Derivative-Free Optimization: A Brief Overview and Some Recent Advances

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Joint works with

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Outline

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Why optimize a function without using derivatives?

> I started to write computer programs in Fortran at Harwell in 1962. ... after moving to Cambridge in 1976 ... I became a consultant for IMSL. One product they received from me was the `TOLMIN` package for optimization ... which requires first derivatives ... Their customers, however, prefer methods that are without derivatives, so IMSL forced my software to employ difference approximations ... I was not happy ... Thus there was strong motivation to try to construct some better algorithms.

— M. J. D. Powell

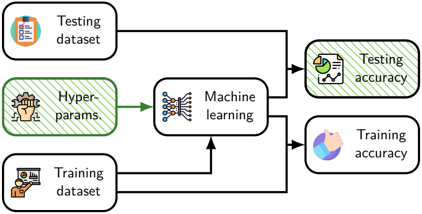
A view of algorithms for optimization without derivatives, 2007, Hong Kong

Derivative-free optimization (DFO)

$$x \longrightarrow \boxed{f} \longrightarrow f(x)$$

- Minimize f using function values, not derivatives (1st-order information).
- A typical case: f is a black box without an explicit formula.
- The dimension of x may be small, but the evaluation of f is expensive.
- Closely related: black-box optimization, simulation-based optimization, gradient-free optimization, zeroth-order optimization.

An example — hyperparameter tuning



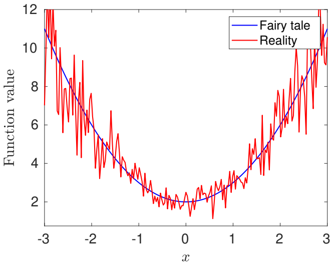
$$\max \{\Pi(x) : x \in \mathcal{X}\}$$

- x represents the hyperparameters for a machine learning model.
- $\Pi(x)$ quantifies the performance of the model (e.g., accuracy) for x.
- Π does not have an explicit formulation.
- The dimension of x is often small, but each evaluation of Π is expensive.
- How to choose x in order to "optimize"/improve the performance?
- A "small" problem defined by big data.

Words of caution

- The reason for not using derivatives is not nonsmoothness but rather the unavailability of the first-order information.
- It is most likely a bad idea to use derivative-free optimization methods if any kind of first-order information is available.
- A real problem is often a gray box instead of a black box. Any known structure should be exploited.

DFO is no fairy-tale world



(Yes, this is your favorite convex quadratic function)

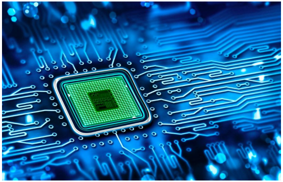
- The black box defining f can be extremely noisy.
- The function evaluation can be extremely expensive.
- The budget can be extremely low.

Be realistic

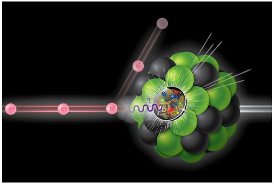
(In real applications) ... one almost never reaches a solution but even 1% improvement can be extremely valuable.

— A. R. Conn

Inversion, history matching, clustering and linear algebra, 2015, Toulouse



Circuit design

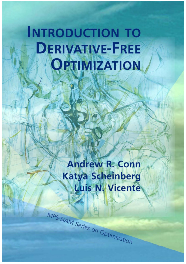


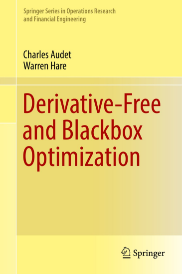
Computational nuclear phsics

Machine learning

- Ciccazzo *et al.*, Derivative-free robust optimization for circuit design, *J. Optim. Theory Appl.*, 2015
- Wild, Sarich, and Schunck, Derivative-free optimization for parameter estimation in computational nuclear physics, *J. Phys. G*, 2015
- Ghanbari and Scheinberg, Black-box optimization in machine learning with trust region based derivative free algorithm, arXiv:1703.06925, 2017

Well-developed theory and methods





- Powell, Direct search algorithms for optimization calculations, 1998
- Powell, A view of algorithms for optimization without derivatives, 2007
- Conn, Scheinberg, and Vicente, *Introduction to Derivative-Free Optimization*, 2007
- Audet and Warren, *Derivative-Free and Blackbox Optimization*, 2017
- Larson, Menickelly, and Wild, Derivative-free optimization methods, 2019

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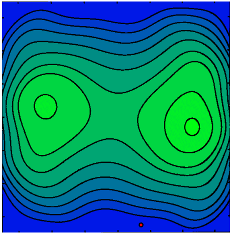
Two main classes of methods

- Model-based methods:
  iterates are determined according to models built using function values
  - Powell's trust-region DFO methods
  - SOLNP and SOLNP+ by Ye *et al*
- Direct search methods:
  iterates are determined by simple comparison of objective function values
  - Nelder-Mead simplex method

Methods not covered by these two classes:

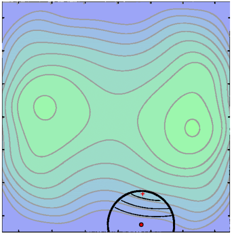
Bayesian optimization, genetic methods, simulated annealing, grid search, ...



$$x_{k+1} \approx x_k + \underset{\|d\| \leq \Delta_k}{\arg\min}\, m_k(x_k + d)$$

- m_k is the trust-region model (surrogate)
  - $m_k(x) \approx f(x)$ around x_k
  - m_k interpolates f on a set $\mathcal{X}_k$ consisting of previous iterates
- $\|d\| \leq \Delta_k$ is the trust-region constraint
  - If "things work well", increase Δ_k
  - Otherwise, decrease Δ_k

Trust-region DFO methods based on interpolation models



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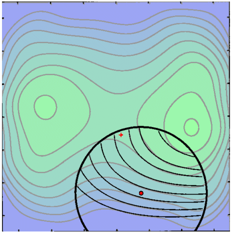

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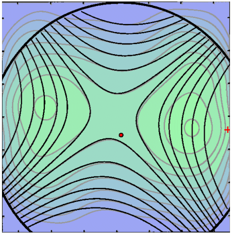

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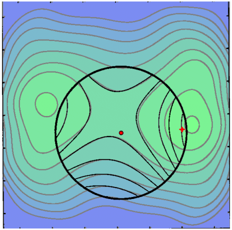

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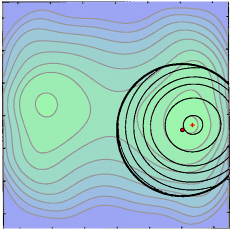

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Maintenance of the interpolation set

The interpolation set $\mathcal{X}_k$ must be updated with care.

- $\mathcal{X}_k$ should reuse previous iterates as much as possible.
- The geometry of $\mathcal{X}_k$ must be good enough so that the problem

$$m_k(x) = f(x) \qquad x \in \mathcal{X}_k$$

  is well conditioned.
- Normally, $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{x_{k+1}\} \setminus \{$a "bad" point$\}$.
- When m_k does not work well and the geometry of $\mathcal{X}_k$ is "bad", geometry-improving steps must be taken.

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Curse of dimensionality

"Large" problems are challenging in DFO:

- Trust-region methods normally employ quadratic models of f:

$$f(x) \approx m_k(x) \equiv c_k + {g_k}^\top (x - x_k) + \frac{1}{2}(x - x_k)^\top B_k (x - x_k).$$

  m_k has $\mathcal{O}(n^2)$ degrees of freedom. Difficult to construct if n is large.

- Directional direct search methods typically search along $\mathcal{O}(n)$ directions at each iteration, necessitating $\mathcal{O}(n)$ function evaluations per iteration.

How to reduce the cost by randomization?

Randomized trust-region method: random interpolation set

Idea: construct sparse quadratic models by interpolating f on randomly sampled interpolation sets with much less than $\mathcal{O}(n^2)$ points.

- Bandeira, Scheinberg, and Vicente, Computation of sparse low degree interpolating polynomials and their application to derivative-free optimization, *Math. Program.*, 2012

Under some conditions, the models constructed in this way are "second-order approximations" of f in a probabilistic sense.

Randomized trust-region method: random interpolation set

Global convergence of methods using such models:

- Bandeira, Scheinberg, and Vicente, Convergence of trust-region methods based on probabilistic models, *SIAM J. Optim.*, 2014

Tool: martingale theory.

Worst-case complexity of methods using such models:

- Gratton, Royer, Vicente, and Zhang, Complexity and global rates of trust-region methods based on probabilistic models, *IMA J. Numer. Anal.*, 2017

Tool: measure concentration inequalities (Chernoff).

There are many other results in this direction. See Dr. Cao Liyuan's talk.

- Cartis and Scheinberg, Global convergence rate analysis of unconstrained optimization methods based on probabilistic models, *Math. Program.*, 2018

Randomized trust-region method: random subspace

Idea: Randomly choose a subspace of dimension $\mathcal{O}(1)$, optimize f using a trust-region method (models are cheap), and iterate.

- Cartis and Roberts, Scalable subspace methods for derivative-free nonlinear least-squares optimization, *Math. Program.*, 2022

Tool: Johnson-Lindenstrauss Embeddings

Randomized direct search method

Idea:

- Traditional: search along a deterministic set of directions $\mathcal{D}$, $|\mathcal{D}| = \mathcal{O}(n)$.
- Randomized: search along a random set of directions $\mathcal{D}_k$, $|\mathcal{D}_k| = \mathcal{O}(1)$.

It turns out that $|\mathcal{D}_k| = 2$ is enough in the unconstrained case, no matter how large is the problem.

- Gratton, Royer, Vicente, Zhang, Direct search based on probabilistic descent, *SIAM J. Optim.*, 2015
- Gratton, Royer, Vicente, Zhang, Direct search based on probabilistic feasible descent for bound and linearly constrained problems, *Comput. Optim. Appl.*, 2019

Tool: measure concentration inequalities (Chernoff).

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算法 5.18. (NEWUOAs)

步 *1.* 取正数序列 $\{h_k\}$、$\{p_k\}$ 和常数 $\varepsilon \geq 0$. 确定初始点 x_1; $s_0 := 0$; $k := 1$.

步 *2.* 选取整数 $m_k \in [n+1, (n+1)(n+2)/2]$, 调用 MODEL($x_k$, h_k, m_k), 获得 x_k 处的近似梯度 $\tilde{g}_k$. 若 $h_k < \varepsilon$ 且 $\|\tilde{g}_k\| < \varepsilon$, 终止. 令

$$\mathcal{S}_k = \operatorname{span}\{\tilde{g}_k, s_{k-1}\}. \tag{5.59}$$

步 *3.* 设置 RHOEND $= p_k$, 调用 NEWUOA 求解子问题

$$\min_{d \in \mathcal{S}_k} f(x_k + d) \tag{5.60}$$

得到 d_k.

步 *4.* 若 $f(x_k + d_k) < f(x_k)$, 则 $x_{k+1} := x_k + d_k$, $s_k := d_k$; 否则 $x_{k+1} := x_k$, $s_k := s_{k-1}$. $k := k+1$. 转步 *2.*

NEWUOAs (screen-shot taken from Sec. 5.3.3 of my Ph.D. thesis, 2012)

More information on NEWUOAs

- NEWUOAs is fully described in Sec. 5.3 of
  Zhang, *On Derivative-Free Optimization Methods* (无导数优化方法的研究), Ph.D. thesis, Chinese Academy of Sciences, Beijing, 2012
- A general framework for subspace methods is given in Sec. 5.3.1 of the thesis.
- Implementation details of NEWUOAs are presented in Sec. 5.3.5 of the thesis.
- The MATLAB implementation of NEWUOAs is available at

  `https://github.com/newuoas/newuoas` .

- NEWUOAs is included as a DFO solver in the open-source package cm3 at

  `https://github.com/modula3/cm3`

  under `caltech-other/newuoa/src/NewUOAs.m3` .

`github.com/newuoas` `github.com/cm3`

NEWUOAs solving some 2000-dimensional Problems

	f_{start}	f_{best}	$\#f$	CPU (s)
ARWHEAD	5.997000E+03	0.000000E+00	16095	6.42
BRYBND	7.200000E+04	6.486038E−09	50000	26.09
DIXMAANE	1.471453E+04	1.000000E+00	36264	21.12
DIXMAANF	2.734976E+04	1.000000E+00	36384	31.07
DIXMAANG	5.069653E+04	1.000000E+00	36393	22.72
DQRTIC	6.376035E+15	1.214880E−38	40854	14.70
GENHUMPS	5.122260E+07	1.624799E−26	36467	23.54
LIARWHD	1.170000E+06	2.428807E−24	16208	6.73
POWER	2.668667E+09	1.423292E−11	20130	19.19
SPARSQUR	5.627812E+05	6.381755E−30	16209	9.87

N.B.: These results are from 2012. In 2023, we can do much better.

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Powell's algorithms and software

- COBYLA: solving general nonlinearly constrained problems using linear models; code released in 1992; paper published in 1994
- UOBYQA: solving unconstrained problems using quadratic models; code released in 2000; paper published in 2002
- NEWUOA: solving unconstrained problems using quadratic models; code released in 2004; paper published in 2006
- BOBYQA: solving bound constrained problems using quadratic models; code released and paper written in 2009
- LINCOA: solving linearly constrained problems using quadratic models; code released in 2013; no paper written

How do these algorithms look like?

DIRECT SEARCH CONSTRAINED OPTIMIZATION 55

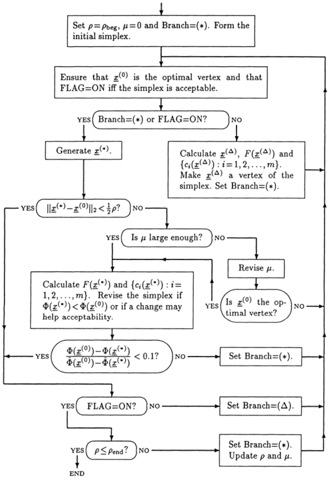
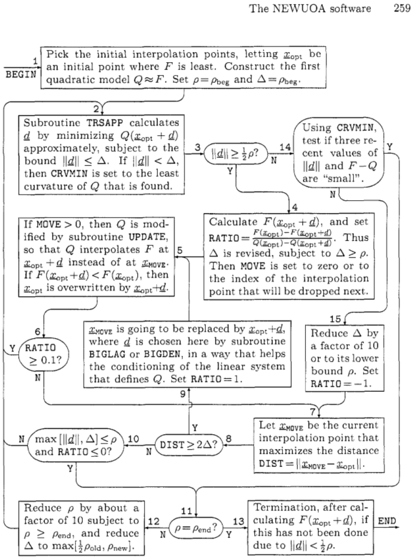


Figure 1: A summary of the algorithm

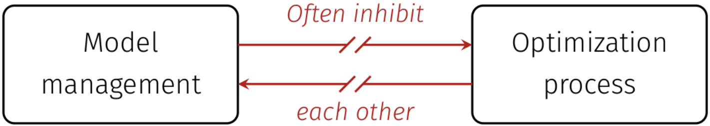
COBYLA

How do these algorithms look like?



NEWUOA

The central difficulty



Implementation of these methods is HARD

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

— M. J. D. Powell

The NEWUOA software for unconstrained optimization without derivatives, 2006

Powell's implementation

- Powell implemented all his five methods into publicly available solvers.
- The solvers are widely used by scientists and engineers.
- They are the default benchmarks when designing new algorithms.
- However, the implementation was in Fortran 77, with plenty of GOTOs: in total, 7939 lines of code with 249 GOTOs!

A modernized implementation is greatly needed.

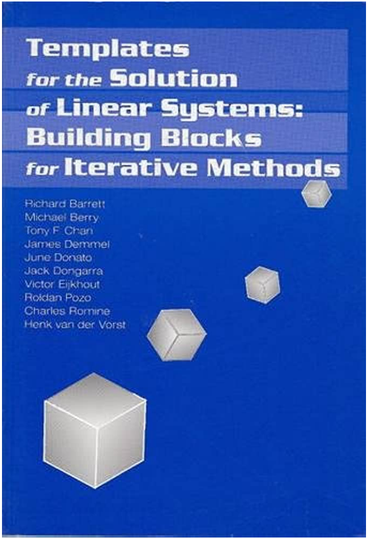
libprima.net

PRIMA is a acronym for

"Reference Implementation for Powell's Methods
with Modernization and Amelioration",

"P" for Powell.

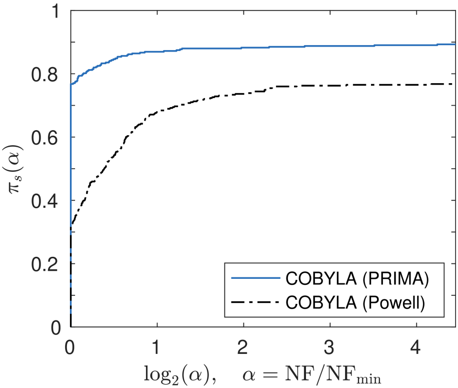
An inspiration



Features of PRIMA

- A structured and modularized way so that they are understandable, maintainable, extendable, fault tolerant, and future proof.
- The code will have no GOTO and will use matrix-vector procedures instead of loops whenever possible.
- The implementation is mathematically equivalent to Powell's except for the bug fixes and improvements we introduce intentionally.
- The implementation is extensively tested by GitHub Actions. The total testing time has exceeded 20 years as of May 2023.
- The inclusion of PRIMA into SciPy is under discussion, and the major SciPy maintainers are positive about it.

The improvement of PRIMA over Powell's implementation



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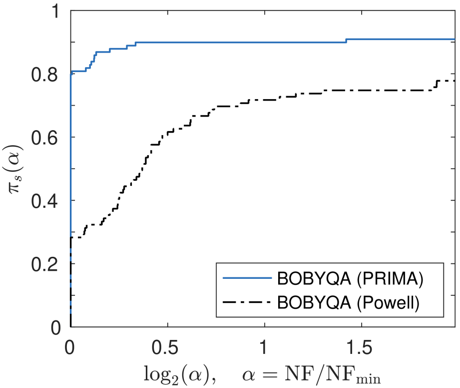

Summary

- Motivation of derivative-free optimization (DFO)
- Basic methods of DFO
- Randomization strategy for scaling DFO methods to larger problems
- Subspace strategy for scaling DFO methods to larger problems
- Software packages: NEWUOAs, PRIMA, and COBYQA

`github.com/newuoas` `libprima.net` `cobyqa.com`

Thank you!