Blockwise Direct-Search Methods

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Derivative-free optimization (DFO): what and why?

What is DFO?

Solve an optimization problem

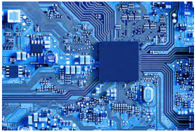
$$\min_{x \in \mathbb{R}^n} f(x)$$

using function values but not derivatives (classical or generalized).

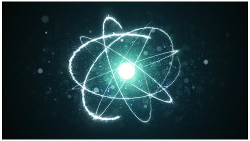
Why do we use DFO?

- Derivatives are not available even though f may be smooth.
- "not available": the evaluation is impossible or too expensive.

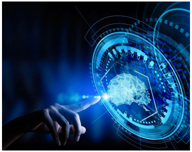
Examples of DFO problems



Circuit Design



Nuclear Energy



Machine Learning

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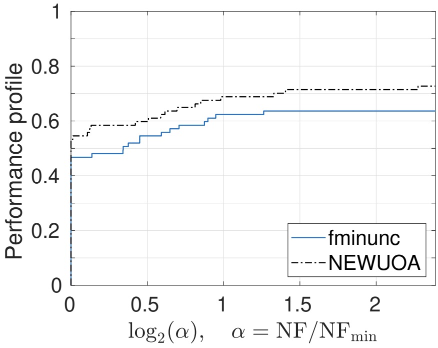
2. More et al., Nuclear energy density optimization. *Phys. Rev.*, 2010.
3. Ghanbari and Scheinberg, Black-box optimization in machine learning with trust region based derivative free algorithm, arXiv:1703.06925, 2017.

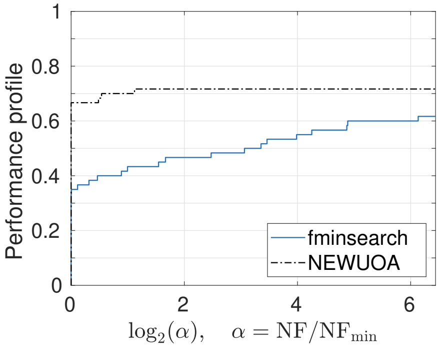
A powerful DFO solver: NEWUOA

- A derivative-free solver for unconstrained problems
- Developed by M.J.D. Powell
- Widely used by engineers and scientists

NEWUOA: performance is excellent



NEWUOA v.s. BFGS



NEWUOA v.s. simplex

(Unconstrained CUTEst problems, $6 \le n \le 100$)

NEWUOA: implementation and understanding is HARD

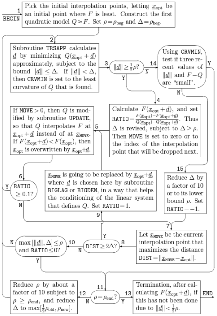


Figure 1: An outline of the method, where Y = Yes and N = No

Outline of NEWUOA's code

NEWUOA: implementation and understanding is HARD

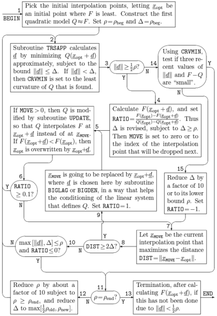


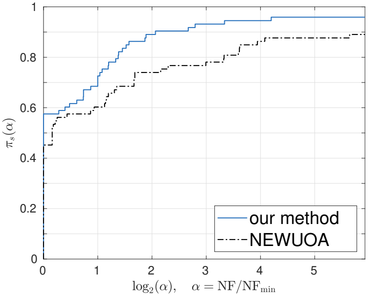
Figure 1: An outline of the method, where Y = Yes and N = No

Outline of NEWUOA's code

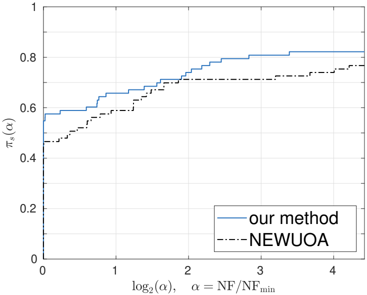
From Powell (2006)

The development of NEWUOA has taken nearly three years. The work was very frustrating . . .

Performance of the new method we introduce



(a) $\tau = 10^{-2}$



(b) $\tau = 10^{-4}$

(Unconstrained CUTEst problems, $6 \le n \le 100$)

Six months v.s. Three frustrating years!

492 lines of MATLAB code v.s. 2497 lines of Fortran code!

Outline

1. Classical direct-search methods
2. Blockwise direct-search methods
3. Implementation and Experiments
4. Conclusions and Future work

Outline

A classical direct-search framework

What is direct search?

- Not construct any models of objective functions explicitly.
- Only relying on simple comparisons to decide the point to visit.

Algorithm 1: Direct Search (DS)

Input: $x_0 \in \mathbb{R}^n$, $0 < \theta < 1 \leq \gamma$, $\alpha_0 \in (0, \infty)$, and searching set $\mathcal{D} \subset \mathbb{R}^n$.

for $k = 0, 1, \ldots$ **do**
  if $f(x_k + \alpha_k d) < f(x_k) - \rho(\alpha_k)$ for some $d \in \mathcal{D}$ **then**
    Set $\alpha_{k+1} = \gamma \alpha_k$ and $x_{k+1} = x_k + \alpha_k d$.
  else
    Set $\alpha_{k+1} = \theta \alpha_k$ and $x_{k+1} = x_k$.

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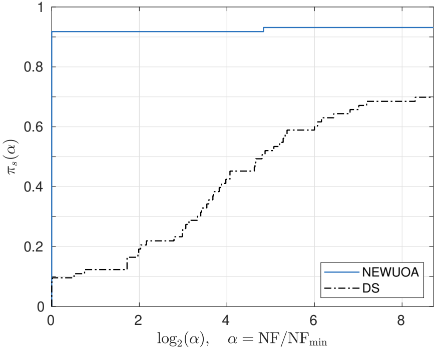
Simple, but performs poorly!

Unsatisfactory performance of direct-search methods



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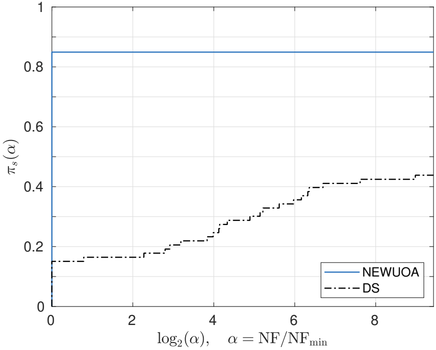

$\tau = 10^{-4}$

Flaws of the classical direct-search method

- One step size for every direction is unfair.
- Rewarding "bad" directions does not make sense.

How to improve it?

Flaws of the classical direct-search method

- One step size for every direction is unfair.
- Rewarding "bad" directions does not make sense.

How to improve it?

- Divide the searching set into many blocks.
- Each block has its own step size.

Outline

The framework of blockwise direct-search method

Algorithm 2: Cyclic Blockwise Direct Search (CBDS)

Input: $x_0 \in \mathbb{R}^n$, $0 < \theta < 1 \le \gamma$, $\alpha_0^1, \ldots, \alpha_0^m \in (0, \infty)$, and searching set $\mathcal{D}^1, \ldots, \mathcal{D}^m \subset \mathbb{R}^n$.

for $k = 0, 1, \ldots$ **do**

  Set $y_k^1 = x_k$.

  for $i = 1, \ldots, m$ **do**

    if $f(y_k^i + \alpha_k^i d_k^i) < f(y_k^i) - \rho(\alpha_k^i)$ for some $d_k^i \in \mathcal{D}^i$ **then**

      Set $\alpha_{k+1}^i = \gamma \alpha_k^i$ and $y_k^{i+1} = y_k^i + \alpha_k^i d_k^i$.

    else

      Set $\alpha_{k+1}^i = \theta \alpha_k^i$ and $y_k^{i+1} = y_k^i$.

  Set $x_{k+1} = y_k^{m+1}$.

Why it is complicated?

There are so many choices needed to select carefully.

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- Gauss-Seidel

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What is the best searching set for each block?

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There are so many choices needed to select carefully.

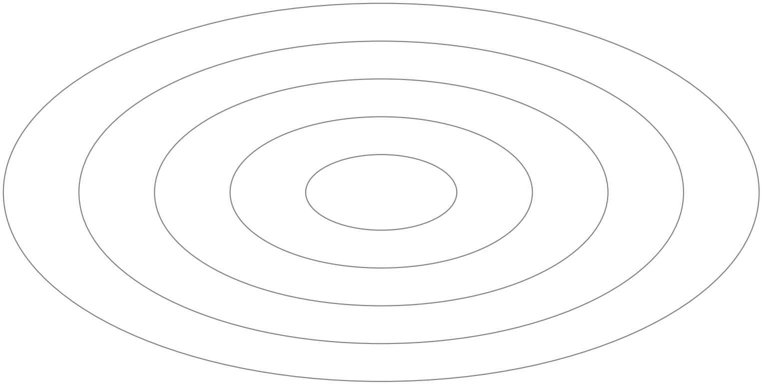
What is the best order to visit the blocks?

- Gauss-Seidel

What is the best searching set for each block?

- Coordinate directions

A simple example of the blockwise direct-search method



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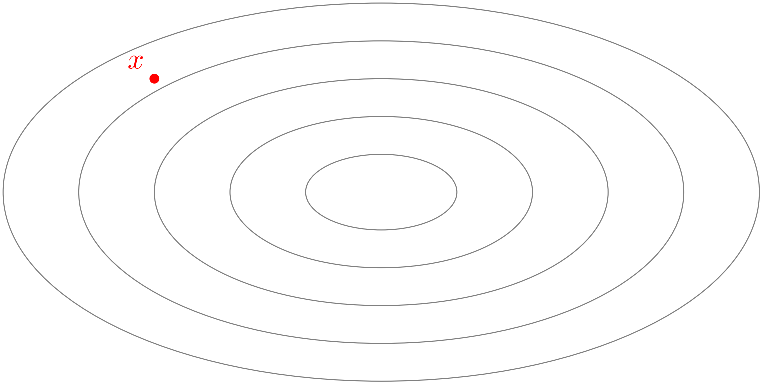

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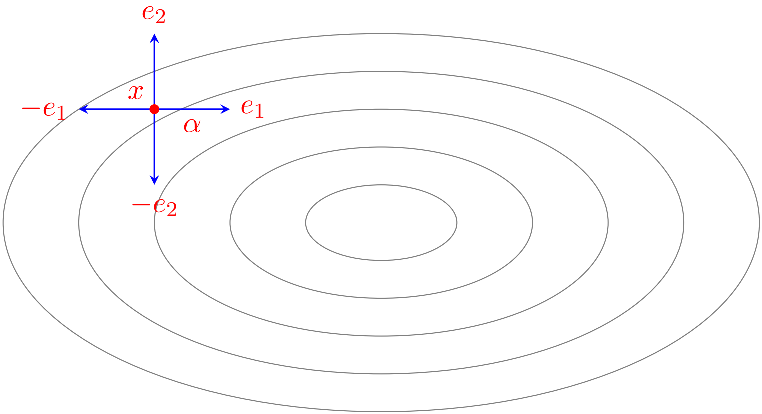

$\mathcal{D}_1 = \{e_1, -e_1\}$ and $\mathcal{D}_2 = \{e_2, -e_2\}$

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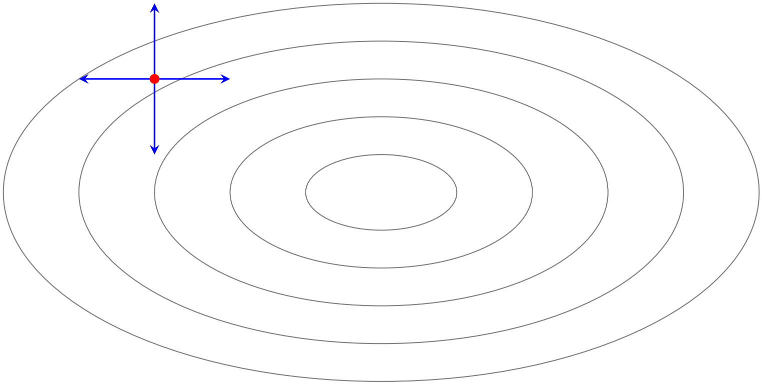

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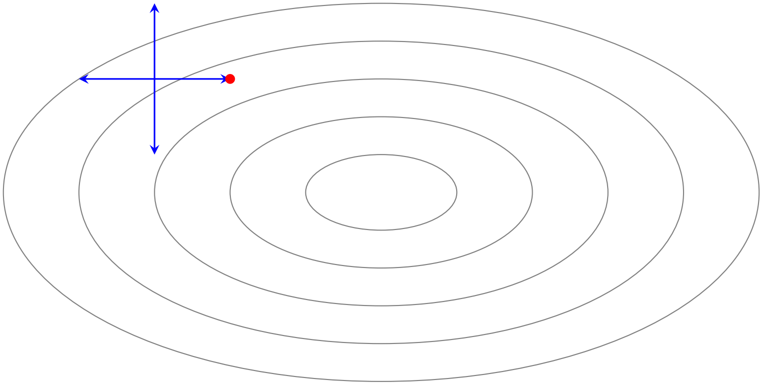

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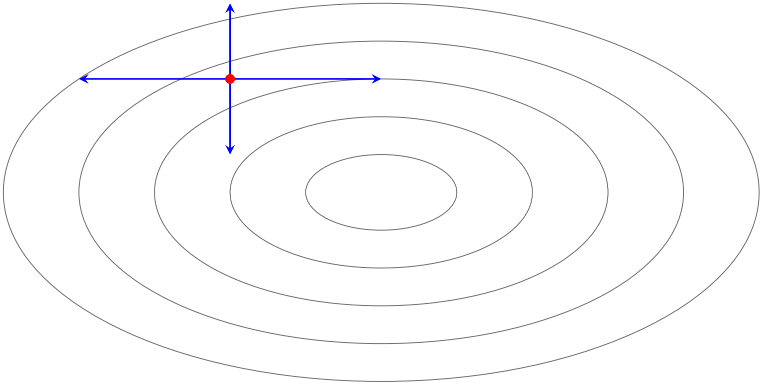

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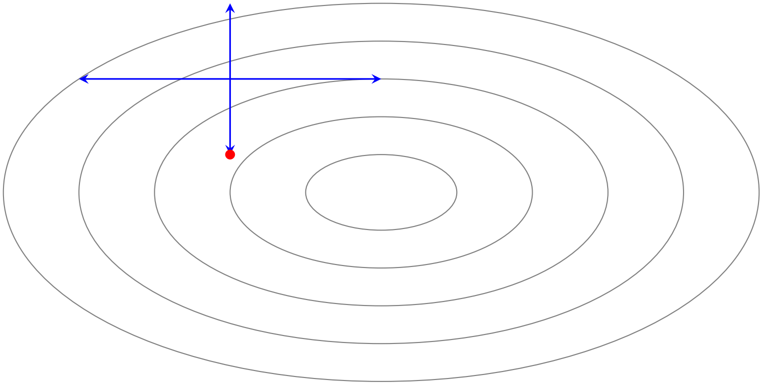

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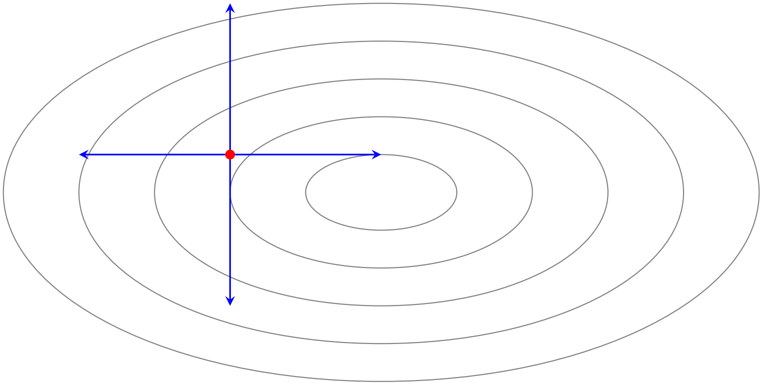

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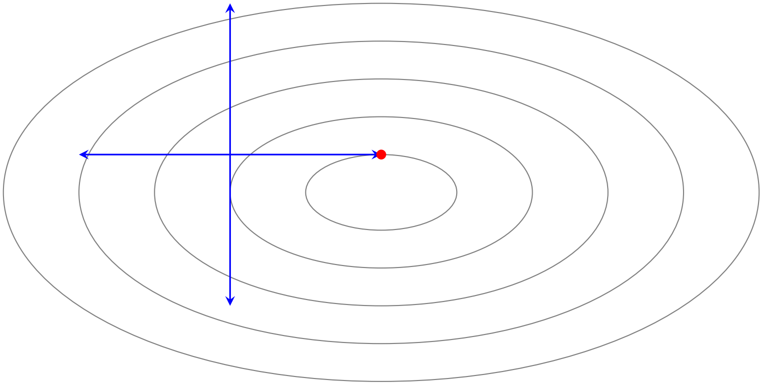

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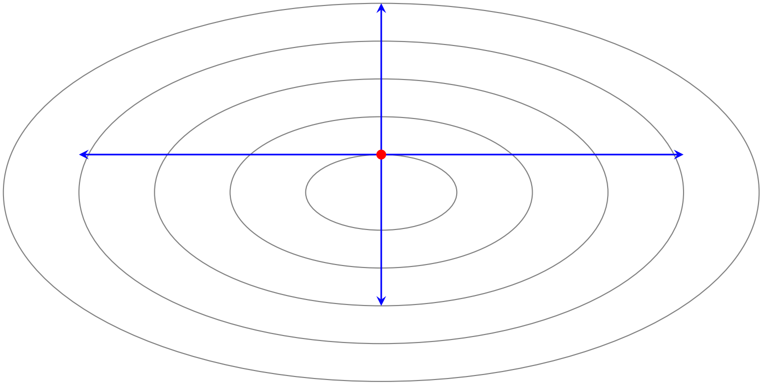

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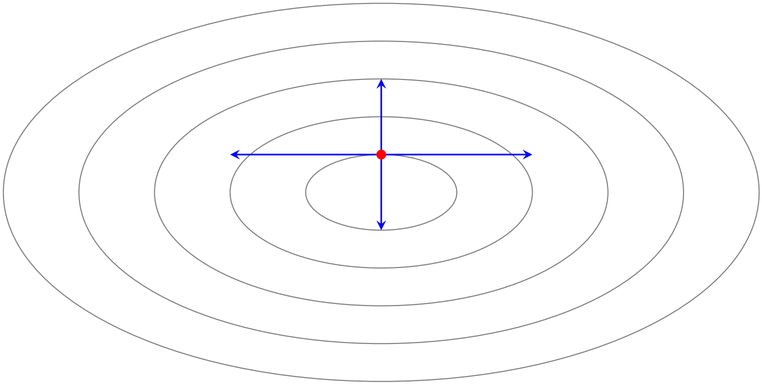

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Comparison between BDS and existing DFO solvers

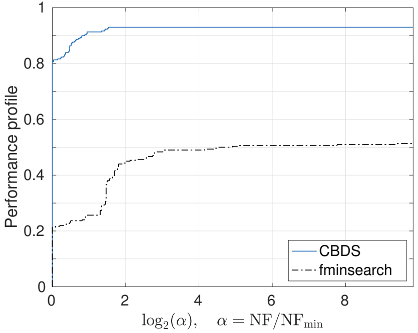
Observed value:

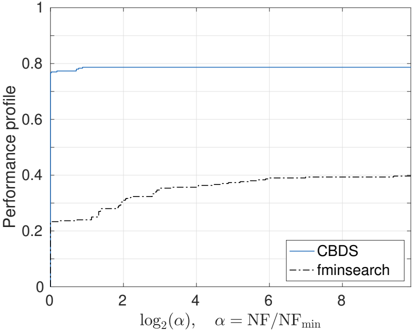
$$\widetilde{f}(x) = \begin{cases} f(x), & \text{there is no noise,} \\ f(x)[1+\epsilon(x)], & \text{there is noise,} \end{cases}$$

where $\epsilon(x) \sim \mathcal{N}(0, \sigma^2)$.
In our experiments:

- problem set: unconstrained problems from CUTEst
- dimensions: $6 \leq n \leq 100$
- noise level: $\sigma = 10^{-3}$
- budget: $1000n$ function evaluations
- number of random experiments: 10

Comparison between BDS and existing DFO solvers





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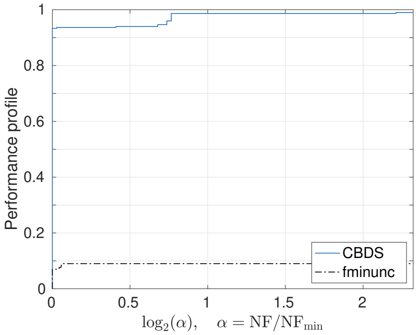

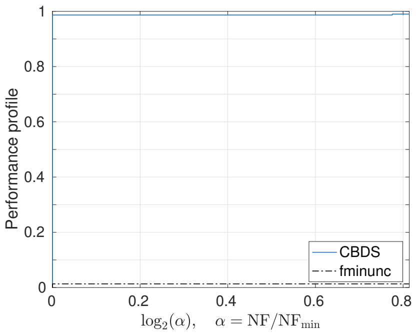

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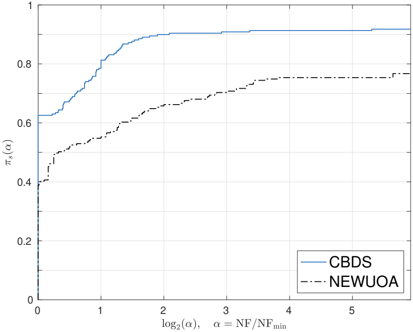

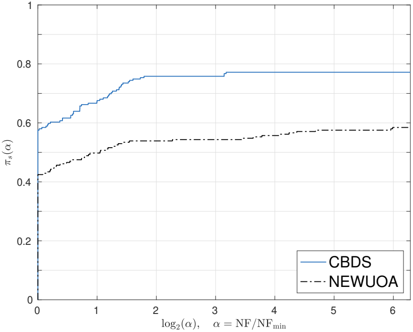

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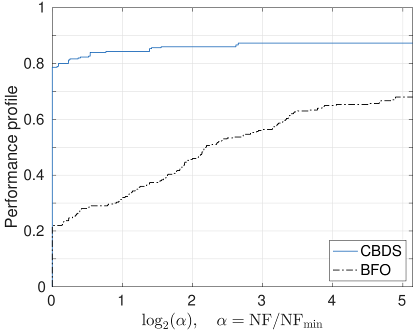

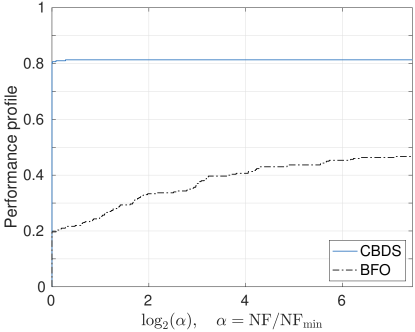

Battle-test!

README.md

Test of BDS.

The tests are **automated** by GitHub Actions.

- Check Spelling passing
- Unit test passing
- Stress test passing
- Parallel test passing
- Recursive test passing
- Test StepTolerance for bds passing
- Test forcing function for bds passing
- Test the technique of initial step size using initial point passing
- Plot performance profiles for BDS, small, testing level of reduction factor passing
- Plot performance profiles for BDS, big, testing level of reduction factor passing
- Plot performance profiles for bds and pbds, big passing
- Plot performance profiles for bds and pbds, small passing
- Plot performance profiles for bds and rbds, small passing
- Plot performance profiles for bds and dspd, big passing
- Plot performance profiles for bds and dspd, small passing
- Plot performance profiles for bds and bfgs, big passing
- Plot performance profiles for bds and bfgs, small passing
- Plot performance profiles for bds and prima, small passing
- Plot performance profiles for bds and simplex, big passing
- Plot performance profiles for bds and simplex, small passing
- Plot performance profiles for bds and nlopt, big passing
- Plot performance profiles for bds and nlopt, small passing
- Plot performance profiles for bds and bfo, small passing

Battle-test, is necessary!

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Is CBDS convergent?

- We do not know the answer yet.
- The analysis of cyclic methods is challenging.
- Is it possible that the vanilla version of CBDS is not convergent?

Conclusions

What we have achieved:

- Our project is open-source and easy to use
- Our method is efficient and adaptive to noise automatically

Future work:

- Convergence and worst-case complexity (of an adapted framework?)
- Finite difference or interpolation using existing iterates
- Apply our algorithm on constrained problems (like bound constraints)
- Apply our algorithm on other programming languages (like Python)

BDS homepage: `github.com/blockwise-direct-search`

Thank you!

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