Blockwise Direct-Search Methods

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

What is DFO?

Solve an optimization problem

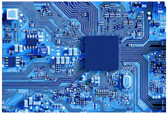
$$\min_{x \in \mathbb{R}^n} f(x)$$

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

When do we use DFO?

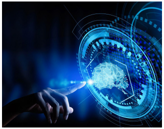
- Derivatives are not available even though f may be smooth.
- "not available": the evaluation is impossible or too expensive.

The applications of DFO



Circuit Design

Photovoltaic



Machine Learning

1. X. Zeng et al., BBGP-sDFO: Batch Bayesian and Gaussian Process Enhanced Subspace Derivative Free Optimization for High-Dimensional Analog Circuit Synthesis, *IEEE Trans. Comput.-Aided Des. Integr. Circuits Syst.*, 2023.
2. Shokralla et al., Parameter estimation of a photovoltaic array using direct search optimization algorithm. *J. Renew. Sustain. Energy*, 2017.
3. Ghanbari and Scheinberg, Black-box optimization in machine learning with trust region based derivative free algorithm, arXiv:1703.06925, 2017.

Two main classes of DFO methods

1. Direct-search methods based on
   - simplex (Nelder-Mead method)
   - directional search (BFO, PDS, NOMAD)
2. Model-based methods based on
   - trust region (Powell's methods)
   - line search

Methods not covered by these two classes:

Bayesian optimization, genetic algorithms, etc.

Model-based methods v.s. Direct-search methods

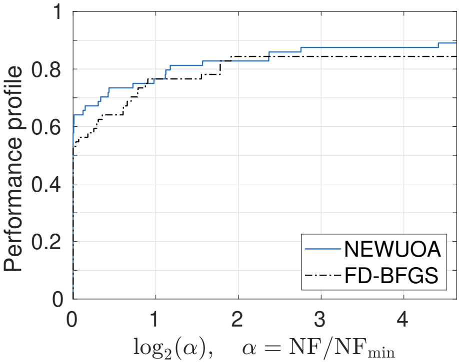
	Model-based	Direct-search
Performance	good	less satisfactory
Implementation	complicated	relatively simple

1. Model-based methods:
   - The optimization process is guided by models.
   - The coupling between modeling and optimization makes the implementation complicated.
2. Direct-search methods:
   - No need to construct models.
   - Iterate is decided by comparing the function values of samples.

An example of DFO solver: NEWUOA

- A derivative-free solver for unconstrained problems
- Developed by M.J.D. Powell
- Widely used by engineers and scientists
- The modernized version (https://github.com/libprima)

NEWUOA: performance is quite good



- FD-BFGS: Forward-finite-difference BFGS method.

NEWUOA: implementation and understanding is HARD

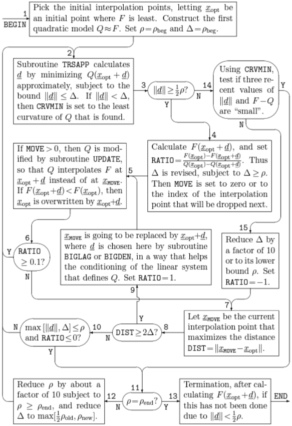


Figure 1: An outline of the method, where Y = Yes and N = No

Framework of NEWUOA

NEWUOA: implementation and understanding is HARD

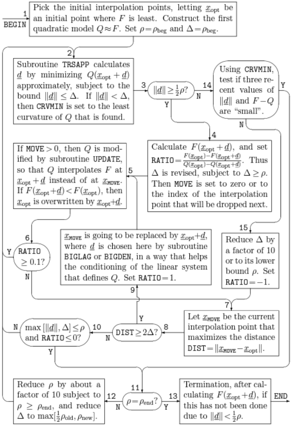


Figure 1: An outline of the method, where Y = Yes and N = No

Framework of NEWUOA

From Powell (2006)

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

Outline

1. Classical direct-search methods

2. Blockwise direct-search methods

3. Implementation and experiments

4. Conclusions and future work

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A classical direct-search framework

What is direct search?

- No explicit models are constructed based on function values.
- Iterations are only decided according to function values.

Algorithm 1: Direct Search (DS) based on sufficient decrease

Input: $x_0 \in \mathbb{R}^n$, $0 < \theta < 1 \leq \gamma$, $\alpha_0 > 0$, $c > 0$, a searching direction set $\mathcal{D} \subset \mathbb{R}^n$.

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

  if $f(x_k + \alpha_k d) < f(x_k) - c\rho(\alpha_k)$ for some $d \in \mathcal{D}$ **then**

    Set $x_{k+1} = x_k + \alpha_k d$ and $\alpha_{k+1} = \gamma\alpha_k$.

  else

    Set $x_{k+1} = x_k$ and $\alpha_{k+1} = \theta\alpha_k$.

Unsatisfactory performance of direct-search methods

Simple, but performs unsatisfactorily!

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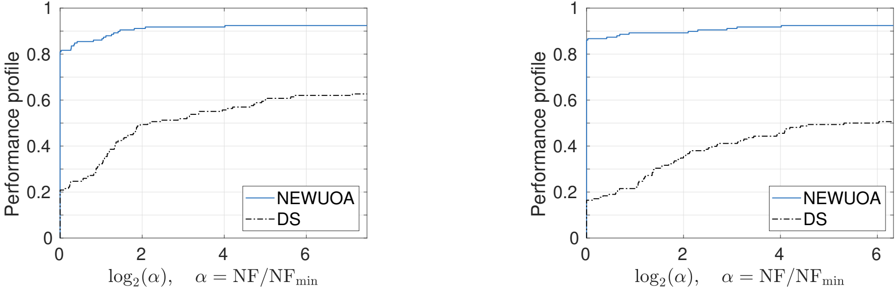

(a) $\tau = 10^{-3}$ (b) $\tau = 10^{-5}$

(Unconstrained CUTEst problems, $1 \leq n \leq 200$)

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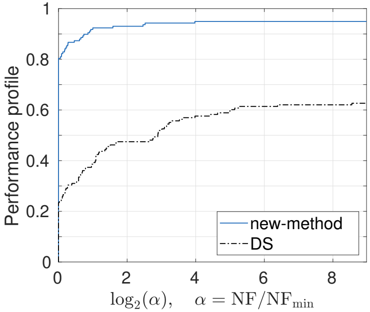
Obvious improvement!



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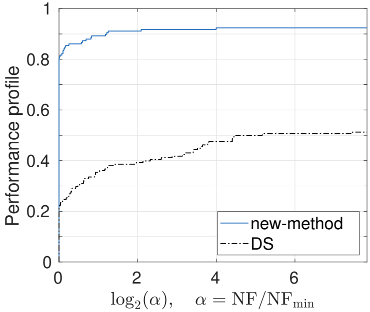

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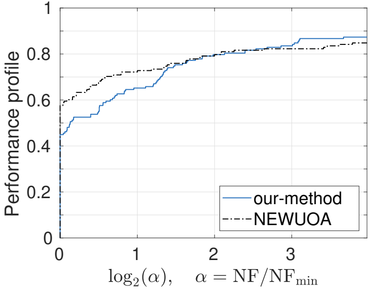
(Unconstrained CUTEst problems, $1 \leq n \leq 200$)

Performance of the new method we introduce



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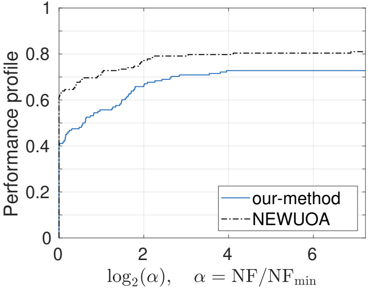

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(Unconstrained CUTEst problems, $1 \leq n \leq 200$)

Flaws of the classical direct-search method

Algorithm 1: Direct Search (DS) based on sufficient decrease

Input: $x_0 \in \mathbb{R}^n$, $0 < \theta < 1 \leq \gamma$, $\alpha_0 > 0$, $c > 0$, searching direction set $\mathcal{D} \subset \mathbb{R}^n$.

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

    if $f(x_k + \alpha_k d) < f(x_k) - c\rho(\alpha_k)$ for some $d \in \mathcal{D}$ **then**

        Set $x_{k+1} = x_k + \alpha_k d$ and $\alpha_{k+1} = \gamma\alpha_k$.

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How to improve it?

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How to improve it?

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

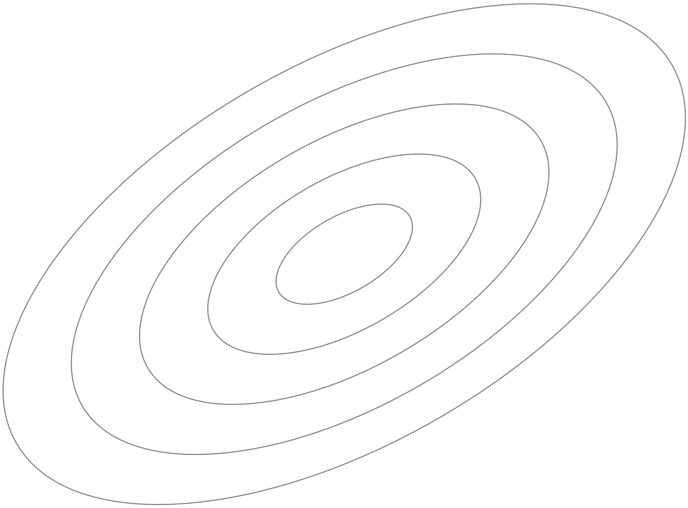
A cyclic framework of blockwise direct-search method

Algorithm 2: Cyclic Blockwise Direct Search (CBDS)

Input: $x_0 \in \mathbb{R}^n$, $0 < \theta < 1 \le \gamma$, $\alpha_0^1, \ldots, \alpha_0^m \in (0, \infty)$, $c > 0$, a searching direction set $\mathcal{D} = \cup_{i=1}^m \mathcal{D}^i \subset \mathbb{R}^n$.

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

A simple example of the blockwise direct-search method



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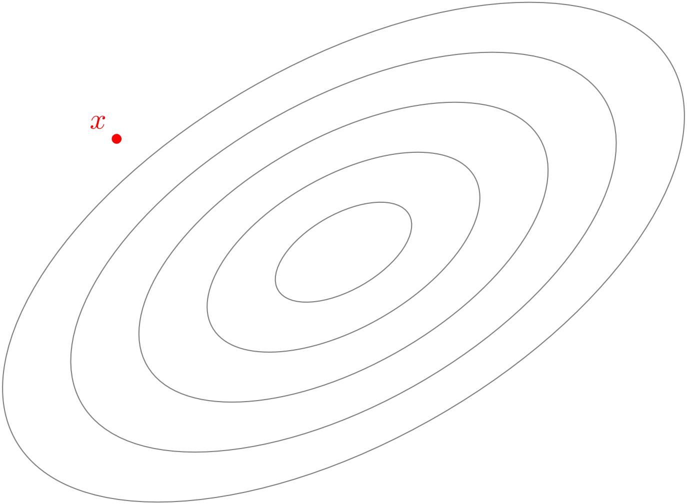

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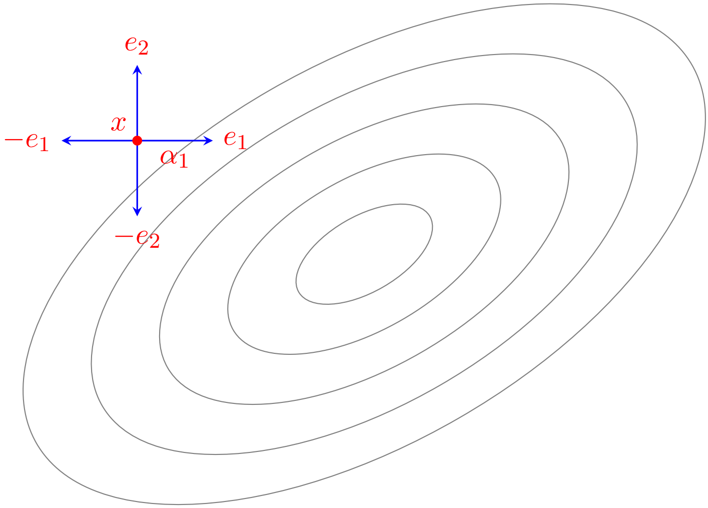

$\mathcal{D}_1 = \{e_1, -e_1\}$ and $\mathcal{D}_2 = \{e_2, -e_2\}$

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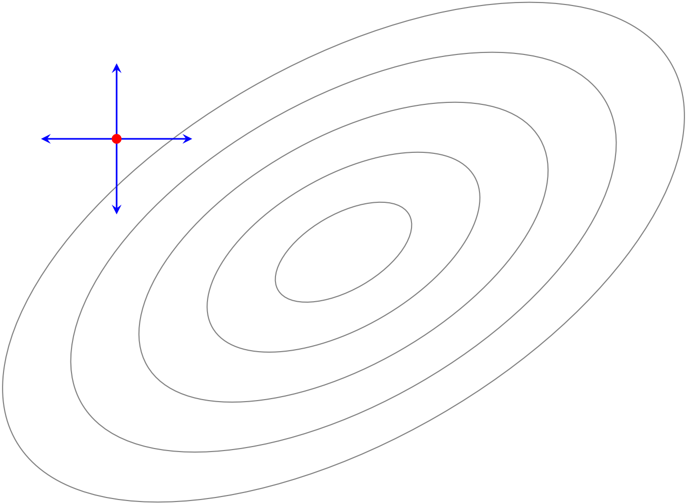

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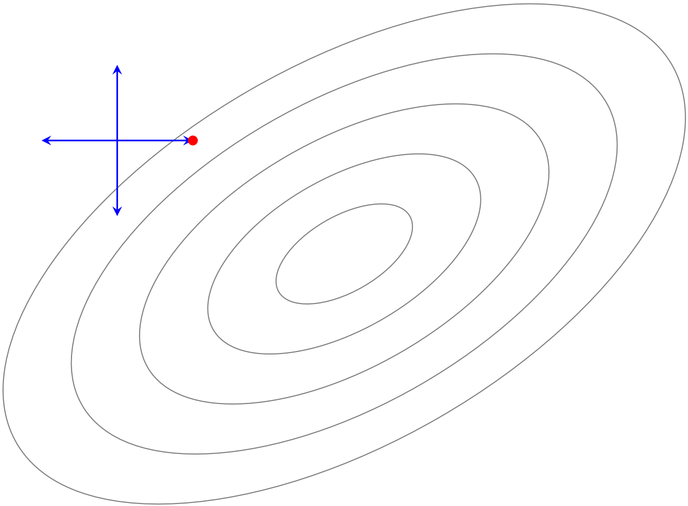

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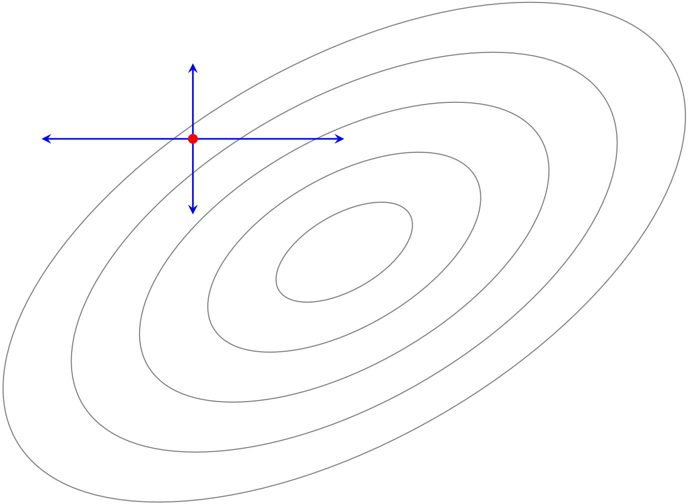

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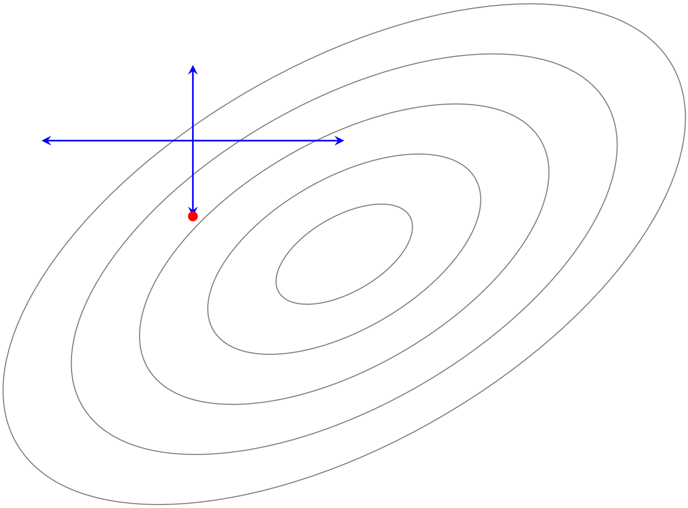

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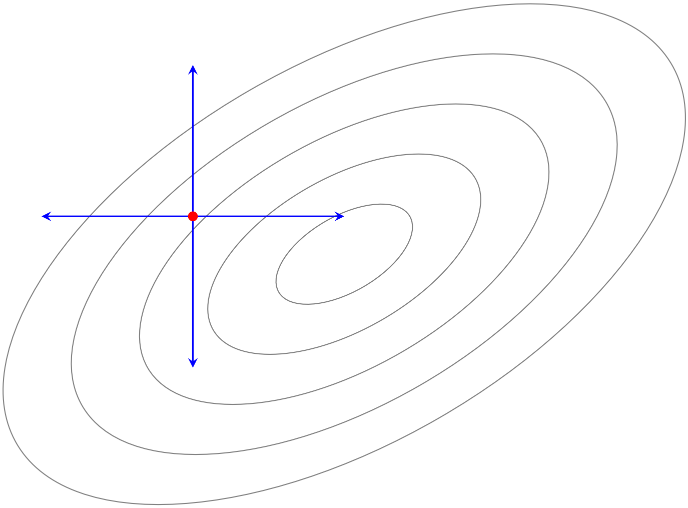

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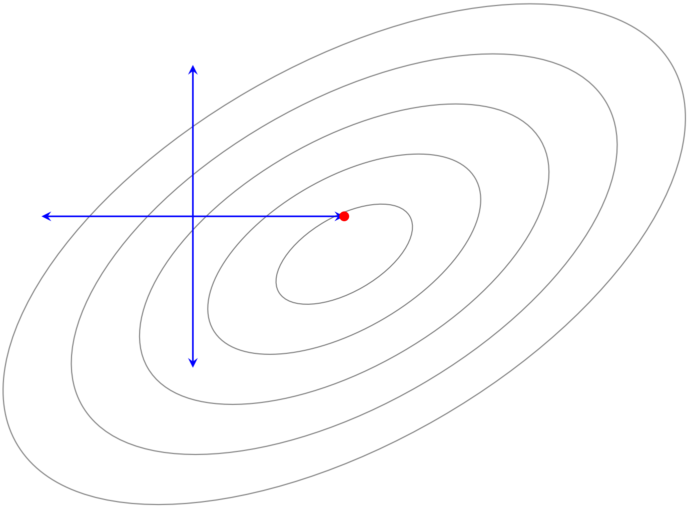

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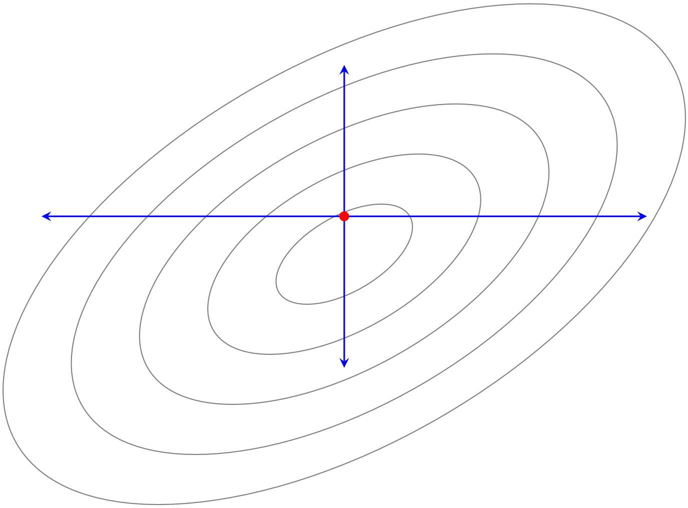

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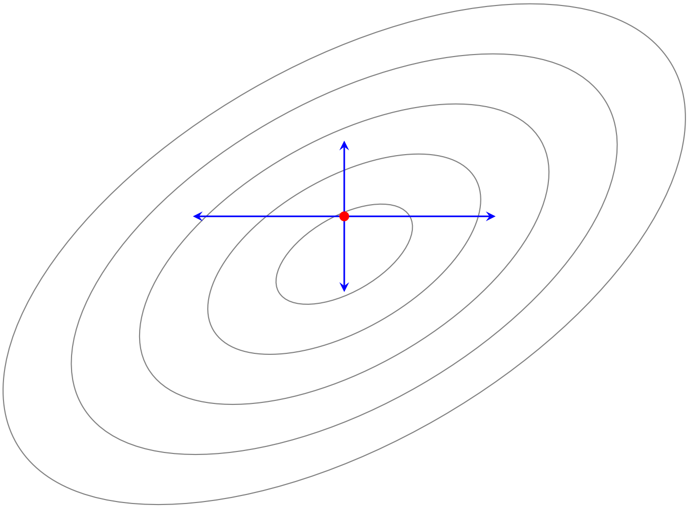

Flexibility of the framework

- The searching direction set: A positive spanning set.
- The division of blocks: any way that "fits the problem".
- The scheme of visiting blocks: Cyclic (Gauss-Seidel), Jacobi, random.

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- The searching direction set: A positive spanning set.
- The division of blocks: any way that "fits the problem".
- The scheme of visiting blocks: Cyclic (Gauss-Seidel), Jacobi, random.

Our implementation takes the following setting as the default:

- $\mathcal{D} = \{e_1, -e_1, \ldots, e_n, -e_n\}$
- $\mathcal{D}^i = \{e_i, -e_i\}$
- Gauss-Seidel scheme

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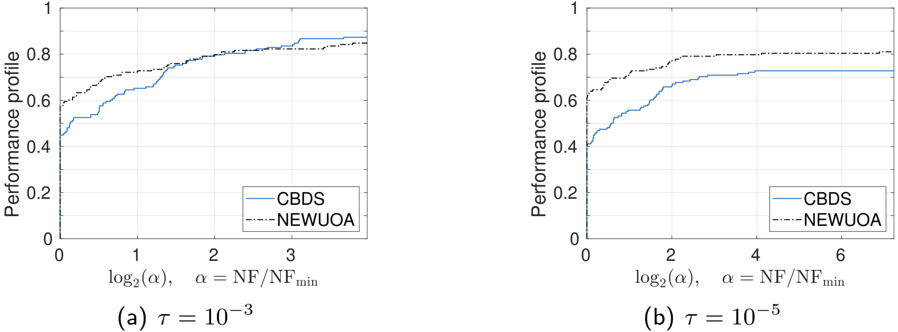
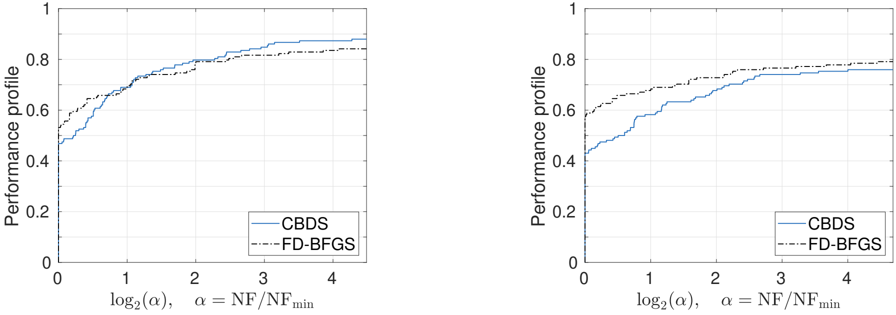
Recapped



(Unconstrained CUTEst problems, $1 \leq n \leq 200$)

Comparison between BDS and existing DFO solvers



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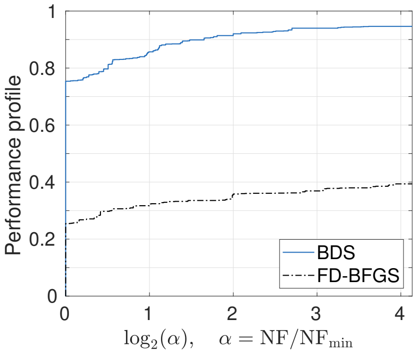
(Unconstrained CUTEst problems, $1 \leq n \leq 200$)

BDS v.s. FD-BFGS



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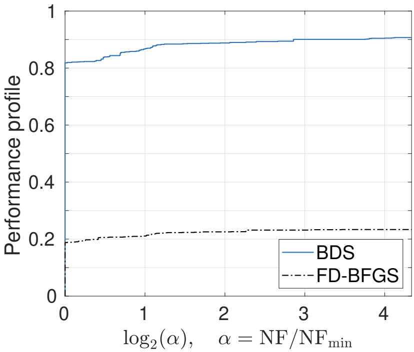
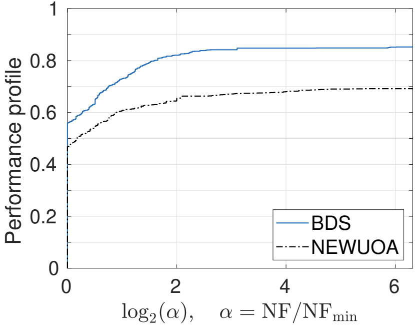


$\tau = 10^{-5}$

Set $h = \sqrt{(\max|f|, 1)\sigma}$ for FD-BFGS.

BDS v.s. NEWUOA



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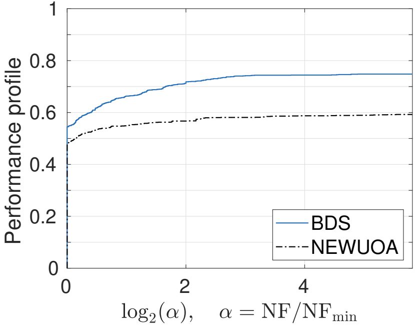
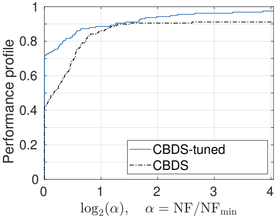


$\tau = 10^{-5}$

Self-tuning can improve the performance! [1]



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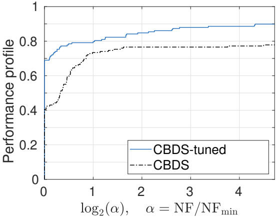

$\tau = 10^{-5}$

In our experiments:

- problem set: unconstrained problems from CUTEst
- dimensions: $1 \le n \le 200$
- hyperparameters: γ, θ, c
- default values: $\gamma = 2$, $\theta = 0.5$, $c =$ eps (machine precision)

[1] Motivated by BFO, A Note on Using Performance and Data Profiles for Training Algorithms, ACM Transactions on Mathematical Software, 2019, Porcelli, M. and Toint, Ph. L.

Self-tuning can improve the performance!

$$\min_{x \in \mathbb{R}^n} f(P_\Omega(x)) + \lambda r(x),$$

where

- $f(x)$: the difference of the integral in the performance profile
- Ω: the feasible set for the hyperparameters
- $P_\Omega(x)$: the projection from x to Ω
- λ: the penalty parameter
- $r(x)$: the residue of x in Ω

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Structured nonsmooth problems

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

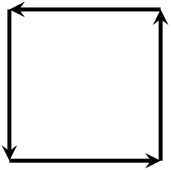
- f is smooth
- Φ is nonsmooth but separable with respect to the blocks

Examples:

- l_p-regularized problems
- bound-constrained problems

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?
- Powell's non-convergent example for cyclic coordinate descent method.



limiting behavior

Conclusions

1. Blockwise Direct Search (BDS) is a substantial improvement over the classical direct search method (based on sufficient decrease)
2. BDS performs well in the following tests:
   - Noise-free problems with a moderate size $(6 \leq n \leq 200)$ and a convergence tolerance that is not too small $(10^{-1} \leq \tau \leq 10^{-5})$
   - Noisy problems with a moderate noise level $(10^{-3} \leq \sigma \leq 10^{-1})$ and a convergence tolerance that is comparable with the noise level
3. BDS is robust under noise without any noise-handling techniques
4. BDS can be tuned to improve its performance
5. BDS is open-source and easy to use

Future work

- Convergence and worst-case complexity (an adapted framework?)
- Make use of the existing iterates (finite difference or interpolation)
- Extend our implementation to other languages (Python, Julia, etc.)

BDS on GitHub

- tested continuously via GitHub Actions
- tested under different platforms

Thank you!

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