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# PDFO: A Cross-Platform Package for Powell's Derivative-Free Optimization Solvers

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*To the memory of the late Professor M. J. D. Powell FRS*

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**Abstract**

The late Professor M. J. D. Powell devised five trust-region derivative-free optimization methods, namely COBYLA, UOBYQA, NEWUOA, BOBYQA, and LINCOA. He also carefully implemented them into publicly available solvers, which are renowned for their robustness and efficiency. However, the solvers were implemented in Fortran 77 and hence may not be easily accessible to some users. We introduce the PDFO package, which provides user-friendly Python and MATLAB interfaces to Powell's code. With PDFO, users of such languages can call Powell's Fortran solvers easily without dealing with the Fortran code. Moreover, PDFO includes bug fixes and improvements, which are particularly important for handling problems that suffer from ill-conditioning or failures of function evaluations. In addition to the PDFO package, we provide an overview of Powell's methods, sketching them from a uniform perspective, summarizing their main features, and highlighting the similarities and interconnections among them. We also present experiments on PDFO to demonstrate its stability under noise, tolerance of failures in function evaluations, and potential in solving certain hyperparameter optimization problems.

**Keywords** Derivative-free optimization · COBYLA · UOBYQA · NEWUOA · BOBYQA · LINCOA

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# 1 Introduction

Most optimization algorithms rely on classical or generalized derivative information of the objective and constraint functions. However, in many applications, such information is not available. This is the case, for example, if the objective function does not have an explicit formulation but can only be evaluated through complex simulations or experiments. Such problems motivate the development of optimization algorithms that use only function values but not derivatives, also known as derivative-free optimization (DFO) algorithms.

Powell devised five algorithms to tackle unconstrained and constrained problems without using derivatives, namely COBYLA [50], UOBYQA [53], NEWUOA [56], BOBYQA [58], and LINCOA. He did not only propose these algorithms but also implemented them into publicly available solvers, paying great attention to the stability and complexity of their numerical linear algebra computations. Renowned for their robustness and efficiency, these solvers are used in a wide spectrum of applications, for instance, aeronautical engineering [25], astronomy [39], computer vision [33], robotics [40], and statistics [5].

However, Powell coded the solvers in Fortran 77, an old-fashion language that damps the enthusiasm of many users to exploit these solvers in their projects. There has been a continued demand from both researchers and practitioners for the availability of Powell's solvers in more user-friendly languages such as Python and MATLAB.

Responding to such a demand, this paper presents a package named PDFO, an acronym for "Powell's Derivative-Free Optimization solvers." PDFO interfaces Powell's Fortran solvers with other languages, enabling users of such languages to call Powell's solvers without dealing with the Fortran code. For each supported language, PDFO provides a simple function that can invoke one of Powell's solvers according to the user's request (if any) or according to the type of the problem to solve. The current release (Version 1.2) of PDFO supports Python and MATLAB, with more languages to be covered in the future. The signature of the Python subroutine is consistent with the `minimize` function of the SciPy optimization library; the signature of the MATLAB subroutine is consistent with the `fmincon` function of the MATLAB Optimization Toolbox. PDFO is cross-platform, available on Linux, macOS, and Windows at

`https://www.pdfo.net`.

It has been downloaded more than 50,000 times as of February 2023, mirror downloads excluded. Moreover, it is one of the optimization engines in GEMSEO [25],[1] an industrial software package for Multidisciplinary Design Optimization (MDO).

PDFO is not the first attempt to facilitate the usage of Powell's solvers in languages other than Fortran. Various efforts have been made in this direction. Py-BOBYQA [9, 10] provides a Python implementation of BOBYQA; NLopt includes multi-language interfaces for COBYLA, NEWUOA, and BOBYQA;[2] minqa wraps UOBYQA, NEWUOA, and BOBYQA in R;[3] SciPy

[1] `https://gemseo.readthedocs.io`.
[2] `https://github.com/stevengj/nlopt`.
[3] `https://CRAN.R-project.org/package=minqa`.

makes COBYLA available in Python under its optimization library.[4] However, PDFO has several features that distinguish it from others.

1. *Comprehensiveness.* To the best of our knowledge, PDFO is the only package that provides all of COBYLA, UOBYQA, NEWUOA, BOBYQA, and LINCOA with a *uniform interface*.
2. *Solver selection.* PDFO can automatically select a solver for a given problem. The selection takes into account the performance of the solvers on the CUTEst [28] problem set.
3. *Problem preprocessing.* PDFO preprocesses the inputs to simplify the problem and reformulate it to meet the requirements of Powell's solvers.
4. *Code patching.* PDFO patches several bugs in the Fortran code. Such bugs can lead to serious problems such as infinite cycling or memory errors.
5. *Fault tolerance.* PDFO tolerates failures of function evaluations. In case of such failures, PDFO will not exit but try to progress.
6. *Additional options.* PDFO includes options for the user to control the solvers in some manners that are useful in practice. For example, the user can request PDFO to scale the problem according to bound constraints on the variables before solving.

In addition to the PDFO package, this paper also provides an overview of Powell's DFO methods. We will not repeat Powell's description of these methods but summarize them from a uniform viewpoint, aiming at easing the understanding of Powell's methods and paving the way for further development based on them.

The analysis of Powell's DFO methods is not within the scope of this paper. Under some assumptions, adapted versions of Powell's algorithms may be covered by existing theory for trust-region DFO methods [18, Chapter 10]. However, it will still be interesting to pursue a tailored theory for Powell's algorithms.

The remaining part of this paper is organized as follows. Section 2 briefly reviews DFO methods in order to provide the context of PDFO. We then present an overview of Powell's DFO methods in Section 3, including a sketch of the algorithms and a summary of their main features. A detailed exposition of PDFO is given in Section 4, highlighting its solver selection, problem preprocessing, bug fixes, and handling of function evaluation failures. Section 5 presents some experiments on PDFO, demonstrating its stability under noise, tolerance of function evaluation failures, and potential in hyperparameter optimization. We conclude the paper with some remarks in Section 6.

## 2 A brief review of DFO methods

Consider a nonlinear optimization problem

$$\min_{x\in\Omega} \ f(x), \tag{2.1}$$

[4] `https://docs.scipy.org/doc/scipy/reference/optimize.minimize-cobyla.html`.

where $f : \mathbb{R}^n \to \mathbb{R}$ is the objective function and $\Omega \subseteq \mathbb{R}^n$ represents the feasible region. As summarized in [18], two strategies have been developed to tackle problem (2.1) without using derivatives, which we will introduce in the following.

The first strategy, known as direct search,[5] samples the objective function $f$ and chooses iterates by simple comparisons of function values, examples including the Nelder-Mead algorithm [43], the MADS methods [2, 37], and BFO [45, 46, 47]. See [35], [18, Chapters 7 and 8], [3, Part 3], and [36, § 2.1] for more discussions on this paradigm, and we refer to [29, 30] for recent developments of randomized methods in this category.

The second strategy approximates the original problem (2.1) by relatively simple models and locates the iterates according to these models. Algorithms applying this strategy are referred to as model-based methods. They often make use of the models within a trust-region framework [17] or a line-search framework [6]. Interpolation and regression are two common ways of establishing the models [52, 15, 16, 74, 4, 7, 65]. Algorithms using finite-difference of gradients can also be regarded as model-based methods, because such gradients essentially come from linear (for the forward and backward differences) or quadratic (for the central difference) interpolation of the function under consideration over rather special interpolation sets [62, § 1.4.3]. Most model-based DFO methods employ linear or quadratic models, examples including Powell's algorithms [50, 53, 56, 58] in PDFO, MNH [73], DFLS [76], DFO-TR [4], and DFO-LS [9, 32], but there are also methods exploiting radial basis functions (RBFs), such as ORBIT [74], CONORBIT [65], and BOOSTERS [44].

Hybrids between direct search and model-based approaches exist, for instance, Implicit Filtering [34, Algorithm 4.7] and MADS with quadratic models [12]. Theories of global convergence and convergence rate have been established for both direct search [71, 35, 72, 29, 22] and model-based methods [13, 17, 59, 26]. Since the objective and constraint functions in DFO problems are commonly expensive to evaluate, the worst-case complexity in terms of function evaluations is a major theoretical aspect of DFO algorithms. Examples of such complexity analysis can be found in [72, 29, 22, 26]. For more extensive discussions on DFO methods and theory, see the monographs [18, 3], the survey papers [66, 20, 36], the recent thesis [62], and the references therein.

[5] In some early papers (e.g., [50, 51]) Powell and many other authors used "direct search" to mean what is known as "derivative-free optimization" today. Powell rarely used the word "derivative-free optimization." The only exceptions known to us are his last paper [61] and his distinguished lecture titled "A parsimonious way of constructing quadratic models from values of the objective function in derivative-free optimization" at the National Center for Mathematics and Interdisciplinary Sciences, Beijing on November 4, 2011 [8].

# 3 Powell's derivative-free algorithms

Powell published in 1964 his first DFO algorithm based on conjugate directions [48].[6] His code for this algorithm is contained in the HSL Mathematical Software Library as subroutine `VA24`.[7] It is not included in PDFO because the code is not in the public domain, although open-source implementations are available (see [14, footnote 4]).

From the 1990s to the final years of his career, Powell developed five model-based DFO algorithms to solve (2.1), namely COBYLA [50] (for nonlinearly constrained problems), UOBYQA [53] (for unconstrained problems), NEWUOA [56] (for unconstrained problems), BOBYQA [58] (for bound-constrained problems), and LINCOA (for linearly constrained problems). Moreover, Powell implemented these algorithms into Fortran solvers and made the code publicly available. They are the cornerstones of PDFO. This section provides an overview of these five algorithms, starting with a sketch in Section 3.1 and then presenting more details afterward.

## 3.1 A sketch of the algorithms

Powell's model-based DFO algorithms are trust-region methods. At iteration $k$, the algorithms construct a linear (for COBYLA) or quadratic (for the other methods) model $f_k$ for the objective function $f$ to meet the interpolation condition

$$f_k(y) = f(y), \quad y \in \mathcal{Y}_k, \tag{3.1}$$

where $\mathcal{Y}_k \subseteq \mathbb{R}^n$ is a finite interpolation set updated along the iterations. COBYLA models the constraints by linear interpolants on $\mathcal{Y}_k$ as well. Instead of repeating Powell's description of these algorithms, we outline them in the sequel, emphasizing the trust-region subproblem, the interpolation problem, and the management of the interpolation set.

### 3.1.1 The trust-region subproblem

In all five algorithms, iteration $k$ places the trust-region center $x_k$ at the "best" point where the objective function and constraints have been evaluated so far. Such a point is selected according to the objective function or a merit function that takes the constraints into account. After choosing the trust-region center $x_k$, with the trust-region model $f_k$ constructed according to (3.1), a trial point $x_k^{\mathrm{t}}$ is then obtained by solving approximately the trust-region subproblem

$$\min_{x \in \Omega_k} \ f_k(x) \quad \text{s.t.} \quad \|x - x_k\| \leq \Delta_k, \tag{3.2}$$

[6] According to Google Scholar, this is Powell's second published paper and also the second most cited work. The earliest and meanwhile most cited one is his paper on the DFP method [23] co-authored with Fletcher and published in 1963. DFP is not a DFO algorithm but the first quasi-Newton method. The least-change property [21] of quasi-Newton methods is a major motivation for Powell to investigate the least Frobenius norm updating [54] of quadratic models in DFO, which is the backbone of NEWUOA, BOBYQA, and LINCOA.

[7] `https://www.hsl.rl.ac.uk`.

where $\Delta_k$ is the trust-region radius, and $\|\cdot\|$ is the $\ell_2$-norm in $\mathbb{R}^n$. In this subproblem, the set $\Omega_k \subseteq \mathbb{R}^n$ is a local approximation of the feasible region $\Omega$. COBYLA defines $\Omega_k$ by linear interpolants of the constraint functions over the set $\mathcal{Y}_k$, whereas the other four algorithms take $\Omega_k = \Omega$.

### 3.1.2 The interpolation problem

**Fully determined interpolation.** The interpolation condition (3.1) is essentially a linear system. Given a base point $y^{\mathrm{b}} \in \mathbb{R}^n$, which may depend on $k$, a linear model $f_k$ takes the form of $f_k(x) = f(y^{\mathrm{b}}) + (x - y^{\mathrm{b}})^{\mathsf{T}} \nabla f_k(y^{\mathrm{b}})$, and hence (3.1) is equivalent to

$$f_k(y^{\mathrm{b}}) + (y - y^{\mathrm{b}})^{\mathsf{T}} \nabla f_k(y^{\mathrm{b}}) = f(y), \ y \in \mathcal{Y}_k, \tag{3.3}$$

which is a linear system with respect to $f(y^{\mathrm{b}}) \in \mathbb{R}$ and $\nabla f(y^{\mathrm{b}}) \in \mathbb{R}^n$, the degrees of freedom being $n + 1$. COBYLA builds linear models by the system (3.3), with $\mathcal{Y}_k$ being an interpolation set of $n + 1$ points updated along the iterations. Similarly, if $f_k$ is a quadratic model, then (3.1) is equivalent to

$$f_k(y^{\mathrm{b}}) + (y - y^{\mathrm{b}})^{\mathsf{T}} \nabla f_k(y^{\mathrm{b}}) + \frac{1}{2}(y - y^{\mathrm{b}})^{\mathsf{T}} \nabla^2 f_k(y^{\mathrm{b}})(y - y^{\mathrm{b}}) = f(y), \ y \in \mathcal{Y}_k, \tag{3.4}$$

a linear system with unknowns $f_k(y^{\mathrm{b}}) \in \mathbb{R}$, $\nabla f_k(y^{\mathrm{b}}) \in \mathbb{R}^n$, and $\nabla^2 f_k(y^{\mathrm{b}}) \in \mathbb{R}^{n \times n}$, the degrees of freedom being $(n+1)(n+2)/2$ due to the symmetry of $\nabla^2 f_k(y^{\mathrm{b}})$. UOBYQA constructs quadratic models by the system (3.4). To decide a quadratic model $f_k$ completely by this system alone, UOBYQA requires that $\mathcal{Y}_k$ contains $(n+1)(n+2)/2$ points, and $f$ should have been evaluated at all these points before the system can be formed. Even though most of these points will be reused at the subsequent iterations so that the number of function evaluations needed per iteration is tiny (see Section 3.1.3), we must perform $(n + 1)(n + 2)/2$ function evaluations during the very first iteration. This is impracticable unless $n$ is small, which motivates the underdetermined quadratic interpolation.

**Underdetermined quadratic interpolation.** In this case, models are established according to the interpolation condition (3.1) with $|\mathcal{Y}_k|$ being less than $(n + 1)(n + 2)/2$, the remaining degrees of freedom being taken up by minimizing a certain functional $\mathcal{F}_k$ to promote the regularity of the quadratic model. More specifically, this means building $f_k$ by solving

$$\min_{Q \in \mathcal{Q}_n} \ \mathcal{F}_k(Q) \quad \text{s.t.} \quad Q(y) = f(y), \ y \in \mathcal{Y}_k, \tag{3.5}$$

where $\mathcal{Q}_n$ is the space of polynomials on $\mathbb{R}^n$ of degree at most 2. NEWUOA, BOBYQA, and LINCOA construct quadratic models in this way, with

$$\mathcal{F}_k(Q) = \left\| \nabla^2 Q - \nabla^2 f_{k-1} \right\|_{\mathsf{F}}^2, \tag{3.6}$$

which is inspired by the least-change property of quasi-Newton updates [21], although other functionals are possible (see [19, 4, 60, 78, 75] for example). The first model $f_1$ is obtained by setting $f_0 = 0$. Powell [60] referred to his approach as the *symmetric Broyden update* of quadratic models (see also [77, § 3.6] and [62, § 2.4.2]). It can be regarded as a derivative-free version of Powell's symmetric Broyden (PSB) quasi-Newton update [49], which minimizes the functional $\mathcal{F}_k$ among all quadratic polynomials that fulfill $Q(x_k) = f(x_k)$, $\nabla Q(x_k) = \nabla f(x_k)$, and $\nabla Q(x_{k-1}) = \nabla f(x_{k-1})$ (see [21, Theorem 4.2]), with $x_k$ and $x_{k-1}$ being the current and the previous iterates, respectively. The interpolation problem (3.5)–(3.6) is a convex quadratic programming problem with respect to the coefficients of the quadratic model.

**Solving the interpolation problem.** Powell's algorithms do not solve the interpolation problems (3.3), (3.4), and (3.5)–(3.6) from scratch. COBYLA maintains the inverse of the coefficient matrix for (3.3) and updates it along the iterations. Since each iteration of COBYLA alters the interpolation set $\mathcal{Y}_k$ by only one point (see Subsection 3.1.3), the coefficient matrix is modified by a rank-1 update, and hence its inverse can be updated according to the Sherman-Morrison-Woodbury formula [31]. UOBYQA does the same for (3.4), except that [53, § 4] describes the update in terms of the Lagrange functions of the interpolation problem (3.4), the coefficients of a Lagrange function corresponding precisely to a column of the inverse matrix. For the underdetermined quadratic interpolation (3.5)–(3.6), NEWUOA, BOBYQA, and LINCOA maintain and update the inverse of the coefficient matrix for the KKT system of (3.5)–(3.6). The update is also done by the Sherman-Morrison-Woodbury formula as detailed in [55, § 2]. In this case, each iteration modifies the coefficient matrix and its inverse by rank-2 updates. In addition, the columns of this inverse matrix readily provide the coefficients of Lagrange functions that make the interpolation problem (3.5)–(3.6) easy to solve (see [54, § 3])

**The base point.** The choice of the base point $y^{\mathrm{b}}$ is also worth mentioning. COBYLA sets $y^{\mathrm{b}}$ to the center $x_k$ of the current trust region. In contrast, the other four algorithms initiate $y^{\mathrm{b}}$ to the starting point provided by the user and keep it unchanged except for occasionally updating $y^{\mathrm{b}}$ to $x_k$, without which the distance $\|y^{\mathrm{b}} - x_k\|$ may become unfavorably large for the numerical solution of the interpolation problem. See [54, § 5] and [56, § 7] for more elaboration.

### 3.1.3 The interpolation set

The strategy to update $\mathcal{Y}_k$ is crucial. It should reuse points from previous iterations, at which the objective and constraint functions have been evaluated. Meanwhile, it needs to maintain the geometry of the interpolation set so that it is well poised, or equivalently, the interpolation problem is well conditioned [18].

At a normal iteration, Powell's methods compute a point $x_k^{\mathrm{t}} \in \mathbb{R}^n$ by solving the trust-region subproblem (3.2), and Powell's DFO methods update the interpolation set as

$$\mathcal{Y}_{k+1} = \left(\mathcal{Y}_k \cup \{x_k^{\mathrm{t}}\}\right) \setminus \{y_k^{\mathrm{d}}\}, \tag{3.7}$$

where $y_k^{\mathrm{d}} \in \mathcal{Y}_k$ is selected after obtaining $x_k^{\mathrm{t}}$, aiming to maintain the well-poisedness of $\mathcal{Y}_{k+1}$. As mentioned, Powell's methods update the inverse of the coefficient matrix for either the interpolation system or the corresponding KKT system by the Sherman-Morrison-Woodbury formula. To keep the interpolation problem well-conditioned, $y_k^{\mathrm{d}}$ is chosen to enlarge the magnitude of the denominator in this formula, which is also the ratio between the determinants of the old and new coefficient matrices.[8] In the fully determined interpolation, this denominator is $\ell_k^{\mathrm{d}}(x_k^{\mathrm{t}})$, where $\ell_k^{\mathrm{d}}$ is the Lagrange function associated with $\mathcal{Y}_k$ corresponding to $y_k^{\mathrm{d}}$ (see equations (10)–(13) and § 2 of [52]). In the underdetermined case, the denominator is lower bounded by $[\ell_k^{\mathrm{d}}(x_k^{\mathrm{t}})]^2$ (see equation (2.12), Lemma 1, and § 2 of [55], where the denominator is $\sigma$, and $\ell_k^{\mathrm{d}}(x_k^{\mathrm{t}})$ is $\tau$). However, Powell's methods do not choose the point $y_k^{\mathrm{d}}$ merely according to this denominator, but also take into account its distance to the trust-region center, giving a higher priority to farther points, as we can see in [53, equation (56)] and [56, equations (7.4)–(7.5)], for example.

An alternative update of the interpolation set takes place when the methods detect that $f_k$ does not represent $f$ well enough, attempting to improve the geometry of the interpolation set. In this case, the methods first select a point $y_k^{\mathrm{d}} \in \mathcal{Y}_k$ to drop from $\mathcal{Y}_k$, and then set

$$\mathcal{Y}_{k+1} = \left(\mathcal{Y}_k \setminus \{y_k^{\mathrm{d}}\}\right) \cup \{x_k^{\mathrm{g}}\}, \tag{3.8}$$

where $x_k^{\mathrm{g}} \in \mathbb{R}^n$ is chosen to improve the well-poisedness of $\mathcal{Y}_{k+1}$. In COBYLA, the choice of $y_k^{\mathrm{d}}$ and $x_k^{\mathrm{g}}$ is guided by the geometrical fact that the interpolation set forms a simplex in $\mathbb{R}^n$, trying to keep $\mathcal{Y}_{k+1}$ away from falling into an $(n-1)$-dimensional subspace, as is detailed in [50, equations (15)–(17)]. The other four methods select $y_k^{\mathrm{d}}$ from $\mathcal{Y}_k$ by maximizing its distance to the current trust-region center $x_k$, and then obtain $x_k^{\mathrm{g}}$ by solving

$$\max_{x\in\Omega} |\ell_k^{\mathrm{d}}(x)| \quad \text{s.t.} \quad \|x - x_k\| \le \bar{\Delta}_k \tag{3.9}$$

for some $\bar{\Delta}_k \in (0, \Delta_k]$. The motivation for this problem is again to enlarge the magnitude of the aforementioned denominator in the Sherman-Morrison-Woodbury updating formula: for UOBYQA, the denominator is $\ell_k^{\mathrm{d}}(x)$, while for NEWUOA, BOBYQA, and LINCOA, the denominator is lower bounded by $[\ell_k^{\mathrm{d}}(x)]^2$. In addition, NEWUOA maximizes this denominator directly if (3.9) fails to make its magnitude large enough, which rarely happens [56, § 6].

Given the two possible updates (3.7) and (3.8) of the interpolation set, it is clear that the number of interpolation points remains constant. As mentioned earlier, this number is $n+1$ in COBYLA and $(n+1)(n+2)/2$ in UOBYQA. NEWUOA, BOBYQA, and LINCOA set it to an integer in $[n+2, (n+1)(n+2)/2]$, with the default value being $2n+1$, which is proved optimal in terms of the well-poisedness of the initial interpolation set chosen by Powell for NEWUOA [64].

[8] Suppose that $W$ is a square matrix and consider $W_+ = W + UV^{\mathsf{T}}$, where $U$ and $V$ are two matrices of the same size and $UV^{\mathsf{T}}$ has the same size as $W$. Then $\det(W_+) = \det(W)\det(I + V^{\mathsf{T}}W^{-1}U)$, and the Sherman-Morrison-Woodbury formula is $(W_+)^{-1} = W^{-1} - W^{-1}U(I + V^{\mathsf{T}}W^{-1}U)^{-1}V^{\mathsf{T}}W^{-1}$, assuming that both $W$ and $I + V^{\mathsf{T}}W^{-1}U$ are nonsingular. The number $\det(I + V^{\mathsf{T}}W^{-1}U)$ is the only denominator involved in the numerical computation of the formula.

## 3.2 COBYLA

Published in 1994, COBYLA was the first model-based DFO solver by Powell. The solver is named after "Constrained Optimization BY Linear Approximations." It aims to solve problem (2.1) with the feasible region

$$\Omega \overset{\text{def}}{=} \{x \in \mathbb{R}^n : c_i(x) \geq 0,\ i = 1, \ldots, m\},$$

where $c_i : \mathbb{R}^n \to \mathbb{R}$ denotes the $i$th constraint function for each $i \in \{1, 2, \ldots, m\}$. The same as the objective function, all constraints are assumed to be accessible only through function values.

As mentioned before, iteration $k$ of COBYLA models the objective and the constraint functions with linear interpolants on the interpolation set $\mathcal{Y}_k$ of $n + 1$ points. Once the linear models $c_{k,i}$ of $c_i$ are built for $i \in \{1, \ldots, m\}$, the trust-region subproblem (3.2) is formed with

$$\Omega_k \overset{\text{def}}{=} \{x \in \mathbb{R}^n : c_{k,i}(x) \geq 0,\ i = 1, \ldots, m\}. \tag{3.10}$$

This subproblem may not be feasible, as the trust region and the region (3.10) may not intersect. COBYLA handles the trust-region subproblem in two stages. In the first stage, it solves

$$\min_{x \in \mathbb{R}^n} \max_{1 \leq i \leq m} [c_{k,i}(x)]_- \quad \text{s.t.} \quad \|x - x_k\| \leq \Delta_k,$$

where $[t]_- = \max\{0, -t\}$ for any $t \in \mathbb{R}$. In doing so, the method attempts to reduce the $\ell_\infty$-violation of the linearized constraints within the trust region. If the first stage finds a point in the interior of the trust region, then the second stage uses the resultant freedom in $x$ to minimize the linearized objective function $f_k$ within the trust region subject to no increase in any greatest violation of the linearized constraints.

COBYLA assesses the quality of points and updates the trust-region radius according to an $\ell_\infty$-merit function and a reduction ratio based on it (see [50, equations (5), (9), and (10)]). It never increases the trust-region radius, and reduces the radius if the geometry of $\mathcal{Y}_k$ is acceptable but the trust-region trial point $x_k^+$ is too close to $x_k$ or does not render a big enough reduction ratio [50, equation (11)].

## 3.3 UOBYQA

In 2002, Powell published UOBYQA [53], named after "Unconstrained Optimization BY Quadratic Approximation." It aims at solving the nonlinear optimization problem (2.1) in the unconstrained case, i.e., when $\Omega = \mathbb{R}^n$.

At iteration $k$, UOBYQA constructs the model $f_k$ for the objective function $f$ by the fully determined quadratic interpolation on the interpolation set $\mathcal{Y}_k$ containing $(n + 1)(n + 2)/2$ points. The trust-region subproblem (3.2) is solved with the Moré-Sorensen algorithm [41]. For the geometry-improving subproblem (3.9), Powell developed an inexact algorithm that requires only $\mathcal{O}(n^2)$ operations. See [53, § 2] for more details.

UOBYQA updates the trust-region radius $\Delta_k$ in a noteworthy way. The update is typical for trust-region methods, except that a lower bound $\rho_k$ is imposed on $\Delta_k$. The value of $\rho_k$ can be regarded as an indicator for the current *resolution* of the algorithm. Without imposing $\Delta_k \geq \rho_k$, the trust-region radius $\Delta_k$ may be reduced to a value that is too small for the current resolution, making the interpolation points concentrate too much. The value of $\rho_k$ is never increased and is decreased when the UOBYQA decides that the work for the current value of $\rho_k$ is finished. It decides so if $\Delta_k$ reaches its lower bound $\rho_k$, the current trust-region trial step does not perform well, and the current interpolation set seems adequate for the current resolution. See [53, § 3] for more information on the updates of $\Delta_k$ and $\rho_k$.

### 3.4 NEWUOA, BOBYQA, and LINCOA

Later on, based on the underdetermined quadratic interpolation introduced in Subsection 3.1.2, Powell developed his last three DFO solvers, namely NEWUOA [56, 57], BOBYQA [58], and LINCOA. BOBYQA and LINCOA are named respectively after "Bound Optimization BY Quadratic Approximation" and "LINearly Constrained Optimization Algorithm", but Powell [56, 57] did not specify the meaning of NEWUOA, which is likely an acronym for "NEW Unconstrained Optimization Algorithm." It is worth mentioning that Powell *never* published a paper to introduce LINCOA, and [61] discusses only how to solve its trust-region subproblem.

NEWUOA, BOBYQA, and LINCOA aim at solving unconstrained, bound-constrained, and linearly constrained problems respectively. They all set $\Omega_k$ in the trust-region subproblem (3.2) to be $\Omega$, corresponding to the whole space for NEWUOA, a box for BOBYQA, and a polyhedron for LINCOA.

To solve the trust-region subproblem (3.2), NEWUOA employs the Steihaug-Toint truncated conjugate gradient (TCG) algorithm [69, 70]; if the boundary of the trust region is reached, then NEWUOA may make further changes to the trust-region step, each one obtained by searching in the two-dimensional space spanned by the current step and the corresponding gradient of the trust-region model [56, § 5]. BOBYQA solves (3.2) by an active-set variant of the TCG algorithm, and it may also improve the TCG step by two-dimensional searches if it reaches the trust-region boundary [58, § 3]. LINCOA uses another active-set variant of TCG to solve the trust-region subproblem (3.2) with linear constraints [61, § 3 and § 5]. An accessible description of the TCG algorithms employed by BOBYQA and LINCOA can be found in [62, § 6.2.1 and § 6.2.2]. NEWUOA, BOBYQA, and LINCOA manage the trust-region radius in a way similar to UOBYQA, imposing a lower bound $\rho_k$ on $\Delta_k$ when updating $\Delta_k$.

When solving the geometry-improving subproblem (3.9), NEWUOA first takes $x_k \pm \bar{\Delta}_k(y_k^{\mathrm{d}} - x_k)/\|y_k^{\mathrm{d}} - x_k\|$, with the sign that provides the larger value of $\ell_k^{\mathrm{d}}$, and then revises it by a procedure similar to the two-dimensional searches that improve the TCG step for (3.2) (see [56, § 6]). BOBYQA computes two approximate solutions to (3.9) and chooses the better one: the first one solves (3.9) with an additional constraint that $x$ is located on the straight lines through $x_k$ and another point in $\mathcal{Y}_k$, and the second is obtained by a Cauchy step for (3.9)

(see [58, § 3]). The geometry-improving step of LINCOA is more complex, as it is chosen from three approximate solutions to (3.9):

1. the point that maximizes $|\ell_k^{\mathrm{d}}|$ within the trust region on the lines through $x_k$ and another point in $\mathcal{Y}_k$,
2. a point obtained by a gradient step that maximizes $|\ell_k^{\mathrm{d}}|$ within the trust region, and
3. a point obtained by a projected gradient step that maximizes $|\ell_k^{\mathrm{d}}|$ within the trust region, the projection being made onto the null space of the constraints that are considered active at $x_k$.

Note that the first two cases disregard the linear constraints (i.e. $x \in \Omega_k = \Omega$), while the third case considers only the active constraints. LINCOA first selects the point among the first two alternatives for a larger value of $|\ell_k^{\mathrm{d}}|$; further, this point is replaced with the third alternative if the latter nearly satisfies the linear constraints $x \in \Omega$ while rendering a value of $|\ell_k^{\mathrm{d}}|$ that is not too small compared with the above one.

BOBYQA respects the bound constraints $x \in \Omega$ when solving the trust-region subproblem (3.2) and the geometry-improving subproblem (3.9), even though these problems are solved approximately. It also chooses the initial interpolation set $\mathcal{Y}_1$ within the bounds. Therefore, BOBYQA is a feasible method. In contrast, LINCOA may violate the linear constraints when solving the geometry-improving subproblem and when setting up the initial interpolation set. Consequently, LINCOA is an infeasible method, which requires $f$ to be defined even when the linear constraints are not satisfied.

# 4 The PDFO package

This section details the main features of PDFO, in particular the signature of the main function, solver selection, problems preprocessing, bug fixes, and handling failures of function evaluations. For more features of PDFO, we refer to its homepage at `https://www.pdfo.net`.

Before starting, we emphasize that PDFO does not re-implement Powell's solvers but rather enables Python and MATLAB to call Powell's Fortran implementation. At a low level, it uses F2PY [9] to interface Python with Fortran, and MEX to interface MATLAB with Fortran, although users never need such knowledge to employ PDFO.

[9] `https://numpy.org/doc/stable/f2py`.

## 4.1 Signature of the main function

The philosophy of PDFO is simple: providing a single function named `pdfo` to solve DFO problems with or without constraints, calling Powell's Fortran solvers in the backend. It takes for input an optimization problem of the form

$$\min_{x\in\mathbb{R}^n} \ f(x) \tag{4.1a}$$

$$\text{s.t. } l \le x \le u, \tag{4.1b}$$

$$A_{\text{I}}x \le b_{\text{I}}, \ A_{\text{E}}x = b_{\text{E}}, \tag{4.1c}$$

$$c_{\text{I}}(x) \le 0, \ c_{\text{E}}(x) = 0, \tag{4.1d}$$

where $f$ a real-valued objective function, while $c_{\text{E}}$ and $c_{\text{I}}$ are vector-valued constraint functions. The bound constraints are given by $n$-dimensional vectors $l$ and $u$, which may take infinite values. The linear constraints are formulated by real matrices $A_{\text{E}}$ and $A_{\text{I}}$ together with real vectors $b_{\text{E}}$ and $b_{\text{I}}$ of proper sizes. We allow one or more of the constraints (4.1b)–(4.1d) to be absent. Being a specialization of (2.1), problem (4.1) is broad enough to cover numerous applications of DFO.

In the Python version of PDFO, the signature of the `pdfo` function is compatible with the `minimize` function available in the `scipy.optimize` module of SciPy. It can be invoked in exactly the same way as `minimize` except that `pdfo` does not accept derivative arguments. The MATLAB version of PDFO designs the `pdfo` function following the signature of the `fmincon` function available in the Optimization Toolbox of MATLAB. In both Python and MATLAB, users can check the detailed syntax of `pdfo` by the standard `help` command.

## 4.2 Automatic selection of the solver

When invoking the `pdfo` function, the user may specify which solver to call in the backend. However, if the user does not do so or chooses a solver that is incapable of solving the problem (e.g., UOBYQA cannot solve constrained problems), then `pdfo` selects the solver as follows.

1. If the problem is unconstrained, then UOBYQA is selected when $2 \le n \le 8$, and NEWUOA is selected when $n = 1$ or $n > 8$.
2. If the problem is bound-constrained, then BOBYQA is selected.
3. If the problem is linearly constrained, then LINCOA is selected.
4. Otherwise, COBYLA is selected.

The problem type is detected automatically according to the input. In the unconstrained case, we select UOBYQA for small problems because it is more efficient, and the number 8 is set according to our experiments on the CUTEst [28] problems. Note that Powell's implementation of UOBYQA cannot handle univariate unconstrained problems, for which NEWUOA is chosen.

In addition to the `pdfo` function, PDFO provides functions named `cobyla`, `uobyqa`, `newuoa`, `bobyqa`, and `lincoa`, which invoke the corresponding solvers directly, but it is highly recommended to call the solvers via the `pdfo` function.

## 4.3 Problem preprocessing

PDFO preprocesses the input of the user in order to fit the data structure expected by Powell's Fortran code.

For example, LINCOA needs a feasible starting point to work properly, unless the problem is infeasible. If the starting point is not feasible, then LINCOA would modify the right-hand sides of the linear constraints to make it feasible and then solve the modified problem. Therefore, for linearly constrained problems, PDFO attempts to project the user-provided starting point onto the feasible region before passing the problem to the Fortran code, so that a feasible problem will not be modified by LINCOA.

Another noticeable preprocessing of the constraints made by PDFO is the treatment of the linear equality constraints in (4.1c). As long as these constraints are consistent, we eliminate them and reduce (4.1) to an $(n - \operatorname{rank} A_{\mathrm{E}})$-dimensional problem. This is done by a QR factorization of $A_{\mathrm{E}}$. The main motivation for this reduction comes again from LINCOA, which accepts only linear inequality constraints. An alternative approach is to write a linear equality constraint as two inequalities, but our approach reduces the dimension of the problem, which is beneficial for the efficiency of DFO solvers in general.

## 4.4 Bug fixes in the Fortran source code

The current version of PDFO patches several bugs in the original Fortran source code, particularly the following ones.

1. The solvers may encounter infinite loops. This happens when the exit conditions of a loop can never be met because variables involved in these conditions become NaN due to floating point exceptions. The user's program will never end if this occurs.
2. The Fortran code may encounter memory errors due to uninitialized indices. This is because some indices are initialized according to conditions that can never be met due to NaN, similar to the previous case. The user's program will crash if this occurs.

In our extensive tests based on the CUTEst problems, these bugs take effect from time to time but not often. They are activated only when the problem is rather ill-conditioned or the inputs are rather extreme. This has been observed, for instance, on the CUTEst problems DANWOODLS, GAUSS1LS, and LAKES with some perturbation and randomization.

Even though these bugs are rarely observed in our tests, it is vital to patch them for two reasons. First, their consequences are severe once they occur. Second, application problems are often more irregular and savage than the testing problems we use, and hence the bugs may be triggered more often than we expect. Nevertheless, PDFO allows the users to call Powell's

original Fortran code without these patches by setting the option `classical` to true, which is highly discouraged.

### 4.5 Handling failures of function evaluations

PDFO tolerates NaN values returned by function evaluations. Such a value can be used to indicate failures of function evaluations, which are common in applications of DFO.

To cope with NaN values, PDFO applies a *moderated extreme barrier*. Suppose that $f(\tilde{x})$ is evaluated to NaN at a certain $\tilde{x} \in \mathbb{R}^n$. PDFO takes the view that $\tilde{x}$ violates a hidden constraint [38, 1]. Hence it replaces NaN with a large but finite number `HUGEFUN` (e.g., $10^{30}$) before passing $f(\tilde{x})$ to the Fortran solver, so that the solver can continue to progress while penalizing $\tilde{x}$. Indeed, since Powell's solvers construct trust-region models by interpolation, all points that are close to $\tilde{x}$ will be penalized. Similar things are done when the constraint functions return NaN. A caveat is that setting $f(\tilde{x})$ to `HUGEFUN` may lead to extreme values or even NaN in the coefficients of the interpolation models, but Powell's solvers turn out to be quite tolerant of such values.

The original extreme barrier approach [18, equation (13.2)] sets `HUGEFUN` to $\infty$, which is inappropriate for methods based on interpolation. In fact, we also moderate $f(\tilde{x})$ to `HUGEFUN` if it is actually evaluated to $\infty$. Our approach is clearly naive, but it is better than terminating the solver once the function evaluation fails In our experiments, this simple approach significantly improves the robustness of PDFO with respect to failures of function evaluation, as will be demonstrated in Subsection 5.2. There do exist other more sophisticated approaches [1], which will be explored in the future.

## 5 Numerical results

This section presents numerical experiments on PDFO. Since Powell's solvers are widely used as benchmarks in DFO, extensive comparisons with standard DFO solvers are already available in the literature [42, 66]. Instead of repeating such comparisons, which is unnecessary, the purpose of our experiments is the following.

1. Demonstrate the fact the PDFO is capable of adapting to noise without fine-tuning according to the noise level, in contrast to methods based on finite differences. This is done in Subsection 5.1 by comparing PDFO with finite-difference CG and BFGS on unconstrained CUTEst problems.
2. Verify the effectiveness of the moderated extreme barrier mentioned in Subsection 4.5 for handling failures of function evaluations. This is done in Subsection 5.2 by testing PDFO with and without the barrier on unconstrained CUTEst problems.
3. Illustrate the potential of PDFO in hyperparameter optimization problems from machine learning, echoing the observations made in [27] about trust-region DFO methods for such

problems. This is done in Subsection 5.3 by comparing PDFO with two solvers from the Python package `hyperopt`.[10]

Our experiments are carried out in double precision based on the Python version of PDFO 1.2. The finite-difference CG and BFGS are provided by SciPy 1.10.0. The version of `hyperopt` is 0.2.7. All these packages are tested with the latest stable version at the time of writing. We conduct the test on a ThinkStation P620 with an AMD Ryzen Threadripper PRO 3975WX CPU and 64 GB of memory, the operating system being Ubuntu 22.04, and the Python version being 3.10.6.

## 5.1 Stability under noise

We first compare PDFO with finite-difference CG and BFGS on unconstrained problems with multiplicative Gaussian noise. We take the view that multiplicative noise makes more sense if the scale of the objective function changes widely, as is often the case in applications.

SciPy provides both CG and BFGS under the `minimize` function in the `scipy.optimize` module. Invoked with the default configurations in SciPy without derivatives, CG and BFGS approximate gradients by forward differences with the default difference parameter $h = \sqrt{u} \approx 1.5 \times 10^{-8}$, where $u$ is the unit roundoff. For PDFO, we specify NEWUOA as the solver, while setting all the other options to the default. In particular, the initial trust-region radius is 1, the final trust-region radius is $10^{-6}$, and the number of interpolation points is $2n+1$, with $n$ being the dimension of the problem being solved. We perform the comparison on 158 unconstrained problems with $n \leq 50$ from the CUTEst [28] problem set using PyCUTEst 1.4 [24]. For each testing problem, the starting point is set to the one provided by CUTEst, and the maximal number of function evaluations is set to $500n$.

Let $\sigma \geq 0$ be the noise level to test. For a testing problem with the objective function $f$, we define

$$\tilde{f}_\sigma(x) = [1 + \sigma R(x)] f(x), \tag{5.1}$$

with $R(x) \sim \mathrm{N}(0, 1)$ being independent and identically distributed when $x$ varies. If $\sigma = 0$, then $\tilde{f}_\sigma = f$, corresponding to the noise-free case. In general, $\sigma$ equals the standard deviation of the noise.

Given a noise level $\sigma \geq 0$ and a convergence tolerance $\tau \in (0, 1)$, we will plot the performance profiles [42] of the solvers on the testing problems. We run all the solvers on all the problems, every objective function being evaluated by its contaminated version (5.1). For each solver, the performance profile displays the proportion of problems solved with respect to the normalized cost to solve the problem up to the convergence tolerance $\tau$. For each problem, the cost to solve the problem is the number of function evaluations needed to achieve

$$f(x_0) - f(x_k) \geq (1 - \tau)[f(x_0) - f_*], \tag{5.2}$$

[10] `https://hyperopt.github.io/hyperopt`.

and the normalized cost is this number divided by the minimum cost of this problem among all solvers; we define the normalized cost as infinity if the solver fails to achieve (5.2) on this problem. Here, $x_0$ represents the starting point, and [42, § 2.1] suggests that the value $f_*$ should be the least value of $f$ obtained by all solvers. Note that the convergence test (5.2) uses the values of $f$ and not those of $\tilde{f}_\sigma$. This means that we assess the solvers according to the true objective function values, even though the solvers can only evaluate $\tilde{f}_\sigma$, which is contaminated unless $\sigma = 0$.

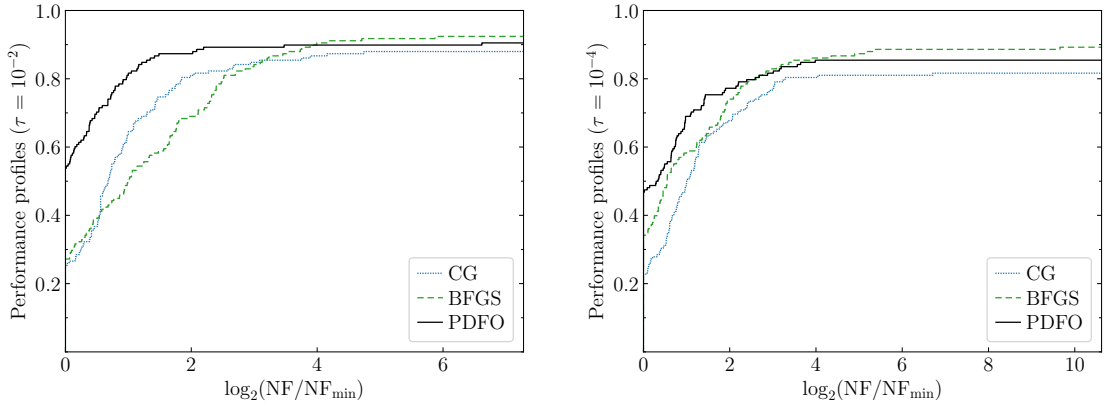
To make our results more reliable, when $\sigma > 0$, the final performance profile is obtained by averaging the profiles obtained via the above procedure over ten independent runs. In addition, the value $f_*$ in the convergence test (5.2) is set to the least value of $f$ obtained by all solvers during all these ten runs plus a run with $\sigma = 0$. Finally, for better scaling of the profiles, we plot the binary logarithm of the normalized cost on the horizontal axis, instead of the normalized cost itself.

Figure 1 shows the performance profiles of the solvers for the noise levels $\sigma = 0$, $\sigma = 10^{-10}$, and $\sigma = 10^{-8}$. Two profiles are included for each noise level, with the convergence tolerance being $\tau = 10^{-2}$ and $\tau = 10^{-4}$ respectively.

In the noise-free case ($\sigma = 0$), PDFO is more efficient than finite-difference CG and BFGS, although the distinction is less visible when $\tau$ is smaller, and BFGS can solve slightly more problems than PDFO. When there is noise ($\sigma > 0$), the advantage of PDFO becomes significant. The performances of CG and BFGS deteriorate considerably under noise, even if the noise level is not high and the convergence tolerance is not demanding. We do not include results with larger values of $\sigma$, as CG and BFGS will barely solve any problem, while PDFO can still tackle a significant proportion of them up to a reasonable precision.

However, given the fact that CG and BFGS take the finite difference parameter $h \approx 10^{-8}$, their unfavorable performance is not surprising. It does not contradict the observations in [67, 68], where $h$ is chosen more carefully according to the noise level and the smoothness of the problems. Our experiment does not include such fine-tuning but adopts the default settings of CG and BFGS in SciPy, as well as the default configurations of PDFO.

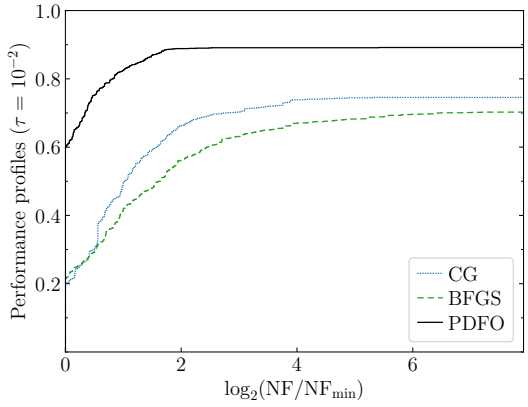
To summarize, the performance of finite-difference CG and BFGS is encouraging when there is no noise, yet much more care is needed when the problems are noisy. In contrast, PDFO adapts to noise automatically in our experiment, demonstrating good stability under noise without requiring knowledge about the noise level. This is because Powell's methods (NEWUOA in this experiment) gradually adjust the geometry of the interpolation set during the iterations, making progress until the interpolation points are too close to distinguish noise from true objective function values. This is not specific to Powell's methods but also applies to other algorithms that sample the objective function on a set of points with adaptively controlled geometry, including finite-difference methods with well-chosen difference parameters [67].



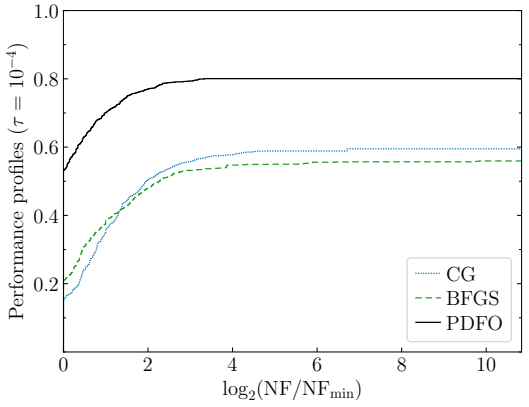

(a) $\sigma = 0$, $\tau = 10^{-2}$



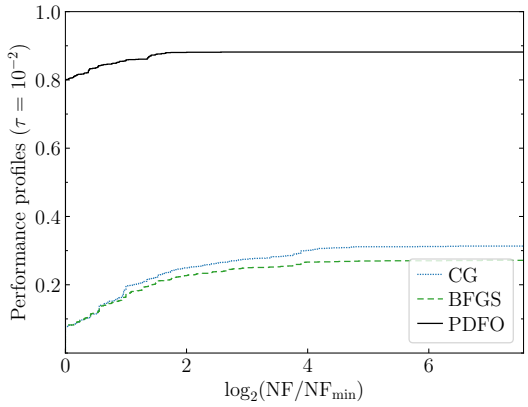

(b) $\sigma = 0$, $\tau = 10^{-4}$



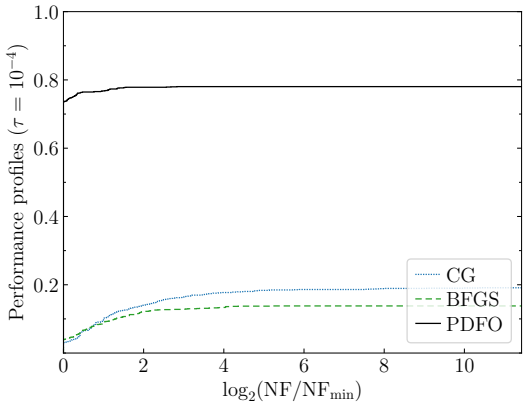

(c) $\sigma = 10^{-10}$, $\tau = 10^{-2}$




(d) $\sigma = 10^{-10}$, $\tau = 10^{-4}$




(e) $\sigma = 10^{-8}$, $\tau = 10^{-2}$




(f) $\sigma = 10^{-8}$, $\tau = 10^{-4}$

Figure 1: Performance profiles of CG, BFGS, and PDFO on unconstrained problems with the objective functions evaluated by $\tilde{f}_\sigma$ in (5.1)

## 5.2 Robustness with respect to failures of function evaluations

We now test the robustness of the solvers when function evaluations fail from time to time. We assume that the objective function returns NaN if the evaluation fails, which occurs randomly with a certain probability. As mentioned in Section 4.5, PDFO uses a moderated extreme barrier to handle such failures. To verify the effectiveness of this approach, we compare PDFO with its variant that does not apply the barrier. To make the experiment more informative, we also include the finite-difference CG and BFGS tested before, which do not handle evaluation failures particularly. The solvers are set up in the same way as in the previous experiment, and we still employ the 158 unconstrained CUTEst problems used previously.

Let $p \in [0, 1]$ be the failure probability of function evaluations. For a testing problem with the objective function $f$, we define

$$\hat{f}_p(x) = \begin{cases} f(x) & \text{if } U(x) \geq p, \\ \text{NaN} & \text{otherwise,} \end{cases} \tag{5.3}$$

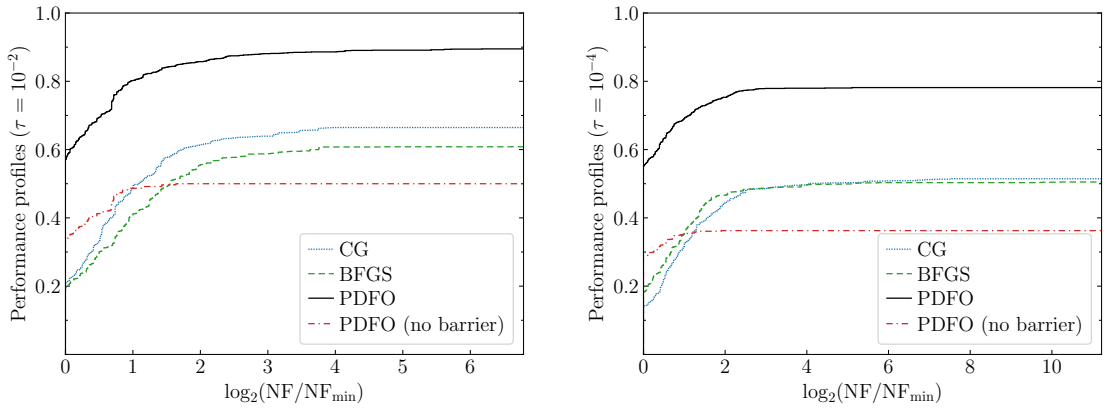
where $U(x)$ follows the uniform distribution on $[0, 1]$, being independent and identically distributed when $x$ varies. Note that $\hat{f}_0 = f$. In the experiment, the solvers can evaluate $f$ only via $\hat{f}_p$. We plot the performance profiles of the solvers in a way that is similar to the previous experiment. The profiles are also averaged over ten independent runs. For each problem, the value $f_*$ in the convergence test (5.2) is set to the least value of $f$ obtained by all solvers during these ten runs plus a run with $p = 0$.

Figure 2 shows the performance profiles of the solvers with $p = 0.01$ and $p = 0.05$. Two profiles are included for each $p$, with the convergence tolerance being $\tau = 10^{-2}$ and $\tau = 10^{-4}$ respectively.

The contrast is clear. Compared with finite-difference CG and BFGS, PDFO is more efficient and solves significantly more problems given the same convergence tolerance. Moreover, comparing PDFO and its no-barrier counterpart, we see that the moderated extreme barrier improves evidently the robustness of PDFO with respect to failures of function evaluations, even though it is a quite naive approach. When $p = 0.05$, the function evaluation fails roughly once every 20 times, but PDFO can still solve almost 60% of the problems up to the convergence tolerance $\tau = 10^{-4}$ in the sense of (5.2), whereas all its competitors solve less than 25%. We speculate that the moderated extreme barrier will also benefit other model-based DFO methods, including those based on finite differences. It deserves further investigation in the future.

## 5.3 An illustration of hyperparameter optimization with PDFO

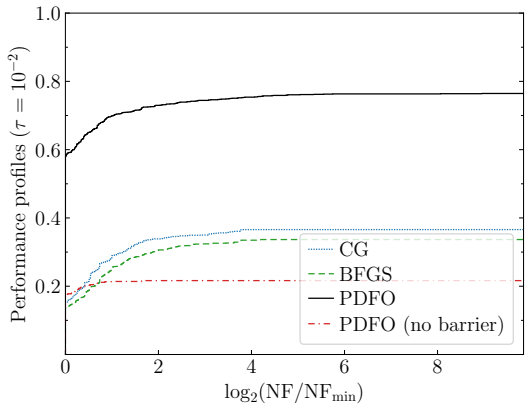
We now consider a hyperparameter optimization problem from machine learning and illustrate the potential of PDFO for such problems. We compare PDFO with Random Search (RS) and Tree-Structured Parzen Estimator (TPE), two solvers from the Python package `hyperopt` for hyperparameter optimization.



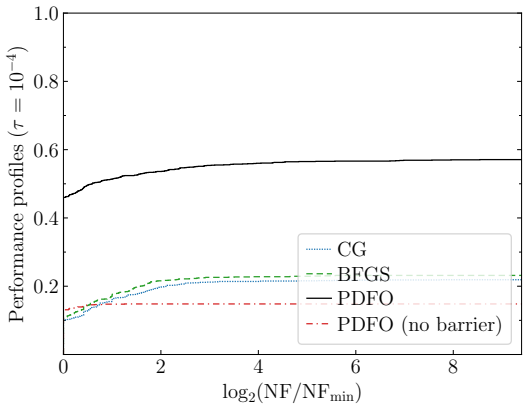

(a) $p = 0.01$, $\tau = 10^{-2}$




(b) $p = 0.01$, $\tau = 10^{-4}$




(c) $p = 0.05$, $\tau = 10^{-2}$




(d) $p = 0.05$, $\tau = 10^{-4}$

Figure 2: Performance profiles of CG, BFGS, PDFO, and PDFO without barrier on unconstrained problems with the objective functions evaluated by $\hat{f}_p$ in (5.3)

Our experiment is inspired by [27, § 5.3], which investigates the application of trust-region DFO methods to hyperparameter optimization. Similar to [27, § 5.3], we tune the $C$-SVC model detailed in [11, § 2.1] for binary classifications. Given a dataset $\{(u_i, z_i)\}_{i=1}^N$, with $u_i \in \mathbb{R}^d$ being a vector of features and $z_i \in \{-1, 1\}$ being the corresponding label, the $C$-SVC constructs a classifier by solving

$$\min_{\alpha} \ \frac{1}{2}\alpha^\top Q\alpha - \alpha^\top \mathbb{1} \quad \text{s.t.} \quad 0 \le \alpha \le C, \ \alpha^\top z = 0, \ \alpha \in \mathbb{R}^N, \tag{5.4}$$

where $C \in (0, \infty)$ is a hyperparameter, $z \in \mathbb{R}^N$ is the vector whose $i$th entry is $z_i$, $\mathbb{1} \in \mathbb{R}^N$ is the vector of all ones, and $Q \in \mathbb{R}^{N\times N}$ is the matrix whose $(i, j)$ entry is $K(u_i, u_j)$ with a kernel function $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$. We take the Gaussian kernel $K(u, v) = \exp(-\gamma\|u - v\|^2)$, where $\gamma \in (0, \infty)$ is another hyperparameter. See [11, § 2.1] for more details.

As suggested by [11, § 9], we tune $C$ and $\gamma$ for the performance of the $C$-SVC. We model this process as solving the problem

$$\max \ P(C, \gamma) \quad \text{s.t.} \quad C > 0, \ \gamma > 0, \tag{5.5}$$

where $P(C, \gamma)$ measures the performance corresponding to parameters $(C, \gamma)$. In our experiment, we define $P$ based on the AUC score [27, § 3], which lies in $[0, 1]$ and measures the quality of a classifier on a dataset, the higher the better. More precisely, $P(C, \gamma)$ is set to a five-fold cross-validation AUC score as follows. Split the training dataset $\mathcal{S}$ into five folds, and train the $C$-SVC five times, each time solving (5.4) on a union of four distinct folds. After each training, calculate the AUC score of the resulting classifier on the fold not involved in the training, leading to five scores, the average of which is $P(C, \gamma)$.

Our experiment is based on binary classification problems from LIBSVM,[11] where we adopt three datasets detailed in Table 1. LIBSVM divides each dataset $\mathcal{D}$ into two disjoint subsets, namely a training dataset $\mathcal{S}$ and a testing dataset $\mathcal{T}$. Given $\mathcal{D}$, we evaluate $P$ based on $\mathcal{S}$ by the procedure described above, with (5.4) being handled by the SVC class of the Python package scikit-learn.[12] Then we solve (5.5) by PDFO, RS, or TPE to obtain the tuned parameters $(\bar{C}, \bar{\gamma})$. As in [27, § 5.3], we modify the constraints of (5.5) to $C \in [10^{-6}, 1]$ and $\gamma \in [1, 10^3]$. For better scaling of the problem, we perform the maximization with respect to $(\log_{10} C, \log_{10} \gamma)$ instead of $(C, \gamma)$, the initial guess being chosen randomly from $[-6, 0] \times [0, 3]$. The solver of PDFO is BOBYQA, for which we set the maximal number of function evaluations to 100. For RS and TPE, we try both 100 and 300 for the maximal number of function evaluations, and they do not terminate until this number is reached.

To assess the quality of the tuned parameters $(\bar{C}, \bar{\gamma})$, we solve (5.4) on $\mathcal{S}$ with $(C, \gamma) = (\bar{C}, \bar{\gamma})$, and calculate both the AUC score and accuracy of the resulting classifier on $\mathcal{T}$, the latter being the fraction of correctly classified data points. Note that $\mathcal{T}$ is not involved in the tuning process.

[11] `https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets`.
[12] `https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html`.

Table 1: Datasets from LIBSVM

| Dataset $\mathcal{D}$ | Number of features | Size of $\mathcal{S}$ | Size of $\mathcal{T}$ |
|---|---|---|---|
| splice | 60 | 1,000 | 2,175 |
| svmguide1 | 4 | 3,088 | 4,000 |
| ijcnn1 | 22 | 49,990 | 91,701 |

Tables 2–4 present the results for this experiment, where $\#P$ denotes the number of evaluating the function $P$ and "Time" represents the computing time for obtaining $(\bar{C}, \bar{\gamma})$.

Table 2: Hyperparameter tuning on the dataset "splice"

| Solver | AUC Score ($10^{-1}$) | Accuracy ($10^{-1}$) | $\#P$ | Time (s) |
|---|---|---|---|---|
| RS | 5.00 | 5.20 | 100 | 8.23 |
| RS | 5.00 | 5.20 | 300 | 24.73 |
| TPE | 5.00 | 5.20 | 100 | 8.22 |
| TPE | 5.00 | 5.20 | 300 | 23.57 |
| PDFO | 9.27 | 7.37 | 33 | 5.11 |

Table 3: Hyperparameter tuning on the dataset "svmguide1"

| Solver | AUC Score ($10^{-1}$) | Accuracy ($10^{-1}$) | $\#P$ | Time (s) |
|---|---|---|---|---|
| RS | 9.94 | 9.61 | 100 | 10.22 |
| RS | 9.95 | 9.68 | 300 | 30.75 |
| TPE | 9.95 | 9.65 | 100 | 8.65 |
| TPE | 9.95 | 9.68 | 300 | 22.38 |
| PDFO | 9.95 | 9.66 | 51 | 2.83 |

Table 4: Hyperparameter tuning on the dataset "ijcnn1"

| Solver | AUC Score ($10^{-1}$) | Accuracy ($10^{-1}$) | $\#P$ | Time ($\mathbf{10^3 s}$) |
|---|---|---|---|---|
| RS | 9.97 | 9.82 | 100 | 3.99 |
| RS | 9.97 | 9.77 | 300 | 11.52 |
| TPE | 9.98 | 9.79 | 100 | 3.42 |
| TPE | 9.98 | 9.79 | 300 | 8.81 |
| PDFO | 9.97 | 9.80 | 44 | 2.48 |

In terms of the AUC score and accuracy, PDFO achieves a clearly better result than RS and TPE on the "splice" dataset, and they all attain comparable results on the other datasets. However, PDFO always uses much fewer function evaluations, and hence, much less computing time. The difference in the computing time is particularly visible on the dataset "ijcnn1" in Table 4, as each evaluation of $P$ takes much time due to the large data size.

Note that our intention is not to manifest that PDFO outperforms standard solvers for general hyperparameter optimization problems, which is unlikely the case. Indeed, PDFO is not applicable unless the hyperparameters are continuous variables. Our objective is rather to provide an example that shows the possibility of applying Powell's methods to hyperparameter optimization, which is not well studied up to now. In doing so, we also hope to call for more investigation on DFO methods for machine learning problems in general, as is suggested in [27].

# 6 Concluding remarks

We have presented the PDFO package, which aims at simplifying the use of Powell's DFO solvers by providing user-friendly interfaces. More information about the package can be found on the homepage of the package at `https://www.pdfo.net`, including the detailed syntax of the interfaces, an extensive documentation of the options, and several examples to illustrate the usage.

In addition, we have provided an overview of Powell's methods behind PDFO. The overview does not intend to repeat Powell's description of the methods, but rather to provide a summary of the main features and structures of the methods, highlighting the intrinsic connections and similarities among them. We hope that the overview will ease the understanding of Powell's methods, in the same way as the PDFO package eases the use of these methods.

Besides Powell's solvers, PDFO also provides a unified interface for DFO solvers. Such an interface can facilitate the development and comparison of different DFO solvers. The interface can readily accommodate solvers other than those by Powell, for example, the COBYQA (Constrained Optimization BY Quadratic Approximations) solver for general nonlinearly constrained DFO problems (see [62, Chapters 5–7] and [63]).

Finally, we stress that PDFO does not implement Powell's DFO solvers in Python or MATLAB, but only interfaces Powell's implementation with such languages. The implementation of these solvers in Python, MATLAB, and other languages is a project in progress under the name of PRIMA (Reference Implementation for Powell's methods with Modernization and Amelioration) [79].

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**Data availability.** The source code of the PDFO package is available at `https://www.pdfo.net`. The source code of the numerical experiments is available at `https://www.github.com/pdfo/paper/blob/main/experiments`.

# References


[1] C. Audet, G. Caporossi, and S. Jacquet. Binary, unrelaxable and hidden constraints in blackbox optimization. *Oper. Res. Lett.*, 48:467–471, 2020.

[2] C. Audet and J. E. Dennis, Jr. Mesh adaptive direct search algorithms for constrained optimization. *SIAM J. Optim.*, 17:188–217, 2006.

[3] C. Audet and W. Hare. *Derivative-Free and Blackbox Optimization*. Springer Ser. Oper. Res. Financ. Eng. Springer, Cham, CH, 2017.

[4] A. S. Bandeira, K. Scheinberg, and L. N. Vicente. Computation of sparse low degree interpolating polynomials and their application to derivative-free optimization. *Math. Program.*, 134:223–257, 2012.

[5] D. M. Bates, M. Mächler, B. Bolker, and S. Walker. Fitting linear mixed-effects models using lme4. *J. Stat. Softw.*, 67:1–48, 2015.

[6] A. S. Berahas, R. H. Byrd, and J. Nocedal. Derivative-free optimization of noisy functions via quasi-Newton methods. *SIAM J. Optim.*, 29:965–993, 2019.

[7] S. C. Billups, J. Larson, and P. Graf. Derivative-free optimization of expensive functions with computational error using weighted regression. *SIAM J. Optim.*, 23:27–53, 2013.

[8] M. D. Buhmann, R. Fletcher, A. Iserles, and Ph.L Toint. Michael J. D. Powell. 29 July 1936–19 April 2015. *Biogr. Mems Fell. R. Soc.*, 64:341–366, 2018.

[9] C. Cartis, J. Fiala, B. Marteau, and L. Roberts. Improving the flexibility and robustness of model-based derivative-free optimization solvers. *ACM Trans. Math. Software*, 45:32:1–32:41, 2019.

[10] C. Cartis, L. Roberts, and O. Sheridan-Methven. Escaping local minima with local derivative-free methods: a numerical investigation. *Optimization*, 71:2343–2373, 2022.

[11] C. C. Chang and C. J. Lin. LIBSVM: a library for support vector machines. *ACM TIST*, 2:27:1–27:27, 2011.

[12] A. R. Conn and S. Le Digabel. Use of quadratic models with mesh-adaptive direct search for constrained black box optimization. *Optim. Methods Softw.*, 28:139–158, 2013.

[13] A. R. Conn, K. Scheinberg, and Ph.L Toint. On the convergence of derivative-free methods for unconstrained optimization. In M. D. Buhmann and A. Iserles, editors, *Approximation Theory and Optimization: Tributes to M. J. D. Powell*, pages 83–108, Cambridge, UK, 1997. Cambridge University Press.

[14] A. R. Conn, K. Scheinberg, and Ph.L Toint. Recent progress in unconstrained nonlinear optimization without derivatives. *Math. Program.*, 79:397–414, 1997.

[15] A. R. Conn, K. Scheinberg, and L. N. Vicente. Geometry of interpolation sets in derivative free optimization. *Math. Program.*, 111:141–172, 2008.

[16] A. R. Conn, K. Scheinberg, and L. N. Vicente. Geometry of sample sets in derivative-free optimization: polynomial regression and underdetermined interpolation. *IMA J. Numer. Anal.*, 28:721–748, 2008.

[17] A. R. Conn, K. Scheinberg, and L. N. Vicente. Global convergence of general derivative-free trust-region algorithms to first- and second-order critical points. *SIAM J. Optim.*, 20:387–415, 2009.

[18] A. R. Conn, K. Scheinberg, and L. N. Vicente. *Introduction to Derivative-Free Optimization*. MPS-SIAM Ser. Optim. SIAM, Philadelphia, PA, USA, 2009.

[19] A. R. Conn and Ph.L Toint. An algorithm using quadratic interpolation for unconstrained derivative free optimization. In G. Di Pillo and F. Giannessi, editors, *Nonlinear Optimization and Applications*, pages 27–47, Boston, MA, USA, 1996. Springer.

[20] A. L. Custódio, K. Scheinberg, and L. N. Vicente. Methodologies and software for derivative-free optimization. In T. Terlaky, M. F. Anjos, and S. Ahmed, editors, *Advances and Trends in Optimization with Engineering Applications*, pages 495–506, Philadelphia, PA, USA, 2017. SIAM.

[21] J. E. Dennis, Jr. and R. B. Schnabel. Least change secant updates for quasi-Newton methods. *SIAM Rev.*, 4:443–459, 1979.

[22] M. Dodangeh and L. N. Vicente. Worst case complexity of direct search under convexity. *Math. Program.*, 155:307–332, 2016.

[23] R. Fletcher and M. J. D. Powell. A rapid convergent decent method for minimization. *Comput. J.*, 6:163–168, 1963.

[24] J. Fowkes, L. Roberts, and Á. Bűrmen. PyCUTEst: an open source python package of optimization test problems. *J. Open Source Softw.*, 7:4377, 2022.

[25] F. Gallard et al. GEMS: a Python library for automation of multidisciplinary design optimization process generation. In *2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*, Kissimmee, FL, USA, 2018. AIAA.

[26] R. Garmanjani, D. Jùdice, and L. N. Vicente. Trust-region methods without using derivatives: worst case complexity and the nonsmooth case. *SIAM J. Optim.*, 26:1987–2011, 2016.

[27] H. Ghanbari and K. Scheinberg. Black-box optimization in machine learning with trust region based derivative free algorithm. Technical Report 17T-005, COR@L, Bethlehem, PA, USA, 2017.

[28] 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.

[29] S. Gratton, C. W. Royer, L. N. Vicente, and Z. Zhang. Direct search based on probabilistic descent. *SIAM J. Optim.*, 25:1515–1541, 2015.

[30] S. Gratton, C. W. Royer, L. N. Vicente, and Z. Zhang. Direct search based on probabilistic feasible descent for bound and linearly constrained problems. *Comput. Optim. Appl.*, 72:525–559, 2019.

[31] W. W. Hager. Updating the inverse of a matrix. *SIAM Rev.*, 31:221–239, 1989.

[32] M. Hough and L. Roberts. Model-based derivative-free methods for convex-constrained optimization. *SIAM J. Optim.*, 32:2552–2579, 2022.

[33] H. Izadinia, Q. Shan, and S. M. Seitz. IM2CAD. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 5134–5143, San Juan, PR, USA, 2017. IEEE.

[34] C. T. Kelley. *Implicit Filtering*. Software Environ. Tools. SIAM, Philadelphia, PA, USA, 2011.

[35] 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.

[36] J. Larson, M. Menickelly, and S. M. Wild. Derivative-free optimization methods. *Acta Numer.*, 28:287–404, 2019.

[37] S. Le Digabel. Algorithm 909: NOMAD: nonlinear optimization with the MADS algorithm. *ACM Trans. Math. Software*, 37:44:1–44:15, 2011.

[38] S. Le Digabel and S. M. Wild. A taxonomy of constraints in simulation-based optimization. arXiv:1505.07881, 2015.

[39] G. A. Mamon, A. Biviano, and G. Boué. MAMPOSSt: modelling anisotropy and mass profiles of observed spherical systems I. Gaussian 3D velocities. *Mon. Not. R. Astron. Soc.*, 429:3079–3098, 2013.

[40] K. Mombaur, A. Truong, and J. P. Laumond. From human to humanoid locomotion—an inverse optimal control approach. *Auton. Robot.*, 28:369–383, 2010.

[41] J. J. Moré and D. C. Sorensen. Computing a trust region step. *SIAM J. Sci. Stat. Comp.*, 4:553–572, 1983.

[42] J. J. Moré and S. M. Wild. Benchmarking derivative-free optimization algorithms. *SIAM J. Optim.*, 20:172–191, 2009.

[43] J. A. Nelder and R. Mead. A simplex method for function minimization. *Comput. J.*, 7:308–313, 1965.

[44] R. Oeuvray and M. Bierlaire. BOOSTERS: a derivative-free algorithm based on radial basis functions. *Int. J. Model. Simul.*, 29:29–36, 2009.

[45] 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.

[46] M. Porcelli and Ph.L Toint. Global and local information in structured derivative free optimization with BFO. arxiv:2001.04801, 2020.

[47] M. Porcelli and Ph.L Toint. Exploiting problem structure in derivative free optimization. *ACM Trans. Math. Software*, 48:1–25, 2022.

[48] M. J. D. Powell. An efficient method for finding the minimum of a function of several variables without calculating derivatives. *Comput. J.*, 7:155–162, 1964.

[49] M. J. D. Powell. A new algorithm for unconstrained optimization. In J. B. Rosen, O. L. Mangasarian, and K. Ritter, editors, *Nonlinear Programming*, pages 31–65, London, UK, 1970. Academic Press.

[50] M. J. D. Powell. A direct search optimization method that models the objective and constraint functions by linear interpolation. In S. Gomez and J. P. Hennart, editors, *Advances in Optimization and Numerical Analysis*, pages 51–67, Dordrecht, NL, 1994. Springer.

[51] M. J. D. Powell. Direct search algorithms for optimization calculations. *Acta Numer.*, 7:287–336, 1998.

[52] M. J. D. Powell. On the Lagrange functions of quadratic models that are defined by interpolation. *Optim. Methods Softw.*, 16:289–309, 2001.

[53] M. J. D. Powell. UOBYQA: unconstrained optimization by quadratic approximation. *Math. Program.*, 92:555–582, 2002.

[54] M. J. D. Powell. Least Frobenius norm updating of quadratic models that satisfy interpolation conditions. *Math. Program.*, 100:183–215, 2004.

[55] M. J. D. Powell. On updating the inverse of a KKT matrix. In Y. Yuan, editor, *Numerical Linear Algebra and Optimization*, pages 56–78, Beijing, CN, 2004. Science Press.

[56] M. J. D. Powell. The NEWUOA software for unconstrained optimization without derivatives. In G. Di Pillo and M. Roma, editors, *Large-Scale Nonlinear Optimization*, volume 83 of *Nonconvex Optimization and Its Applications*, pages 255–297, Boston, MA, USA, 2006. Springer.

[57] M. J. D. Powell. Developments of NEWUOA for minimization without derivatives. *IMA J. Numer. Anal.*, 28:649–664, 2008.

[58] M. J. D. Powell. The BOBYQA algorithm for bound constrained optimization without derivatives. Technical Report DAMTP 2009/NA06, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge, UK, 2009.

[59] M. J. D. Powell. On the convergence of trust region algorithms for unconstrained minimization without derivatives. *Comput. Optim. Appl.*, 53:527–555, 2012.

[60] M. J. D. Powell. Beyond symmetric Broyden for updating quadratic models in minimization without derivatives. *Math. Program.*, 138:475–500, 2013.

[61] M. J. D. Powell. On fast trust region methods for quadratic models with linear constraints. *Math. Program. Comput.*, 7:237–267, 2015.

[62] T. M. Ragonneau. *Model-Based Derivative-Free Optimization Methods and Software*. PhD thesis, Department of Applied Mathematics, The Hong Kong Polytechnic University, Hong Kong, 2022.

[63] T. M. Ragonneau and Z. Zhang. COBYQA: Constrained Optimization BY Quadratic Approximations. `https://www.cobyqa.com`, 2023.

[64] T. M. Ragonneau and Z. Zhang. An optimal interpolation set for model-based derivative-free optimization methods. arXiv:2302.09992, 2023.

[65] R. G. Regis and S. M. Wild. CONORBIT: constrained optimization by radial basis function interpolation in trust regions. *Optim. Methods Softw.*, 32:552–580, 2017.

[66] L. M. Rios and N. V. Sahinidis. Derivative-free optimization: a review of algorithms and comparison of software implementations. *J. Global Optim.*, 56:1247–1293, 2013.

[67] H. J. M. Shi, Y. Xie, M. Q. Xuan, and J. Nocedal. Adaptive finite-difference interval estimation for noisy derivative-free optimization. *SIAM J. Sci. Comput.*, 44:A2302–A2321, 2022.

[68] H. J. M. Shi, M. Q. Xuan, F. Oztoprak, and J. Nocedal. On the numerical performance of derivative-free optimization methods based on finite-difference approximations. *Optim. Methods Softw.*, 38:289–311, 2023.

[69] T. Steihaug. The conjugate gradient method and trust regions in large scale optimization. *IMA J. Numer. Anal.*, 20:626–637, 1983.

[70] Ph.L Toint. Towards an efficient sparsity exploiting Newton method for minimization. In I. S. Duff, editor, *Sparse Matrices and Their Uses*, pages 57–88, London, UK, 1981. Academic Press.

[71] V. Torczon. On the convergence of pattern search. *SIAM J. Optim.*, 7:1–25, 1997.

[72] L. N. Vicente. Worst case complexity of direct search. *EURO J. Comput.*, 1:143–153, 2013.

[73] S. M. Wild. MNH: a derivative-free optimization algorithm using minimal norm Hessians. In *The Tenth Copper Mountain Conference on Iterative Methods*, 2008.

[74] S. M. Wild, R. G. Regis, and C. A. Shoemaker. ORBIT: optimization by radial basis function interpolation in trust-regions. *SIAM J. Sci. Comput.*, 30:3197–3219, 2008.

[75] P. Xie and Y. Yuan. Least $H^2$ norm updating quadratic interpolation model function for derivative-free trust-region algorithms. arxiv:2001.04801, 2023.

[76] H. Zhang, A. R. Conn, and K. Scheinberg. A derivative-free algorithm for least-squares minimization. *SIAM J. Optim.*, 20:3555–3576, 2010.

[77] Z. Zhang. *On Derivative-Free Optimization Methods* (in Chinese). PhD thesis, Chinese Academy of Sciences, Beijing, CN, 2012.

[78] Z. Zhang. Sobolev seminorm of quadratic functions with applications to derivative-free optimization. *Math. Program.*, 146:77–96, 2014.

[79] Z. Zhang. PRIMA: Reference Implementation for Powell's methods with Modernization and Amelioration. `http://www.libprima.net`, 2023.