COBYQA

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

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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.

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\end{aligned}
$$

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

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

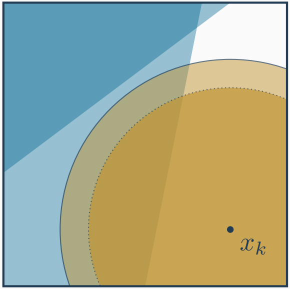
with $\widehat{\mathcal{L}}_k(x, \lambda) = \hat{f}_k(x) + \lambda^\mathsf{T} \hat{g}_k(x)$, given some models $\hat{f}_k$ and $\hat{g}_k$.

- We only require an approximate solution s_k.
- The solution must satisfy $l \le x_k + s_k \le u$.
- 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.



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Reduced trust region

Linear constraints

Standard approach[1] vs. new one.

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

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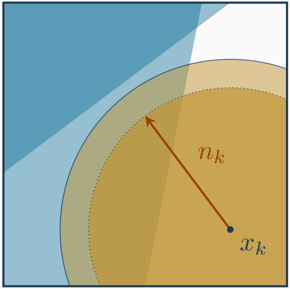

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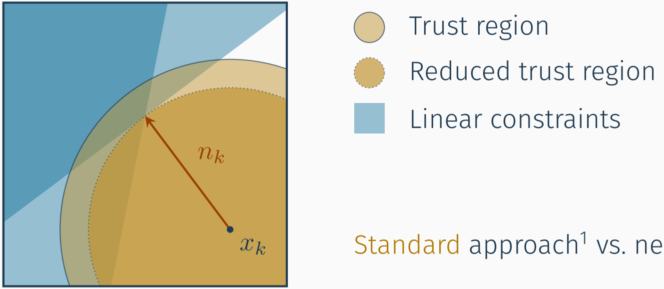

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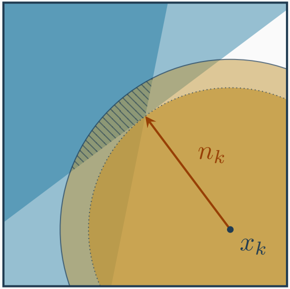

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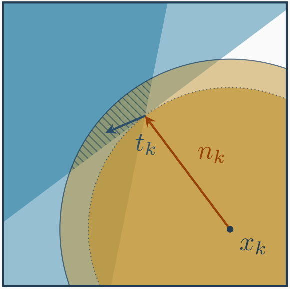

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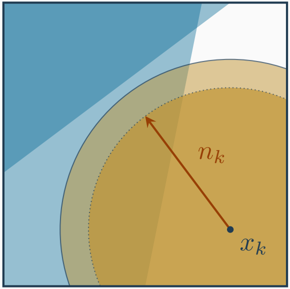

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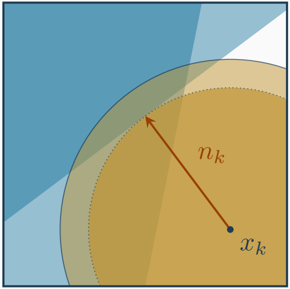

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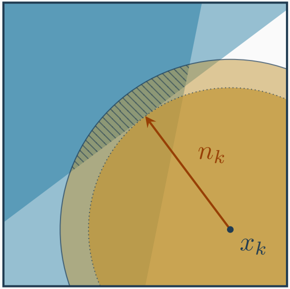

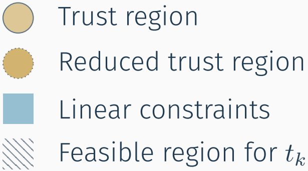

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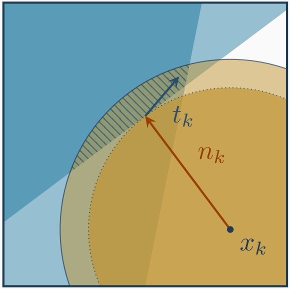

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- Feasible region for t_k

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 $\zeta < 1$)

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

- The tangential step t_k solves approximately

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

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

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

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 kth 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

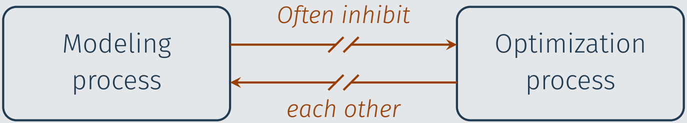
- How to calculate the steps n_k and t_k numerically?
  COBYQA adapts the truncated conjugate gradient method.
- What is the approximate Lagrange multiplier λ_k?
  We choose the least-squares Lagrange multiplier.
- Which merit function should we use?
  COBYQA uses the ℓ_2-merit function.
- How to update 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 Δ_k and a lower bound $\delta_k \le \Delta_k$

- The lower bound δ_k is never increased.
- We update Δ_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 δ_k is an indicator of the current resolution.

- Without $\Delta_k \ge \delta_k$, the value of Δ_k may become too small.
- It prevents the interpolation points from concentrating too much.
- The value of δ_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

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

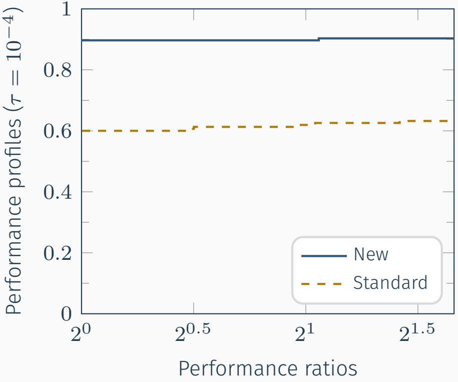
  where v_∞ denotes the ℓ_∞-constraint violation.
- The problems are from the CUTEst set.
- The problems are of dimension at most 50 (this is not small).
- Problems with unrelaxable bounds replace f with

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

Performance of the new Byrd-Omojokun approach

We compare the new and the standard Byrd-Omojokun approaches

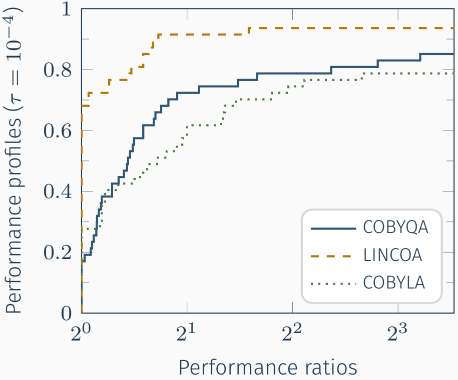
- on linearly and nonlinearly constrained problems,
- in the implementation of COBYQA.



Performance on linearly constrained problems

We compare COBYQA, LINCOA, and COBYLA

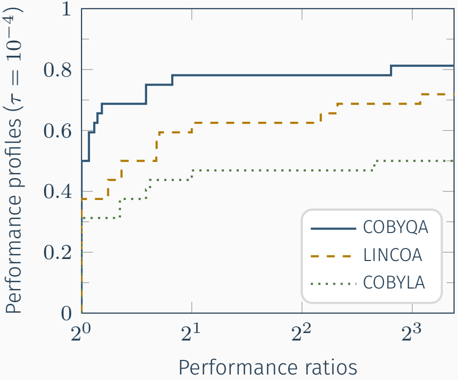
- on linearly constrained problems,



Performance on linearly constrained problems

We compare COBYQA, LINCOA, and COBYLA

- on linearly constrained problems,
- with unrelaxable bounds.



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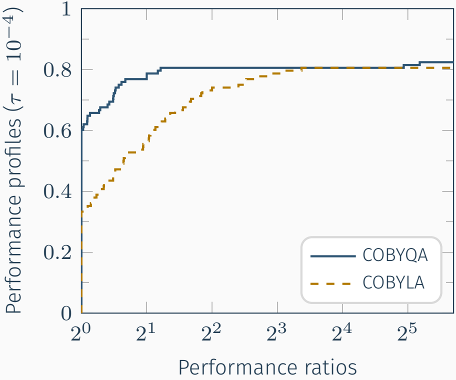

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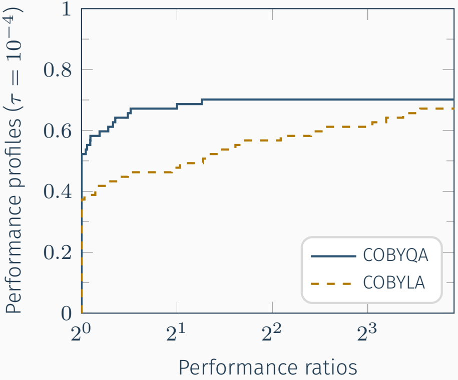
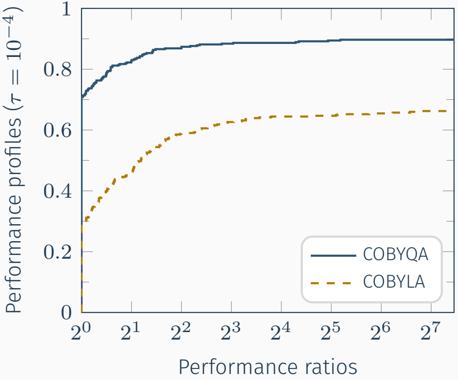


Comparison with COBYLA

We compare COBYQA and COBYLA on all 388 problems.



Conclusion

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- 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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