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A derivative-free trust-region method for optimization on the ellipsoid

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Introduction

Most optimization methods depend on the derivative information about the objective function. However, in practice, we can not obtain the derivative information sometimes, and even the function evaluation is expensive. To optimize without using the derivative, derivative-free optimization (DFO) is proposed, which is also called black-box optimization (BBO). DFO aims to generate a sequence of iteration points $\{\boldsymbol{x}_k\}$ to reach the minimizer with fewer function evaluations.

$$\min_{\boldsymbol{x}\in\Re^n} \ F(\boldsymbol{x}), \ \text{subject to } \boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} + b = 0, \tag{1}$$

Our method is based on the model-based methods [1, 2, 3, 4, 5, 6, 7, 8]. In this paper, we discuss the equality constraint

$$\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} + b = 0, \tag{2}$$

where $\boldsymbol{A} = \operatorname{diag}\{a_1, a_2, \ldots, a_n\}, \ a_i > 0, \ \forall\, i = 1, \ldots, n$, which denotes the ellipsoidal constraint. This kind of problem and the corresponding methods have wide use, such as the electronic structure calculations in materials sciences, of which the essence is solving an energy-minimizing problem with the orthogonality constraints. Besides, the linear eigenvalue problems are also special optimization problems with the orthogonality constraints.

DFO Algorithm 1

For the ellipsoidal constraint (2), we denote $g(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} + b$. The objective function with the Courant penalty function is $P(\boldsymbol{x}, \sigma) = F(\boldsymbol{x}) + \sigma(g(\boldsymbol{x}))^2$. Terminating condition: $|g(\boldsymbol{x}_{k+1})| \le \varepsilon$ or $\|\boldsymbol{x}_k - \boldsymbol{x}_{k-1}\|_2 \le \varepsilon$.

EC_NEWUOA with the Courant penalty

1: Given $\boldsymbol{x}_1 \in \Re^n, \sigma_1 > 0, k := 1, \varepsilon \ge 0$.
2: Use the initial point $\boldsymbol{x}_k$ and NEWUOA to solve $\min_{\boldsymbol{x}} \ P(\boldsymbol{x}, \sigma_k)$, and obtain $\boldsymbol{x}_{k+1}$.
3: If the terminating condition holds, then stop; $\sigma_{k+1} = 10\sigma_k$, $k := k+1$; Go to step 2.

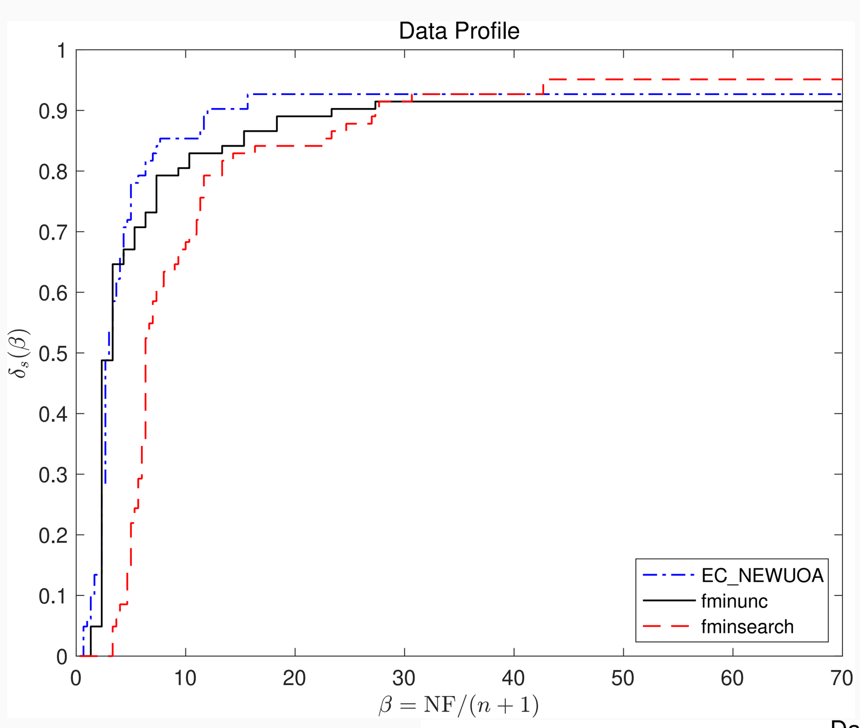
DFO Algorithm 2

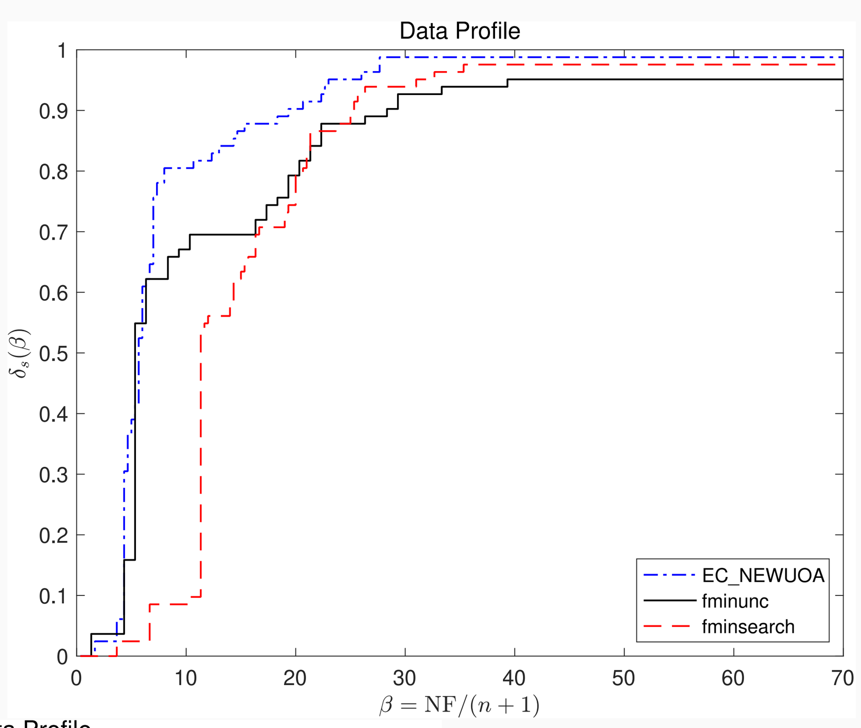
The objective function referring to the augmented Lagrangian method is $L(\boldsymbol{x}, \lambda, \sigma) = F(\boldsymbol{x}) + \lambda g(\boldsymbol{x}) + \frac{1}{2}\sigma(g(\boldsymbol{x}))^2$.

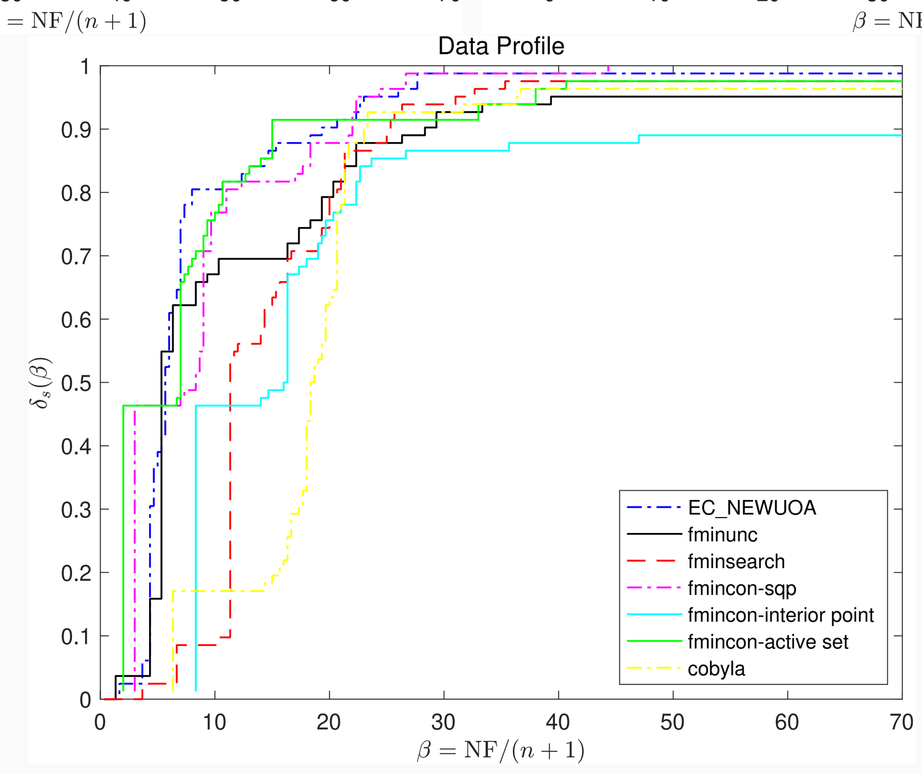
EC_NEWUOA using the augmented Lagrangian method

1: Given $\boldsymbol{x}_1 \in \Re^n, \lambda_1 \in \Re, \ \lambda_1 \ge 0$, and $\varepsilon \ge 0, \sigma_1 > 0, k := 1$.
2: Use the initial point $\boldsymbol{x}_k$ and NEWUOA to solve $\min_{\boldsymbol{x}} \ L(\boldsymbol{x}, \lambda_k, \sigma_k)$, and obtain $\boldsymbol{x}_{k+1}$.
3: If the terminating condition holds, then stop; $\lambda_{k+1} = \lambda_k + \sigma_k g(\boldsymbol{x}_{k+1})$; $\sigma_{k+1} := 10\sigma_k, k := k+1$; Go to step 2.

Numerica Results







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