Blockwise Direct-Search Methods

Haitian Li

The Hong Kong Polytechnic University

Joint work with Zaikun Zhang

The 2nd Derivative-free Optimization Symposium, Padova, Italy

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

What is DFO?

Solve an optimization problem

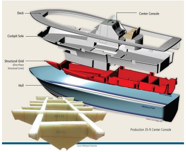
$$\min_{x \in \mathbb{R}^n} f(x)$$

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

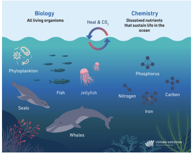
When do we use DFO?

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

The applications of DFO



Ship Design



Machine Learning

Ocean Biogeochemical

1. G. Liuzzi, S. Lucidi, F. Rinaldi et al., Derivative-free global ship design optimization using global/local hybridization of the DIRECT algorithm. *OPTIM ENG*, 2016.
2. Ghanbari and Scheinberg, Black-box optimization in machine learning with trust region based derivative free algorithm, arXiv:1703.06925, 2017.
3. C. Cartis et al., A derivative-free optimisation method for global ocean biogeochemical models. *Geosci. Model Dev*, 2022.

Two main classes of DFO methods

1. Direct-search methods based on
   - simplex (Nelder-Mead method)
   - directions (NOMAD, BFO, PDS,...)
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:
   - Iterate is decided by comparing the function values of samples.
   - No need to construct models.

An example of model-based methods: NEWUOA

- A model-based DFO solver for unconstrained problems
- Developed by M.J.D. Powell
- Widely used by engineers and scientists
- A popular benchmark in the DFO community[1]
- The modernized version: PRIMA (https://github.com/libprima)

[1] Benchmarking derivative-free optimization algorithms, Moré, J. J. and Wild, S. M., SIAM Journal on Optimization, 2009.

NEWUOA: implementation and understanding is HARD

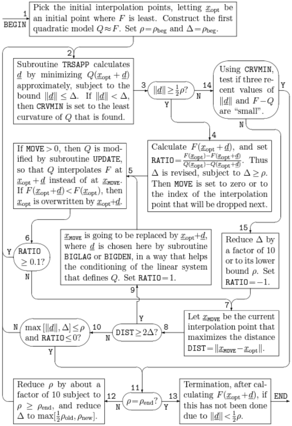


Figure 1: An outline of the method, where Y = Yes and N = No

Framework of NEWUOA

NEWUOA: implementation and understanding is HARD

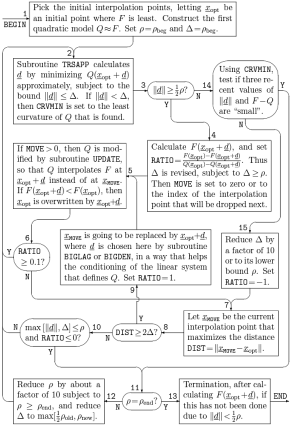


Figure 1: An outline of the method, where Y = Yes and N = No

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. Experiments
4. Conclusions and future work

Outline

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

A classical direct-search framework

What is direct search?

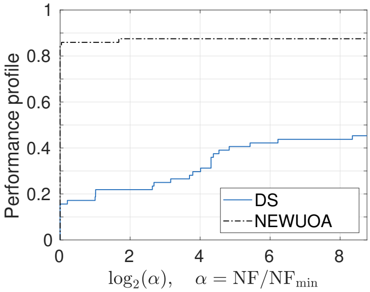
- No explicit models are constructed based on function values.
- Iterations are only decided according to function values.

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

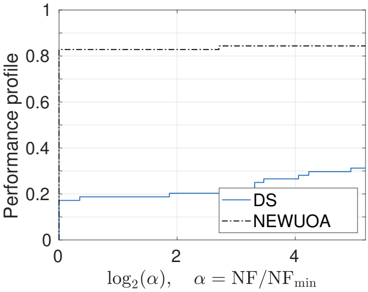
Input: $x_0 \in \mathbb{R}^n$, $0 < \theta < 1 \leq \gamma$, $\alpha_0 > 0$, $c > 0$,
a searching direction set $\mathcal{D} \subset \mathbb{R}^n$.

for $k = 0, 1, \ldots$ **do**
- **if** $f(x_k + \alpha_k d_k) < f(x_k) - \rho(\alpha_k)$ for some $d_k \in \mathcal{D}$ **then**
  - Set $x_{k+1} = x_k + \alpha_k d_k$ 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



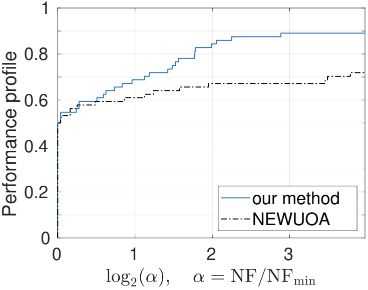
(a) $\tau = 10^{-3}$



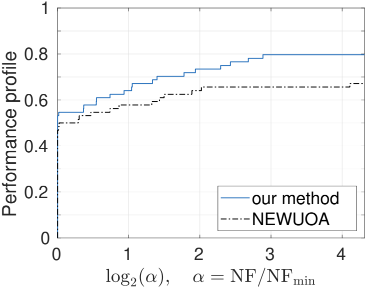
(b) $\tau = 10^{-5}$

Unconstrained CUTEst problems, $6 \leq n \leq 200$

Performance of the new method we will introduce



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



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

Unconstrained CUTEst problems, $6 \le n \le 200$

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

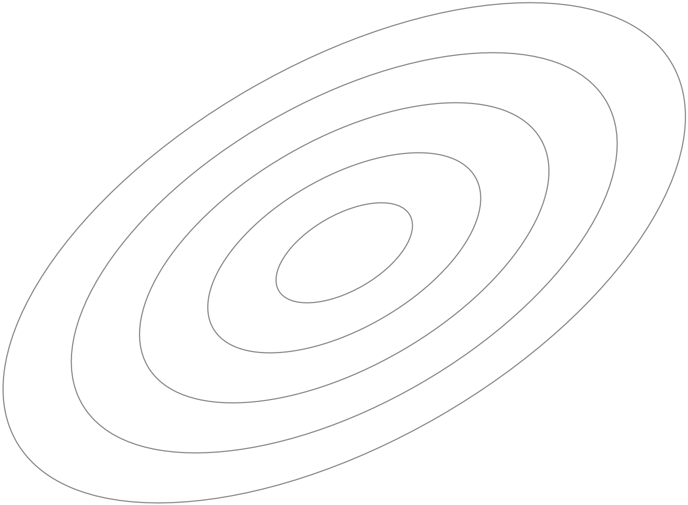
  if $f(x_k + \alpha_k d_k) < f(x_k) - \rho(\alpha_k)$ for some $d_k \in \mathcal{D}$ **then**

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

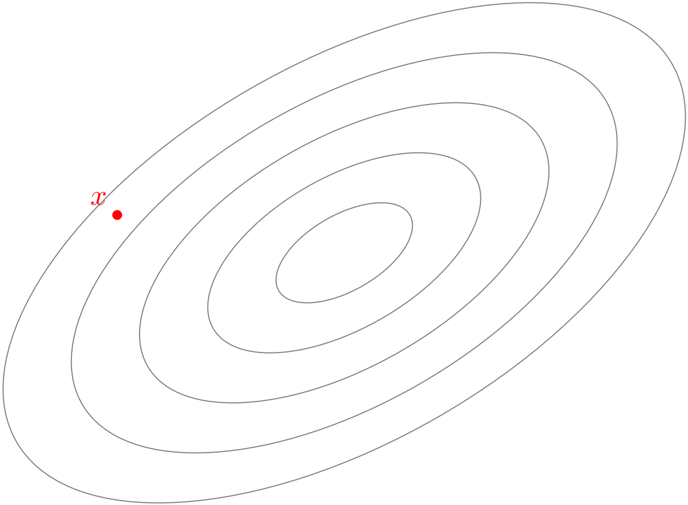
  else

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

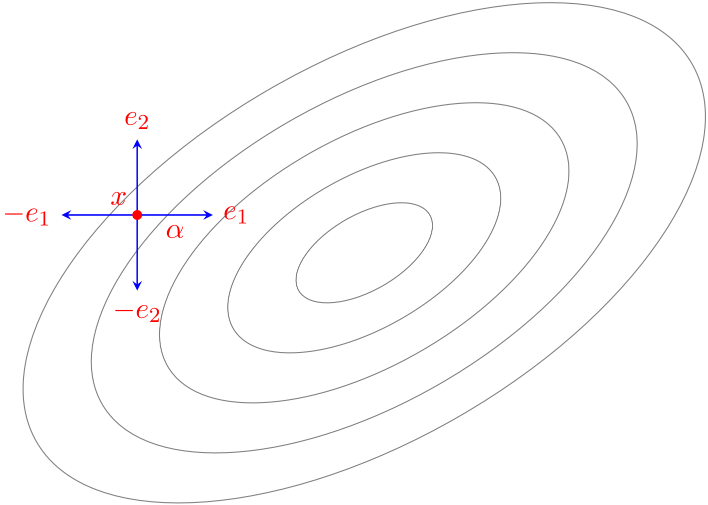
An illustration of the classical direct-search method



An illustration of the classical direct-search method

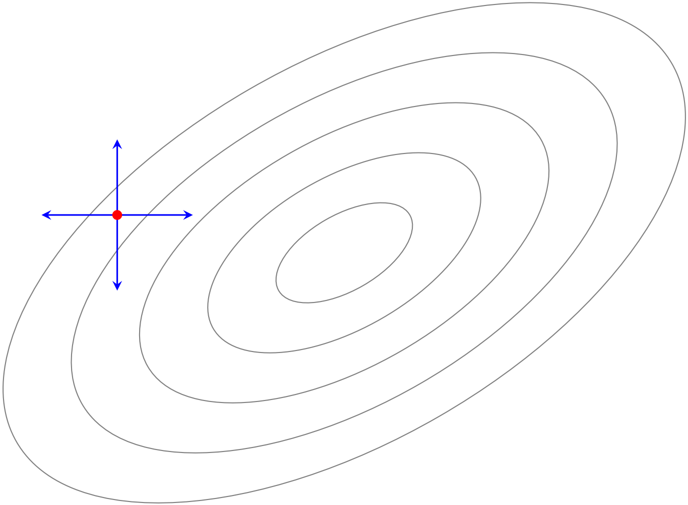


An illustration of the classical direct-search method

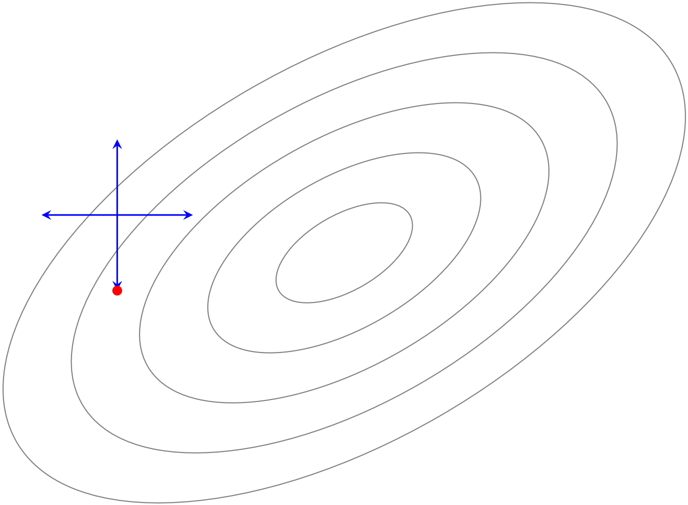


$$\mathcal{D} = \{e_1, -e_1, e_2, -e_2\}$$

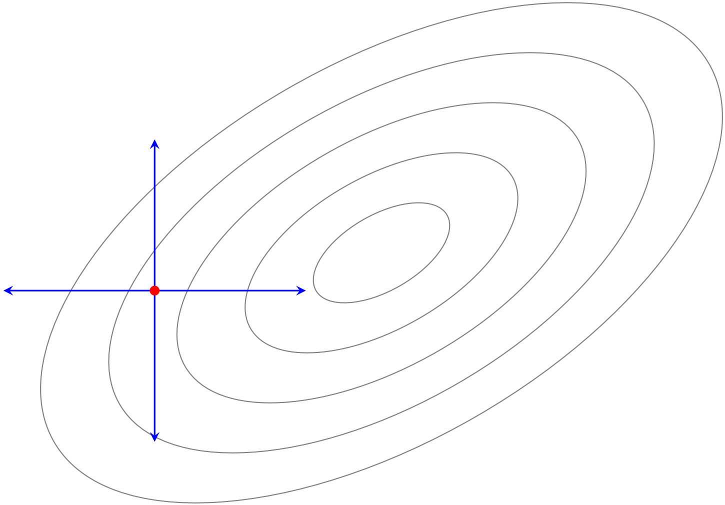
An illustration of the classical direct-search method



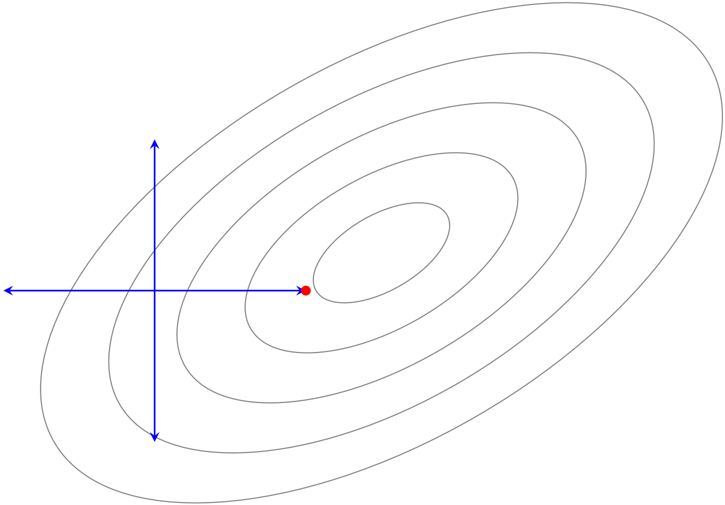
An illustration of the classical direct-search method



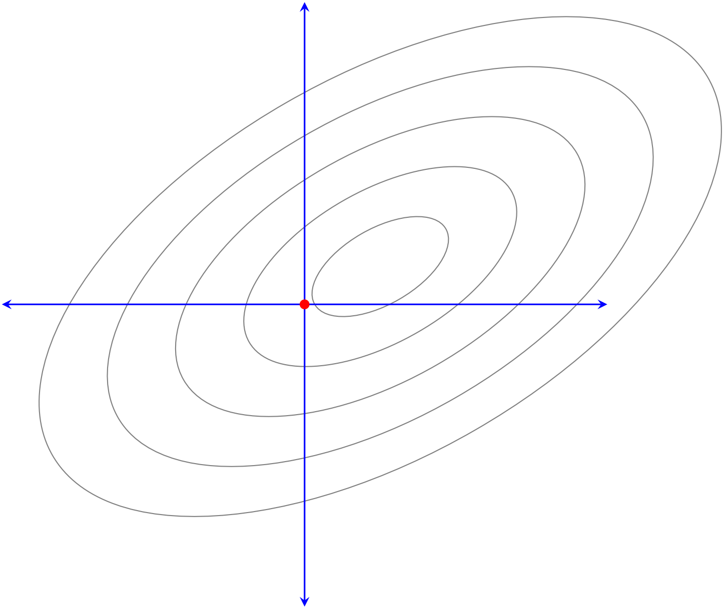
An illustration of the classical direct-search method



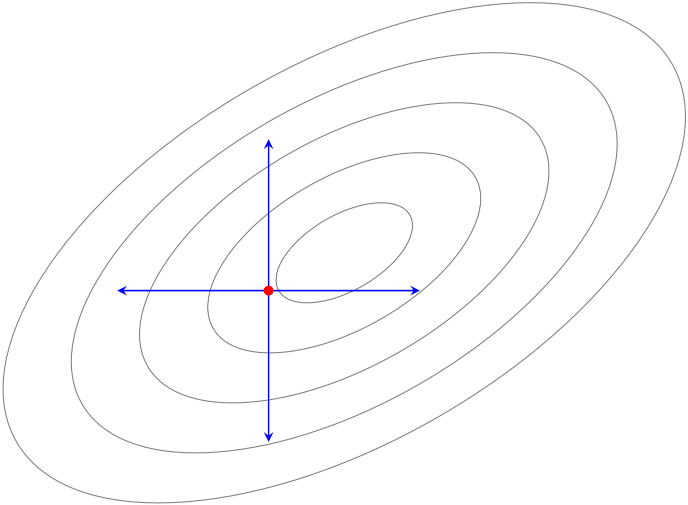
An illustration of the classical direct-search method



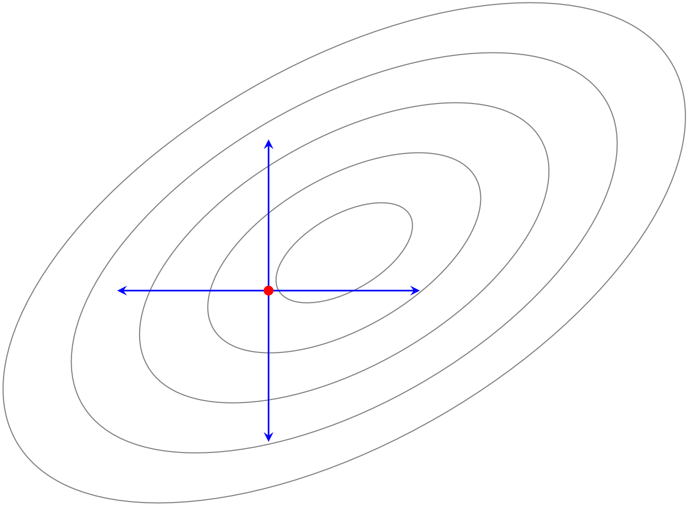
An illustration of the classical direct-search method



An illustration of the classical direct-search method

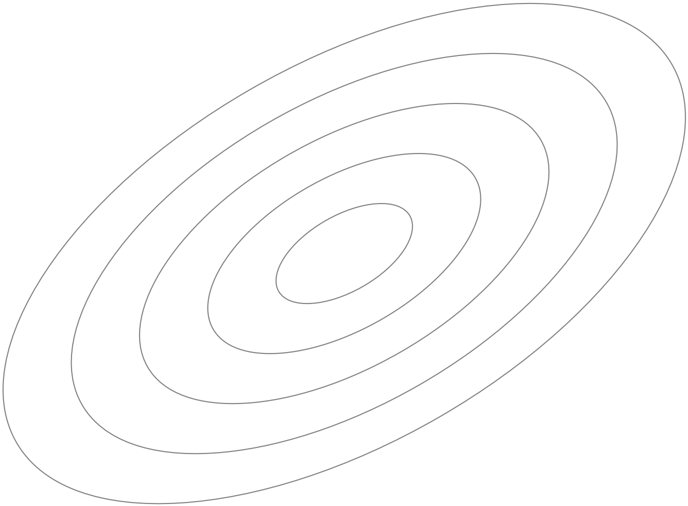


An illustration of the classical direct-search method

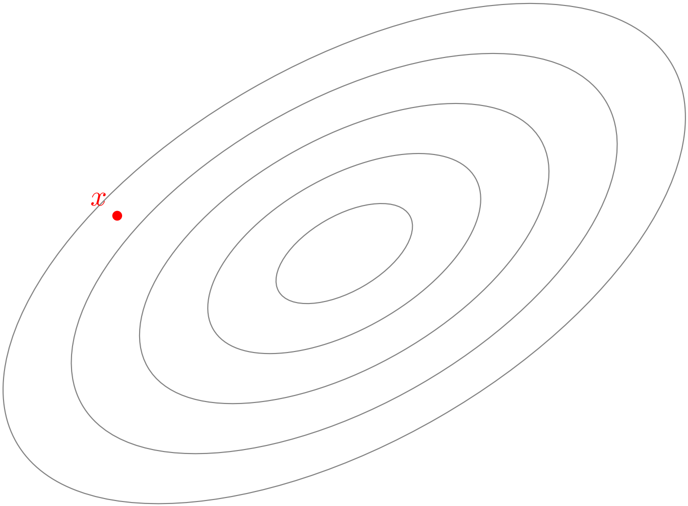


It is not reasonable to have one single stepsize for all directions!

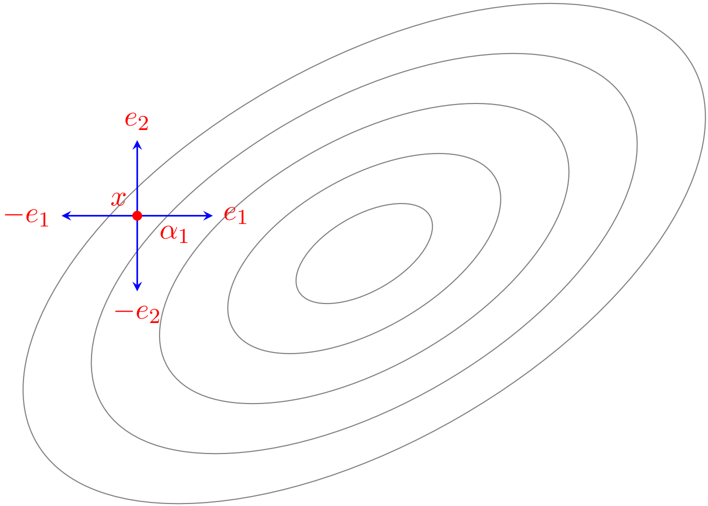
An improved direct-search method?



An improved direct-search method?

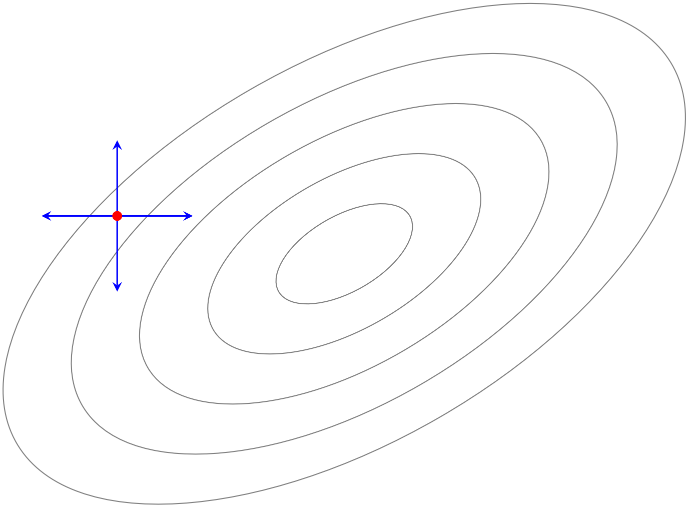


An improved direct-search method?

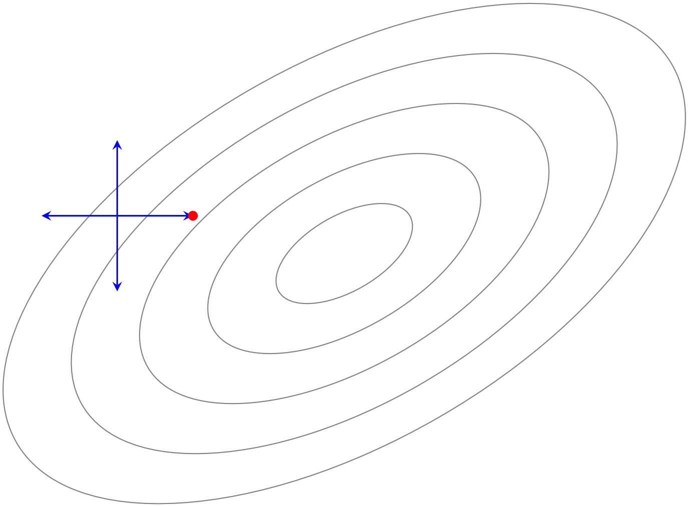


$\mathcal{D}_1 = \{e_1, -e_1\}$ and $\mathcal{D}_2 = \{e_2, -e_2\}$

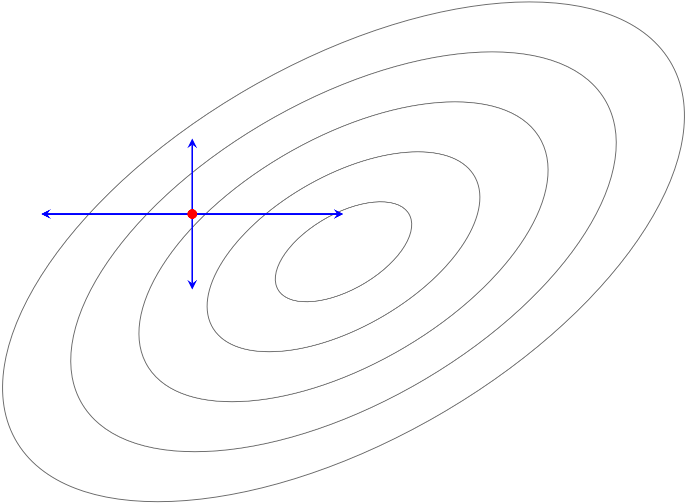
An improved direct-search method?



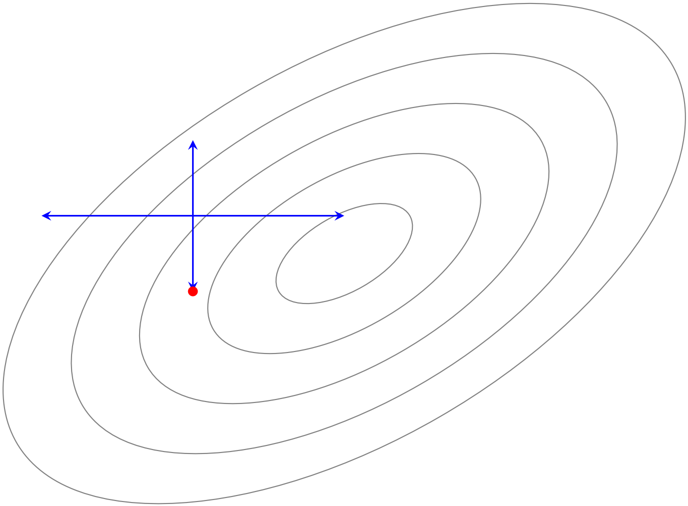
An improved direct-search method?



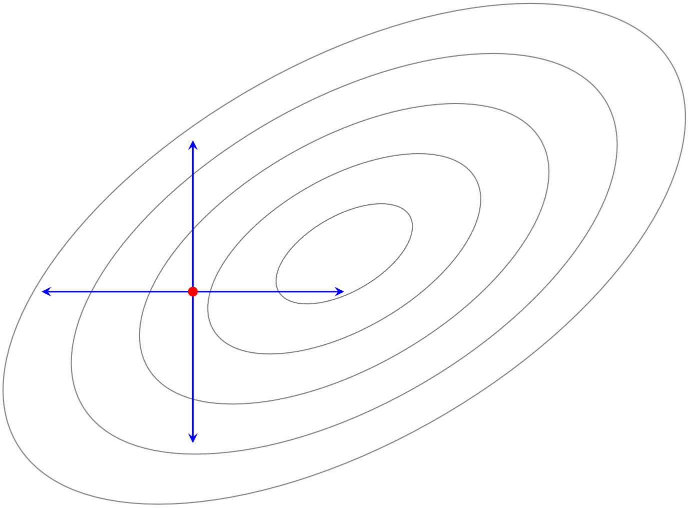
An improved direct-search method?



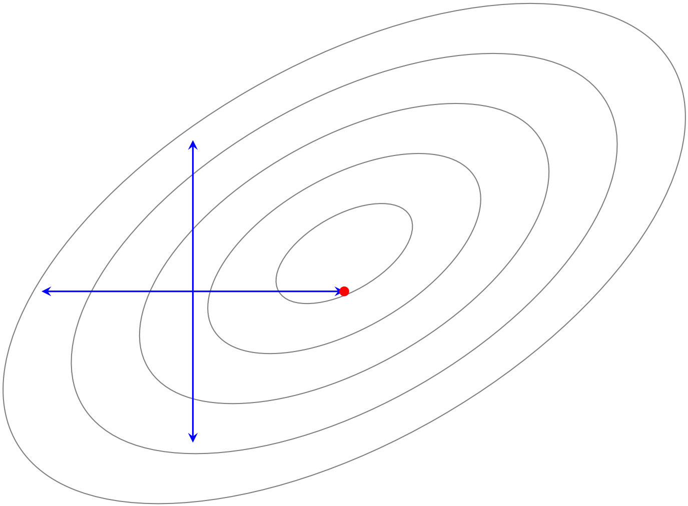
An improved direct-search method?



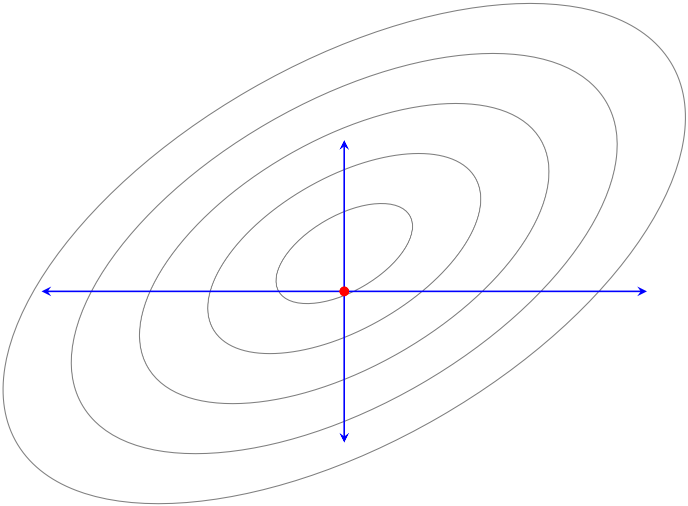
An improved direct-search method?



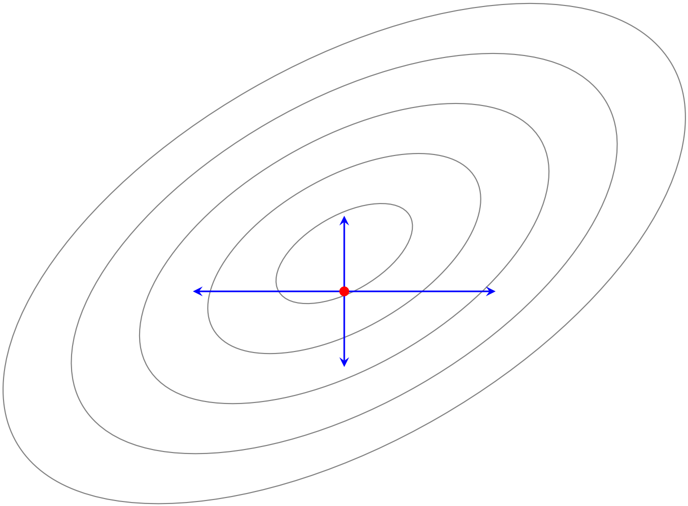
An improved direct-search method?



An improved direct-search method?



An improved direct-search method?



Outline

Blockwise direct-search method

Algorithm 2: Blockwise Direct Search (BDS)

Input: $x_0 \in \mathbb{R}^n$, $0 < \theta < 1 \leq \gamma$, $\alpha_0^1, \ldots, \alpha_0^m \in (0, \infty)$, $c > 0$, 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 $f(y_k^i + \alpha_k^i d_k^i) < f(y_k^i) - \rho(\alpha_k^i)$ 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 $x_{k+1} = y_k^{m+1}$.

The difference from the classical direct search

- The only difference from the classical direct search: blocks
- No backtracking/extrapolating line search like in
  - S. Lucidi and M. Sciandrone, SIAM Journal on Optimization, 2002
  - A. Brilli, M. Kimiaei, G. Liuzzi, and S. Lucidi, arXiv:2302.05274
  - Talk of A. Cristofari, DFOS 2024

Flexibility of the framework

- The searching direction set: A positive spanning set.
- The division of blocks: any (“fits” the problem as much as possible).
- The scheme of visiting blocks: Cyclic (Gauss-Seidel), Jacobi, random.

Flexibility of the framework

- The searching direction set: A positive spanning set.
- The division of blocks: any ("fits" the problem as much as possible).
- 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

Outline

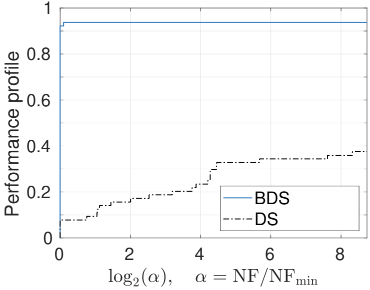
1. Classical direct-search methods

2. Blockwise direct-search methods

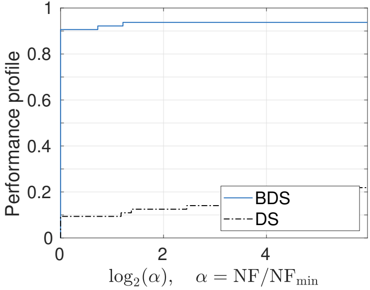
3. Experiments

4. Conclusions and future work

Comparison between BDS and DS



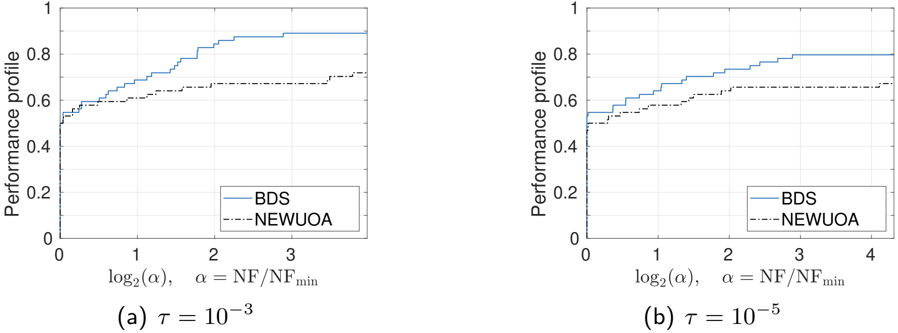
(a) $\tau = 10^{-3}$



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

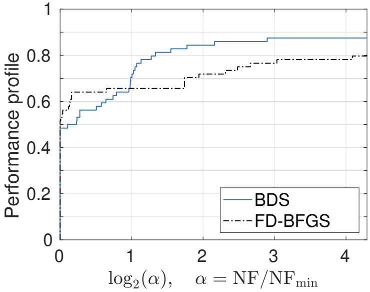
Unconstrained CUTEst problems, $6 \leq n \leq 200$

Comparison betwen BDS and NEWUOA (recapped)

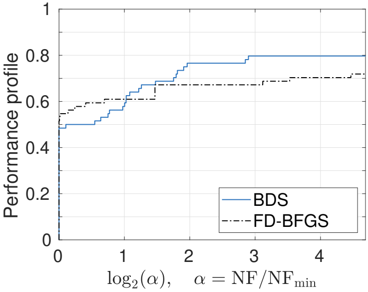


Unconstrained CUTEst problems, $6 \leq n \leq 200$

Comparison between BDS and FD-BFGS



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



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

Unconstrained CUTEst problems, $6 \leq n \leq 200$

- FD-BFGS: Forward-finite-difference BFGS (fminunc in MATLAB).

Performance of BDS under noise

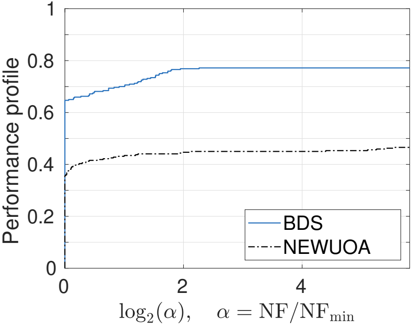
Observed function value:

$$\widetilde{f}(x) = f(x)[1 + \sigma r(x)],$$

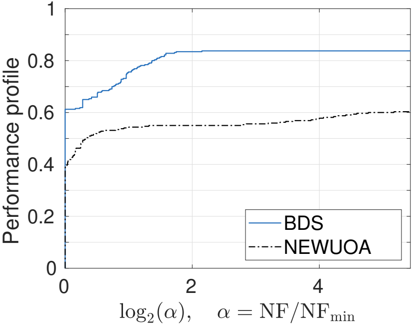
where $r(x) \sim \mathcal{N}(0, 1)$.
In our experiments:

- problem set: unconstrained problems from CUTEst
- dimensions: $6 \leq n \leq 200$
- noise level: $\sigma = 10^{-3}$
- budget: $500n$ function evaluations
- number of random experiments: 5

BDS v.s. NEWUOA

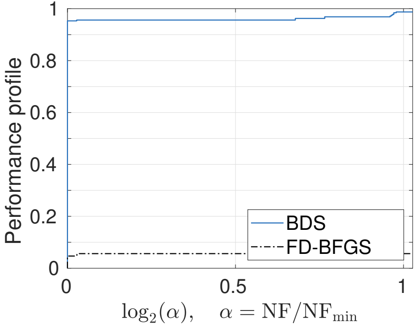


$\tau = 10^{-3}$

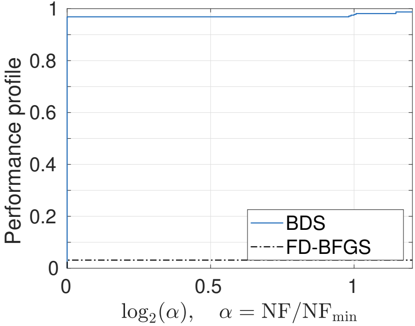


$\tau = 10^{-5}$

BDS v.s. FD-BFGS (fminunc)

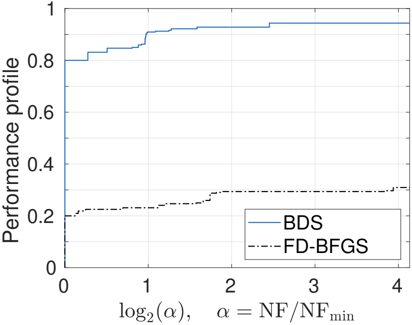


$\tau = 10^{-3}$

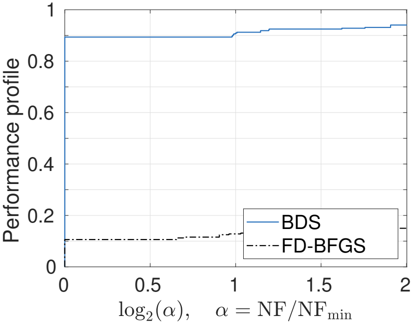


$\tau = 10^{-5}$

BDS v.s. adaptive FD-BFGS



$\tau = 10^{-3}$



$\tau = 10^{-5}$

Adaptive stepsize for FD-BFGS: $h = \sqrt{(\max|f|, 1)\sigma}$

Outline

Structured nonsmooth problems

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

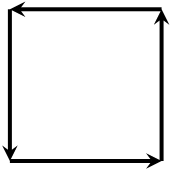
- f is smooth
- Φ is nonsmooth but separable with respect to the blocks

Examples:

- l_p-regularized problems
- bound-constrained problems

Is BDS convergent?

- The analysis of cyclic methods is challenging.
- Powell's non-convergent example of cyclic coordinate descent method[2].



limiting behavior of Powell's example

- We do not know whether BDS is convergent yet.
- Is it possible that the vanilla version of BDS is not convergent?

[2] On search directions for minimization algorithms, Mathematical programming, 1973, Powell, M. J. D.

Conclusions

1. Blockwise Direct Search (BDS) is a substantial improvement over the classical direct search method (based on sufficient decrease)
2. BDS is robust under noise without any noise-handling techniques

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

- open-source and easy to use
- tested continuously via GitHub Actions
- tested under different platforms

Thank you!

References I

- C. Audet and J. E. Dennis Jr.
  Analysis of generalized pattern searches.
  SIAM J. Optim., 13:889–903, 2002.
- C. Audet and J. E. Dennis Jr.
  Mesh adaptive direct search algorithms for constrained optimization.
  SIAM J. Optim., 17:188–217, 2006.
- C. Audet and D. Orban.
  Finding optimal algorithmic parameters using derivative-free optimization.
  SIAM Journal on Optimization, 17(3):642–664, 2006.
- A. S. Bandeira, K. Scheinberg, and L. N. Vicente.
  Convergence of trust-region methods based on probabilistic models.
  SIAM J. Optim., 24:1238–1264, 2014.

References II

- Emilio F Campana, Matteo Diez, Umberto Iemma, Giampaolo Liuzzi, Stefano Lucidi, Francesco Rinaldi, and Andrea Serani.
  Derivative-free global ship design optimization using global/local hybridization of the direct algorithm.
  Optimization and Engineering, 17:127–156, 2016.
- N. I. M. Gould, D. Orban, and Ph. L. Toint.
  CUTEst: a constrained and unconstrained testing environment with safe threads for mathematical optimization.
  Comput. Optim. Appl., 60:545–557, 2015.
- S. Gratton, C. W. Royer, L. N. Vicente, and Z. Zhang.
  Direct search based on probabilistic descent.
  SIAM J. Optim., 25:1515–1541, 2015.

References III

- Tianchen Gu, Wangzhen Li, Aidong Zhao, Zhaori Bi, Xudong Li, Fan Yang, Changhao Yan, Wenchuang Hu, Dian Zhou, Tao Cui, et al.
  Bbgp-sdfo: Batch bayesian and gaussian process enhanced subspace derivative free optimization for high-dimensional analog circuit synthesis.
  IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, 2023.
- T. G. Kolda, R. M. Lewis, and V. Torczon.
  Optimization by direct search: New perspectives on some classical and modern methods.
  SIAM Rev., 45:385–482, 2003.

References IV

- S. Oliver, C. Cartis, I. Kriest, S. F. B. Tett, and S. Khatiwala.
  A derivative-free optimisation method for global ocean biogeochemical models.
  Geoscientific Model Development, 15(9):3537–3554, 2022.
- M. Porcelli and Ph. L. Toint.
  BFO, a trainable derivative-free brute force optimizer for nonlinear bound-constrained optimization and equilibrium computations with continuous and discrete variables.
  ACM Trans. Math. Software, 44:6:1–6:25, 2017.
- M. J. D. Powell.
  The NEWUOA software for unconstrained optimization without derivatives.
  In G. Di Pillo and M. Roma, editors, *Large-scale Nonlinear Optimization*, pages 255–297. Springer, Boston, 2006.

References V

- Michael JD Powell.
  On search directions for minimization algorithms.
  Mathematical programming, 4:193–201, 1973.