right)$, $k := k + 1$, and go to Step 1.

Complexity Analysis

Lemma: The sequence $\{\sigma_k\}$ satisfies

$$\sigma_1 \leq \sigma_k \leq 2\left(L + \frac{\sigma_1}{2}\right) \equiv \sigma_{\max},$$

for all $k \geq 1$.

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Lemma: The sequence $\{\sigma_k\}$ satisfies

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Moreover, the number FE_T of function evaluations performed up to the Tth iteration is bounded as follows

$$FE_T \leq 1 + (n+1)\left[2T + \log_2(\sigma_{\max}) - \log_2(\sigma_1)\right] = \mathcal{O}(nT).$$

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Theorem: Given $\epsilon > 0$, let T be the first iteration index such that

$$\|\nabla f(x_T)\| \leq \epsilon.$$

Then,

$$T \leq 3 + \left(\frac{5L}{4} + \sigma_{\max}\right)^2 \left[\frac{8(f(x_1) - f_{low})}{\sigma_1} + 2\|x_1 - x_0\|^2\right] \epsilon^{-2} = \mathcal{O}(\epsilon^{-2}).$$

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Corollary: $FE_T \leq \mathcal{O}(nT) \leq \mathcal{O}(n\epsilon^{-2})$, i.e., the propose method requires at most $\mathcal{O}\left(n\epsilon^{-2}\right)$ function evaluations to generate x_k such that $\|\nabla f(x_k)\| \leq \epsilon$.

What is the main trick?

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Quadratic Regularization Method: $\mathcal{O}(n\epsilon^{-2})$

Instead of

$$x_{k,i}^{+} = x_k - \left(\frac{1}{2^i \sigma_k}\right) g_{k,i},$$

we can compute $x_{k,i}^{+}$ as an approximate minimizer of the quadratic model

$$M_{x_k, 2^i \sigma_k}(y) = f(x_k) + \langle g_{k,i}, y - x_k \rangle + \frac{1}{2}\langle B_k(y - x_k), y - x_k \rangle + \frac{2^i \sigma_k}{2}\|y - x_k\|^2,$$

where $B_k \in \mathbb{R}^{n \times n}$ is symmetric and positive semidefinite.

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Additional Assumption: $\|B_k\| \leq M$ for all $k \geq 1$.

QRM with Central Finite-Differences: $\mathcal{O}(n\epsilon^{-2})$

We can also use central finite-difference gradients:

$$[g_{k,i}]_j = \frac{f(x_k + h_i e_j) - f(x_k - h_i e_j)}{2h_i}, \quad j = 1, \ldots, n.$$

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If $2^i \sigma_k \geq L_2$, then (5) holds.

Outline

- Introduction and Motivation
- New Methods
- Preliminary Numerical Results

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Four dimensions were considered: $n = 8, 12, 16, 20$.

Total of 120 test problems.

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- $FE(\epsilon)$: Corresponding number of function evaluations.
- $A(\epsilon)$: It is defined as

$$A(\epsilon) = \frac{FE(\epsilon)}{T(\epsilon)(n+1)}.$$

Complexity Analysis

Lemma: The number FE_T of function evaluations performed up to the Tth iteration is bounded as follows

$$FE_T \leq 1 + (n+1)\left[2T + \log_2(\sigma_{\max}) - \log_2(\sigma_1)\right].$$

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Lemma: The number FE_T of function evaluations performed up to the Tth iteration is bounded as follows

$$A_T = \frac{FE_T}{T(n+1)} \leq 2 + \frac{1 + (n+1)\left[\log_2(\sigma_{\max}) - \log_2(\sigma_1)\right]}{T(n+1)}$$

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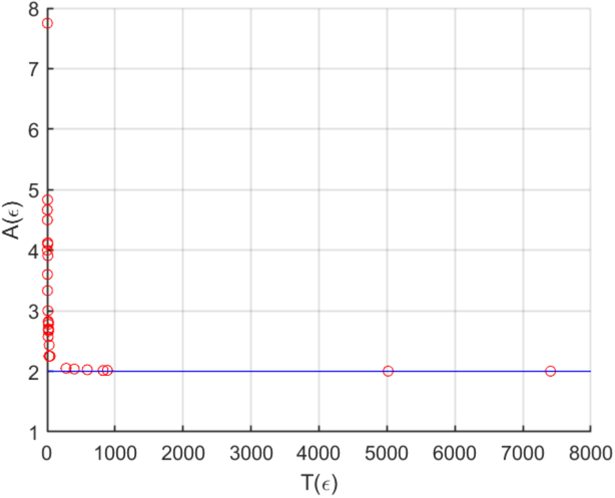
So, when $T \to +\infty$, the upper bound on A_T approaches to 2.

Preliminary Numerical Results: Experiment 1

	$\epsilon = 10^{-1}$			$\epsilon = 10^{-2}$		
PROBLEM	$T(\epsilon)$	$FE(\epsilon)$	$A(\epsilon)$	$T(\epsilon)$	$FE(\epsilon)$	$A(\epsilon)$
1. Extend. Rosenbrock	5017	90450	2.0032	7406	133452	2.0022
2. Extend. Powell Sing.	279	5148	2.0502	886	16074	2.0158
3. Penalty I	14	325	2.5714	14	324	2.5714
4. Penalty II	16	387	2.6875	44	891	2.2500
5. Variably Dim.	399	7317	2.0376	590	10755	2.0254
6. Trigonometric	4	162	4.5000	28	567	2.2500
7. Discrete BV	11	297	3.0000	824	14931	2.0133
8. Discrete IE	3	126	4.6667	5	162	3.6000
9. Broyden Tridiagonal	21	504	2.6667	30	657	2.4333
10. Broyden Banded	16	405	2.8125	20	486	2.7000
11. Brown AL	17	432	2.8235	18	450	2.7778
12. Linear	4	144	4.0000	6	180	3.3333
13. Linear-1	4	279	7.7500	4	279	7.7500
14. Linear-0	10	369	4.1000	11	387	3.9091
15. Chebyquad	6	261	4.8333	8	297	4.1250

Preliminary Numerical Results: Experiment 1

Figure below presents all the pairs $(T(\epsilon), A(\epsilon))$.



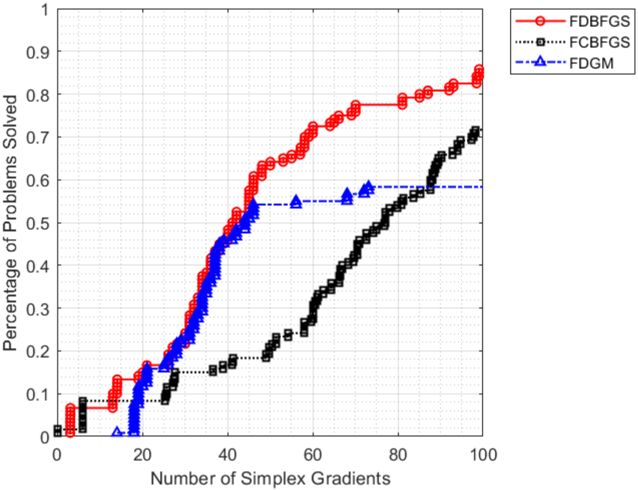
Preliminary Numerical Results: Experiment 2

The following codes were compared in the full set of 120 test problems:

- FDGM: New method with forward finite-difference gradients and $B_k = 0$.
- FDBFGS: New method with forward finite-difference gradients and B_k obtained by the BFGS formula.
- **FCBFGS**: New method with **central finite-difference** gradients and B_k obtained by the **BFGS formula**.

Preliminary Numerical Results

Data Profiles with $\tau = 10^{-7}$ (Moré & Wild, 2009)



Preliminary Numerical Results

- FDBFGS: New method with forward finite-difference gradients and B_k obtained by the BFGS formula.
- DFNLS: derivative-free trust-region method proposed by G., Yuan & Yuan (2016).
- NMSMAX: Nelder-Mead Method.

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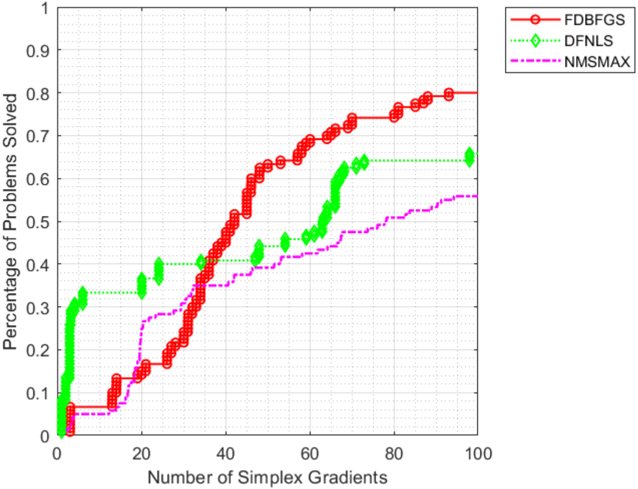

Conclusion

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2. Worst-case evaluation complexity bounds of $\mathcal{O}\left(n\epsilon^{-2}\right)$.
3. Preliminary numerical seem promissing.

Topics for Future Research

1. Generalization to composite nonsmooth optimization problems ($f(x) = \psi(c(x))$, with ψ nonsmooth).

2. Adaptation to noisy problems: Berahas, Byrd & Nocedal (2019), Berahas, Cao, Choromanski & Scheinberg (2021), Berahas, Sohab & Vicente (2021), Shi, Xuan, Oztoprak & Nocedal (2021)...

Reference

G.N.G.: *Quadratic Regularization Methods with Finite-Difference Gradient Approximations*. Optimization Online (November, 2021)

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Happy Lunar New Year!

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