# COBYQA

## A derivative-free trust-region SQP method for nonlinearly constrained optimization

**Tom M. Ragonneau** Zaikun Zhang

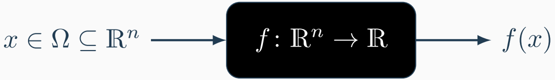
ICNONLA 2023, Taiyuan, Shanxi, China, 2023

Department of Applied Mathematics
The Hong Kong Polytechnic University
Hung Hom, Kowloon, Hong Kong, China

This work was partially supported by the Hong Kong PhD Fellowship Scheme.

# Derivative-free optimization (DFO)

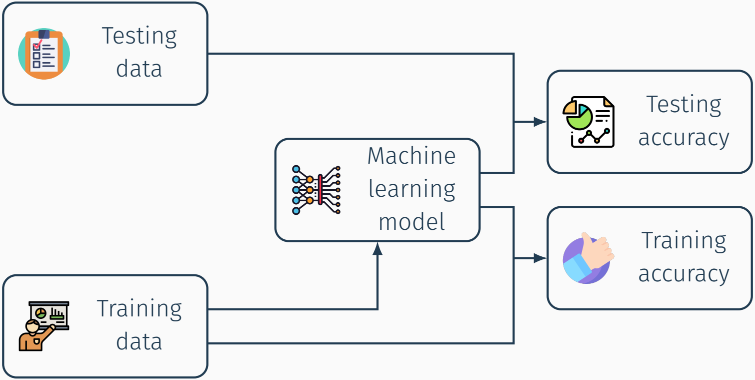
- Minimize a function $f$ using function values but no derivatives.
- $f$ can be a black box resulting from experiments or simulations.



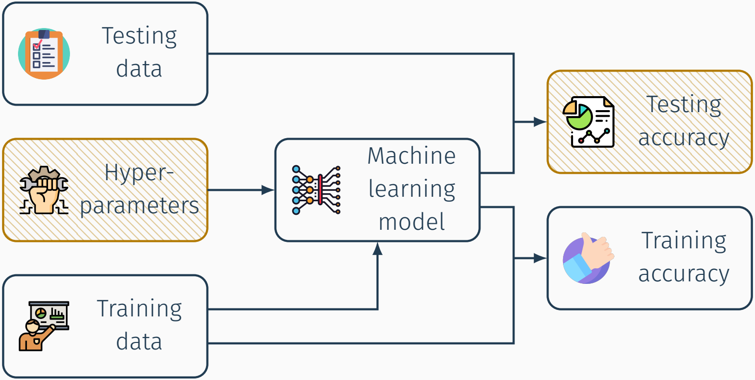

- $f$ may be smooth, but $\nabla f$ cannot be numerically evaluated.
- Evaluations of $f$ are expensive.
- Closely related terms:

*blackbox optimization*
*zeroth-order optimization*
*simulation-based optimization*
*gradient-free optimization*

# An example of a DFO problem



# An example of a DFO problem




### Hyperparameter tuning problem

- How to choose the hyperparameters?
- An idea: optimizing the testing accuracy. What is the gradient?

# General context

We design a method named COBYQA for solving

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \text{s.t.} \quad & g(x) \le 0, \; h(x) = 0, \\ & l \le x \le u, \end{aligned}$$

when derivatives of $f$, $g$, and $h$ are unavailable.

# General context

We design a method named COBYQA for solving

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when derivatives of $f$, $g$, and $h$ are unavailable.

- We omit the equality constraints for simplicity.
- COBYQA aims at being a successor to COBYLA (Powell 1994).
- We implement COBYQA into a Python solver.
- The bound constraints are unrelaxable:
  - They often represent inalienable restrictions.
  - $f$, $g$, or $h$ may not be well-defined outside the bounds.

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# General framework of COBYQA

# A derivative-free trust-region SQP method

COBYQA iteratively solves the trust-region SQP subproblem

$$\begin{aligned} \min_{s \in \mathbb{R}^n} \quad & \nabla f(x_k)^\mathsf{T} s + \frac{1}{2} s^\mathsf{T} \nabla^2_{xx} \mathcal{L}(x_k, \lambda_k) s \\ \text{s.t.} \quad & g(x_k) + \nabla g(x_k) s \le 0, \\ & l \le x_k + s \le u, \\ & \|s\| \le \Delta_k, \end{aligned}$$

with $\mathcal{L}(x, \lambda) = f(x) + \lambda^\mathsf{T} g(x)$.

# A derivative-free trust-region SQP method

COBYQA iteratively solves the trust-region SQP subproblem

$$\begin{aligned}
\min_{s \in \mathbb{R}^n} \quad & \nabla \hat{f}_k(x_k)^{\mathsf{T}} s + \frac{1}{2} s^{\mathsf{T}} \nabla_{xx}^2 \widehat{\mathcal{L}}_k(x_k, \lambda_k) s \\
\text{s.t.} \quad & \hat{g}_k(x_k) + \nabla \hat{g}_k(x_k) s \le 0, \\
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\end{aligned}$$

with $\widehat{\mathcal{L}}_k(x, \lambda) = \hat{f}_k(x) + \lambda^{\mathsf{T}} \hat{g}_k(x)$, given some models $\hat{f}_k$ and $\hat{g}_k$.

- We only require an approximate solution $s_k$.
- The solution must satisfy $l \le x_k + s_k \le u$.
- See Schittkowski and Yuan (2011) and Yuan (2015).

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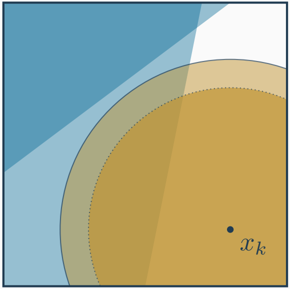
- See Schittkowski and Yuan (2011) and Yuan (2015).

The subproblem may be infeasible. What is a solution?

# A new Byrd-Omojokun approach

We compute $s_k = n_k + t_k$, where

- the normal step $n_k$ reduces the (possible) constraint violation, and
- the tangential step $t_k$ reduces the quadratic objective function.




Trust region

Reduced trust region

Linear constraints

Standard approach[1] vs. new one.

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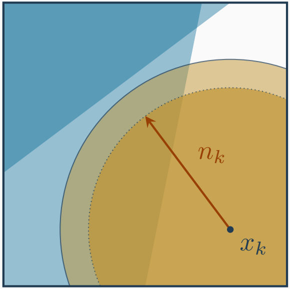


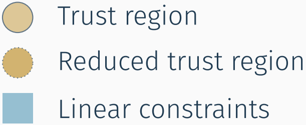


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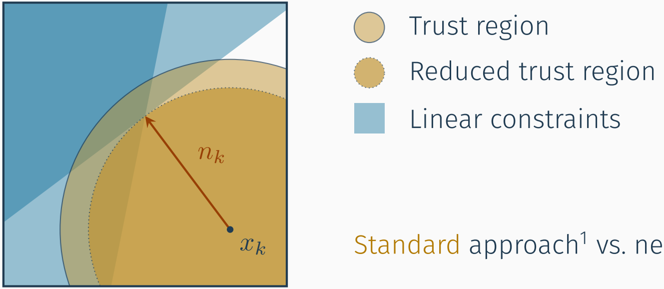


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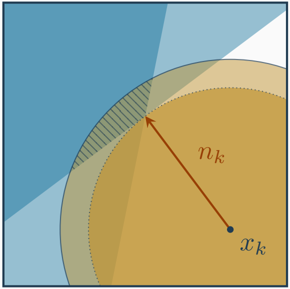


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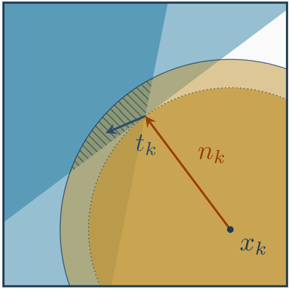



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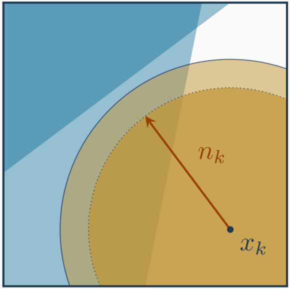


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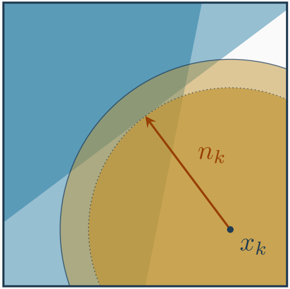


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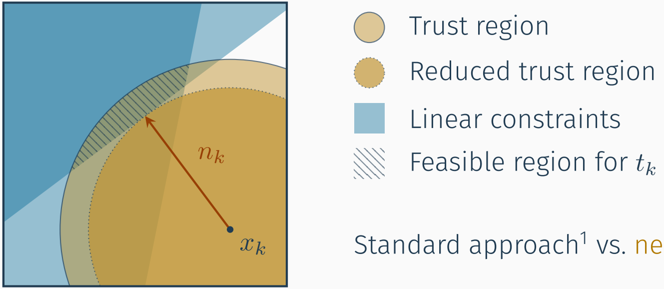


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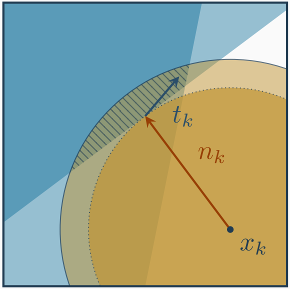



- Trust region
- Reduced trust region
- Linear constraints
- Feasible region for $t_k$

Standard approach[1] vs. new one.

The feasible region for $t_k$ is wider in the new approach.

[1] See Conn, Gould, and Toint (2000, §15.4.4).

# A new Byrd-Omojokun approach (cont'd)

Standard approach:

- The normal step $n_k$ solves approximately (for some $\zeta < 1$)

$$\begin{aligned} \min_{s \in \mathbb{R}^n} \quad & \left\| \left[ \hat{g}_k(x_k) + \nabla \hat{g}_k(x_k) s \right]^+ \right\| \\ \text{s.t.} \quad & l \le x_k + s \le u, \\ & \|s\| \le \zeta \Delta_k. \end{aligned}$$

- The tangential step $t_k$ solves approximately

$$\begin{aligned} \min_{s \in \mathbb{R}^n} \quad & \left[ \nabla \hat{f}_k(x_k) + \nabla^2_{xx} \widehat{\mathcal{L}}_k(x_k, \lambda_k) n_k \right]^\mathsf{T} s + \frac{1}{2} s^\mathsf{T} \nabla^2_{xx} \widehat{\mathcal{L}}_k(x_k, \lambda_k) s \\ \text{s.t.} \quad & \nabla \hat{g}_k(x_k) s \le 0, \\ & l \le x_k + n_k + s \le u, \\ & \|n_k + s\| \le \Delta_k. \end{aligned}$$

# A new Byrd-Omojokun approach (cont'd)

New approach:

- The normal step $n_k$ solves approximately (for some $\zeta < 1$)

$$\begin{aligned} \min_{s \in \mathbb{R}^n} \quad & \left\| \left[ \hat{g}_k(x_k) + \nabla \hat{g}_k(x_k) s \right]^+ \right\| \\ \text{s.t.} \quad & l \leq x_k + s \leq u, \\ & \|s\| \leq \zeta \Delta_k. \end{aligned}$$

- The tangential step $t_k$ solves approximately

$$\begin{aligned} \min_{s \in \mathbb{R}^n} \quad & \left[ \nabla \hat{f}_k(x_k) + \nabla^2_{xx} \widehat{\mathcal{L}}_k(x_k, \lambda_k) n_k \right]^\mathsf{T} s + \frac{1}{2} s^\mathsf{T} \nabla^2_{xx} \widehat{\mathcal{L}}_k(x_k, \lambda_k) s \\ \text{s.t.} \quad & \nabla \hat{g}_k(x_k) s \leq [\hat{g}_k(x_k) + \nabla \hat{g}_k(x_k) n_k]^-, \\ & l \leq x_k + n_k + s \leq u, \\ & \|n_k + s\| \leq \Delta_k. \end{aligned}$$

# Interpolation-based models

# Interpolation-based quadratic models

COBYQA builds quadratic models of $f$ and $g$ by interpolation.

**Derivative-free symmetric Broyden update (Powell 2004)**

The $k$th model $\hat{f}_k$ of $f$ solves

$$\begin{aligned} \min_{Q \in \mathcal{Q}_n} \quad & \left\| \nabla^2 \hat{f}_{k-1} - \nabla^2 Q \right\|_{\mathsf{F}} \\ \text{s.t.} \quad & Q(y) = f(y), \ y \in \mathcal{Y}_k, \end{aligned}$$

for some interpolation set $\mathcal{Y}_k \subseteq \mathbb{R}^n$ (similar for $\hat{g}_k$).

- We recycle $\mathcal{Y}_{k+1} = (\mathcal{Y}_k \cup \{x_k + s_k\}) \setminus \{\bar{y}\}$ for some bad point $\bar{y} \in \mathcal{Y}_k$.
- To compute $\hat{f}_k$, we only need to solve a linear system.

Some alternatives: Conn, Scheinberg, and Toint (1997a,b, 1998), Wild (2008), Custódio, Rocha, and Vicente (2010), Bandeira, Scheinberg, and Vicente (2012), Zhang (2014), and Xie and Yuan (2023).

# Many difficulties arise

# A lot of questions must be addressed

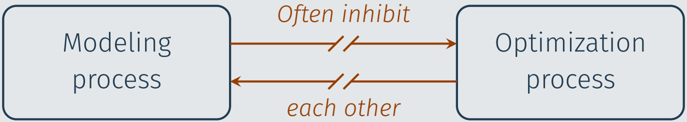
- How to calculate the steps $n_k$ and $t_k$ numerically?
  COBYQA adapts the truncated conjugate gradient method.
- What is the approximate Lagrange multiplier $\lambda_k$?
  We choose the least-squares Lagrange multiplier.
- Which merit function should we use?
  COBYQA uses the $\ell_2$-merit function.
- How to update the penalty parameter?
  The update incorporates
  - a theoretical value for the exactness of the merit function, and
  - a strategy used by Powell in COBYLA.

These questions (and many more) are addressed in Ragonneau (2022).

# A crucial difficulty in the implementation

- What if the interpolation set $\mathcal{Y}_k$ is almost nonpoised?
  A well-known approach: a geometry-improving mechanism.[2]

**This is a central difficulty in the implementation of DFO methods**




- The iterates $\{x^k\}$ likely lie on a particular path.
- The modeling process does not ponder the optimization problem.

[2] See Conn, Scheinberg, and Vicente (2008a,b) and Fasano, Morales, and Nocedal (2009).

# Management of the trust-region radius

**We maintain $\Delta_k$ and a lower bound $\delta_k \le \Delta_k$**

- The lower bound $\delta_k$ is never increased.
- We update $\Delta_k$ in the usual way, but we always have $\Delta_k \ge \delta_k$.
- This strategy is adapted from Powell (2006, 2009) and LINCOA.

The value of $\delta_k$ is an indicator of the current resolution.

- Without $\Delta_k \ge \delta_k$, the value of $\Delta_k$ may become too small.
- It prevents the interpolation points from concentrating too much.
- The value of $\delta_k$ is only decreased when necessary.
- Hence, stopping when $\delta_k \le \delta_{\text{end}}$ is reasonable ($\delta_{\text{end}} > 0$).

# Implementation and experiments

# The Python implementation of COBYQA

**From Powell (2006)**

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

The development of COBYQA was not easier.

We implemented COBYQA in Python and made it publicly available.

www.cobyqa.com

```
$ pip install cobyqa
```

# Comparing COBYQA with existing DFO solvers

- We assess the quality of points based on the merit function

$$\varphi(x) = \begin{cases} f(x) & \text{if } v_\infty(x) \le 10^{-10}, \\ \infty & \text{if } v_\infty(x) \ge 10^{-5}, \\ f(x) + 10^5 v_\infty(x) & \text{otherwise,} \end{cases}$$

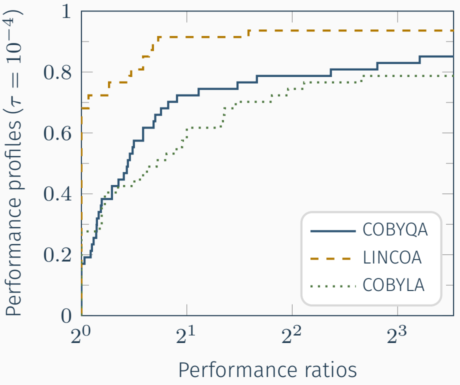
  where $v_\infty$ denotes the $\ell_\infty$-constraint violation.
- The problems are from CUTEst (Gould, Orban, and Toint 2015).
- The problems are of dimension at most $50$ (this is not small).
- Problems with unrelaxable bounds replace $f$ with

$$\tilde{f}(x) = \begin{cases} f(x) & \text{if } l \le x \le u, \\ \infty & \text{otherwise.} \end{cases}$$

# Performance on linearly constrained problems

We compare COBYQA, LINCOA, and COBYLA

- on linearly constrained problems,



# Performance on linearly constrained problems

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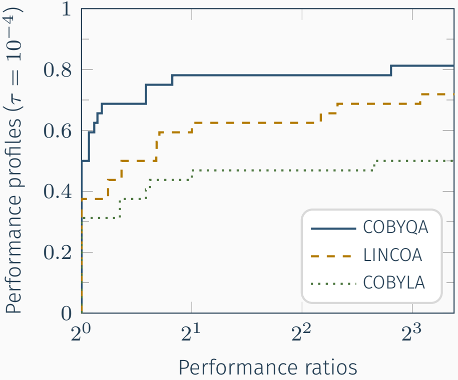

# Performance on nonlinearly constrained problems

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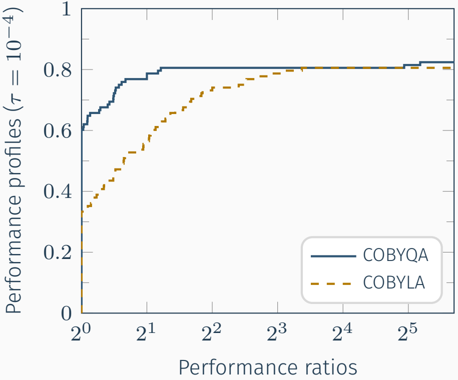

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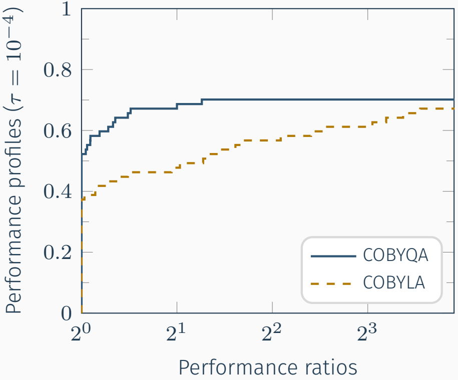
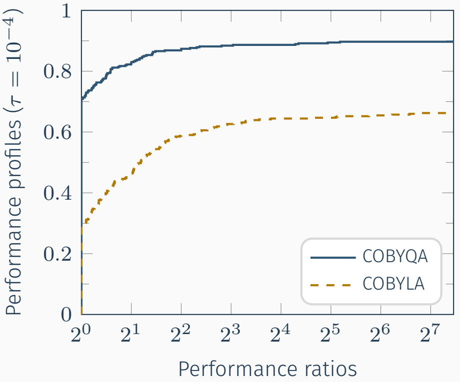


# Comparison with COBYLA

We compare COBYQA and COBYLA on all 388 problems.



# Conclusion

# Conclusion

- COBYQA already received positive feedback from practitioners.
- It will soon be included in
  - PDFO as a successor for COBYLA, and
  - GEMSEO, an industrial software package for MDO.
- We will soon investigate the convergence properties of COBYQA.

For more information, visit:

COBYQA

My website

My thesis

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