PDFO — Cross-Platform Package for Using Powell's Derivative-Free Optimization Solvers

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Abstract

To do.

1 Introduction

Most optimization algorithms rely on classical or generalized derivative information of the objective function and constraints. 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. Optimization problems of such kind arise from automatic error analysis [34, 35], machine learning [29], analog circuit design [42], aircraft engineering [28], and chemical product design [71], to name but a few. These problems motivate the development of optimization algorithms that use only function values but not derivatives.

Between 1994 and 2015, Powell developed five solvers to tackle unconstrained and constrained problems without using derivatives, namely COBYLA, UOBYQA, NEWUOA, BOBYQA, and LINCOA. These solvers were implemented by Powell, with particular attention paid to their numerical stability and algebraic complexity. Renowned for their robustness and efficiency, these solvers are extremely appealing to practitioners and widely used in applications, for instance, aeronautical engineering [27], astronomy [10, 44], computer vision [37], robotics [45], and statistics [7].

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However, Powell coded in Fortran 77, an old-fashion language that damps the enthusiasm of many users to exploit these solvers in their projects. There have been a considerable demand from both researchers and practitioners for the availability of Powell's solvers in more user-friendly languages such as Python, MATLAB®, and Julia. Our aim is to wrap Powell's Fortran code into a package, namely PDFO, which enables users of such languages to call Powell's solvers without any need of dealing with the Fortran code. For each supported language, PDFO provides a simple subroutine 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 1.1) 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 Library™. The package is cross-platform, available on Linux, macOS, and Microsoft Windows at once.

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 in response to the continual demands from both researchers and practitioners: Py-BOBYQA [12] provides a Python implementation of BOBYQA; NLopt [38] includes multi-language interfaces for COBYLA, NEWUOA, and BOBYQA; `minqa` [6] wraps UOBYQA, NEWUOA, and BOBYQA in R; SciPy [73] makes COBYLA available in Python under its optimization library. Nevertheless, PDFO has several features that distinguishes itself 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. In addition to homogenizing the usage, such an interface eases the comparison between these solvers in case multiple of them are able to tackle a given problem. Doing so, we may gain insights that cannot be obtained otherwise into the behavior of the solvers, as will be illustrated in appendix B.
2. *Solver selection.* When using PDFO, the user can specifically call one of Powell's solvers; nevertheless, if the user does not specify any solver, PDFO will select automatically a solver according to the given problem. The selection takes into consideration the performance of the solvers on the CUTEst [30] problem set. Interestingly, it turns out that the solver with the best performance may not be the most intuitive one. For example, NEWUOA is not always the best choice for solving an unconstrained problem. This will be elaborated in appendix B
3. *Code patching.* During the development of PDFO, we spotted in the original Fortran code some bugs, which led to infinite cycling or segmentation faults on some ill-conditioned problems. The bugs have been patched in PDFO. Nevertheless, we provide an option that can enforce the package to use the original code of

Powell without the patches, which is not recommended except for research. In addition, PDFO provides COBYLA in double precision, whereas Powell used single precision when he implemented it in the 1990s. See appendix B for details.

4. *Fault tolerance.* PDFO takes care of failures in the evaluation of the objective or constraint functions when NaN or infinite values are returned. In case of such failures, PDFO will not exit but try to progress. Moreover, PDFO ensures that the returned solution is not a point where the evaluation fails, while the original code of Powell may return a point whose objective function value is numerically NaN. This is explained in appendix B.
5. *Problem preprocessing.* PDFO preprocesses the inputs to simplify the problem and reformulate it to meet the requirements of Powell's solvers. For instance, if the problem has linear constraints $Ax = b$, PDFO can rewrite it into a problem on the null space of A, eliminating such constraints and reducing the dimension. Another example is that the starting point of a linearly-constrained problem is projected to the feasible region, because LINCOA needs a feasible starting point to work properly.
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 the bounds of the variables before solving it.

The organization of this paper is as follows: section 3 presents a brief description of the five Powell's derivative-free optimization (DFO) algorithms and section 4 introduces PDFO, a cross-platform package providing MATLAB® and Python interfaces for using the above-mentioned solvers.

2 A brief review of DFO methods

Consider a nonlinear optimization problem

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

where $f \colon \mathrm{R}^n \to \mathrm{R}$ is the objective function and $\Omega \subseteq \mathrm{R}^n$ refers to the feasible region of the problem. As summarized in [20], two strategies have been developed to tackle the problem (2.1) without using derivatives, which we will sketch in the sequel.

The first strategy, known as direct search,[1] explores the objective function f and chooses iterates by simple comparisons of function values, examples including the Nelder-Mead algorithm [48], the MADS methods [1, 2, 43], and BFO [**Porcelli_Toint_2020b**,

[1]In some early papers (e.g., [55, 56]), Powell used the word "direct search" to mean what is known as "derivative-free optimization" today.

51, 52]. See [40], [20, Chapters 7 and 8], [3, Part 3], and [41, Section 2.1] for more discussions on this paradigm, and we refer to [31, 33] for recent developments on randomized methods in this category.

The second strategy approximates the original problem (2.1) by relatively simple models and locates the iterates according to such models. Algorithms with this strategy are referred to as model-based methods, and they often make use of the models within a trust-region framework [**Conn_Gould_Toint_2000**, 19, 76], but line search methods also exist [8, 69]. Interpolation and regression are two common ways of establishing the models [**Billups_Larson_Graf_2013**, 4, 17, 57, 59, 65, 75]. It is worth noting that algorithms using finite-difference approximations of gradients can also be regarded as model-based methods, because such approximations essentially come from linear (for forward and backward finite differences) or quadratic (for central finite difference) interpolation of the function under consideration over rather special interpolation sets. A crucial aspect of methods using interpolation models is the strategy they employ to update the interpolation set. The strategy should recycle points from previous iterations, at which the objective function has already been evaluated; meanwhile, it needs to maintain the well poisedness [20, 67] of the interpolation set in order to guarantee the accuracy of the interpolants and ensure the convergence of the optimization algorithm [17, 18, 25, 68]. Most model-based DFO methods employ polynomial models that are linear or quadratic, examples including Powell's methods [55, 58, 61, 63, 64], MNH [74], DFLS [77], DFO-TR [4], and DFO-LS [12], but there are also successful cases exploiting radial basis functions (RBFs), such as ORBIT [75], CONORBIT [65], and BOOSTERS [49]. Model-based DFO is one of the motivations for studying trust-region or line search methods with randomized models, for which we refer to [5, 11, 32] as examples.

Hybrids between direct search and model-based approaches exist, for example [23], [39, Algorithm 4.7], and [14]. For more extensive discussions on DFO methods and theory, see the monographs [3, 20], the survey papers [22, 41, 66], and the references therein.

3 Powell's derivative-free methods

Powell published hist first DFO algorithm based on conjugate directions in 1964 [53].[2] His code for this algorithm is contained in the HSL Mathematical Software Library [36] as subroutine `VA24`. It is not included in PDFO because the code is not in the public domain, although open-source implementations are available (see [15, footnote 4]).

From the 1990s to the final days of his career, Powell developed five DFO trust-region

[2]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 [**Fletcher_Powell_1963**], co-authored with Flethcer and published in 1963.

algorithms, namely COBYLA [55], UOBYQA [58], NEWUOA [61], BOBYQA [63], and LINCOA [64]. In addition, Powell coded these algorithms into Fortran solvers and made them publicly available. We provide a brief overview on these algorithms in the sequel.

Powell's DFO trust-region algorithms uses linear or quadratic interpolation models. At iteration k, the algorithms determine a finite set $\mathcal{Y}_k \subseteq \mathrm{R}^n$ of interpolation points lying in a region around the iterate x_k, construct a model $\widehat{f}_k$ satisfying the interpolation conditions

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

and obtain a trial point by solving approximately

$$\begin{aligned} \min_{x \in \Omega_k} \quad & \widehat{f}_k(x) && \text{(3.2a)} \\ \text{s.t.} \quad & \|x - x_k\| \le \Delta_k, && \text{(3.2b)} \end{aligned}$$

where x_k is the current iterate, $\widehat{f}_k$ stands for a model of the objective function f, Δ_k denotes the trust-region radius, $\|\cdot\|$ is a norm in R^n, and Ω is replaced by a local approximation $\Omega_k \subseteq \mathrm{R}^n$, which can be Ω itself. The trial point is then accepted if it satisfies some sufficient decrease condition.

3.1 COBYLA

At the dawn of the modern DFO, Powell introduced in 1994 his solver COBYLA [55], named after "constrained optimization by linear approximation". It attempts to solve the optimization problem (2.1) when the feasible region Ω is general and expressed as

$$\Omega \stackrel{\text{def}}{=} \{x \in \mathrm{R}^n \colon c_i(x) \ge 0,\ i = 1, ..., m\},$$

where $c_i \colon \mathrm{R}^n \to \mathrm{R}$ denotes the ith nonlinear constraint function, with $i \in \{1, 2, \dots, m\}$. At each iteration, it approximates the objective and constraint functions with linear models obtained by fully-determined interpolations on $\mathcal{Y}_k$, whose cardinal is fixed to $n{+}1$. In this context, the poisedness [67, §1] of the interpolation set, i.e., the geometrical condition on $\mathcal{Y}_k$ required to ensure the uniqueness of the models, can be seen as the volume of the n-simplex engendered by $\mathcal{Y}_k$ to be nonzero. Once the linear models $\widehat{c}_{i,k}$ of the constraint functions c_i for $i \in \{1, 2, \dots, m\}$ are built, an approximation Ω_k of Ω is obtained as the intersection of the half-spaces generated by the linear approximations of the constraint functions, that is

$$\Omega_k \stackrel{\text{def}}{=} \{x \in \mathrm{R}^n \colon \widehat{c}_{i,k}(x) \ge 0,\ i = 1, ..., m\}, \tag{3.3}$$

and the trust-region subproblem (3.2) is then solved. As a linear programming problem, the trust-region subproblem is solved in the following way. Solving sequentially the problems (3.2) by replacing the trust-region radius Δ_k by a constant continuously evolving from 0 to Δ_k would generate a continuous piecewise linear path from x_k to the solution of the subproblem. The strategy of COBYLA is to compute this path, by updating the active sets of the constraint models. However, the trust-region condition (3.2b) and the region (3.3) may contradict each others, in which case the trial point is chosen to solve approximately

$$\begin{aligned} \max_{x \in \mathrm{R}^n} \quad & \min_{i=1,2,\dots,m} \widehat{c}_{i,k}(x) \\ \text{s.t.} \quad & \|x - x_k\| \le \Delta_k. \end{aligned}$$

In doing so, the method attempts to reduce some violation of the constraint models while ensuring that the trial point lies in the trust region, as it is needed by most global convergence properties.

3.2 UOBYQA

Later on, in 2002, Powell developed UOBYQA [58], named after "unconstrained optimization by quadratic approximation". It aims at solving the nonlinear optimization problem (2.1) in the unconstrained case, i.e., when $\Omega = \mathrm{R}^n$. To do so, at each iteration, it models the objective function with a quadratic of the form (3.6), obtained by fully-determined interpolation on the set $\mathcal{Y}_k$ containing $N = (n+1)(n+2)/2$ points. The set $\mathcal{Y}_{k+1}$ differs from $\mathcal{Y}_k$ of at most one point. During a classical iteration, a trial point, i.e., an approximate solution of the trust-region subproblem (3.2) replaces an interpolation of $\mathcal{Y}_k$. As we already mentioned, it is essential to maintain some geometrical properties of $\mathcal{Y}_k$ to ensure the existence and the uniqueness of the models from a computational viewpoint. Hence, UOBYQA may undertake geometry-improvement steps whenever the models seem not to be accurate, led a remarkable result pointed out in [57]. It states that given a point $\bar{y} \in \mathcal{Y}_k$ to remove from the interpolation set, its most suitable substitute to build $\mathcal{Y}_{k+1}$ solves the subproblem

$$\begin{aligned} \max_{x \in \mathrm{R}^n} \quad & |\ell_{\bar{y}}(x)| \\ \text{s.t.} \quad & \|x - x_k\| \le \Delta_k, \end{aligned} \tag{3.4}$$

where $\ell_{\bar{y}} \colon \mathrm{R}^n \to \mathrm{R}$ denotes the Lagrange function associated with $\bar{y}$, defined by $\ell_{\bar{y}}(y) = \delta_{\bar{y},y}$ for each $y \in \mathcal{Y}_k$, where $\delta_{\bar{y},y}$ is the Kronecker delta. Since UOBYQA requires only a rough solution of the geometry-improvement subproblem (3.4), Powell developed an algorithm that requires only $\mathcal{O}(n^2)$ operations, based on an estimation of $|\ell_{\bar{y}}(\cdot)|$. Once such a point is calculated, the solver continues with a classical trust-region step, and the subproblem (3.2) is solved with the Moré-Sorensen algorithm [46], as it controls the accuracy of the solution.

3.3 NEWUOA, BOBYQA, and LINCOA

The major flaw of UOBYQA is the amount of required interpolation points, which can become prohibitively huge when n increases. Therefore, Powell designed a mechanism to define quadratic models of the form (3.6) that requires fewer interpolation points [59]. Given the set $\mathcal{Y}_k$, containing typically $\mathcal{O}(n)$ points (the default value $2n+1$ being recommended), the model $\widehat{f}_k$ is the quadratic satisfying the interpolation conditions whose Hessian's update is least in Frobenius norm, that is

$$
\begin{aligned}
\widehat{f}_k \stackrel{\text{def}}{=} \operatorname*{arg\,min}_{Q \in \mathcal{P}_{n,2}} \quad & \|\nabla^2 Q - \nabla^2 \widehat{f}_{k-1}\|_{\mathsf{F}} \\
\text{s.t.} \quad & Q(y) = f(y), \quad y \in \mathcal{Y}_k,
\end{aligned}
\tag{3.5}
$$

where $\mathcal{P}_{n,d}$ is the space of n-variate polynomials of degree at most d and $\nabla^2 \widehat{f}_{-1}$ is set to be zero. If the number of interpolation points was less than or equal to $n+1$, the models would remain linear, so that Powell requires the number of points in $\mathcal{Y}_k$ to be at least $n+2$ and at most $(n+1)(n+2)/2$. As we mentioned earlier, the choice of the variational problem (3.5) is fostered by the fact that it occurs in the quasi-Newton update for unconstrained optimization when the first derivative of the objective function is available [26, §3.6]. As in the fully-determined case, the geometry of the interpolation set plays a crucial role, as it influences the accuracy of the quadratic models, and the geometry-improvement steps (3.4) should be also entertained.

The last three DFO solvers of Powell are NEWUOA [61, 62], BOBYQA [63], and LINCOA [64]. BOBYQA and LINCOA are named respectively after "bound optimization by quadratic approximation" and "linearly-constrained optimization algorithm", but the meaning of the acronym NEWUOA is not known (even though most people agree on "new unconstrained optimization algorithm"). Powell never published a paper introducing LINCOA, and [64] discusses only the resolution of its trust-region subproblem. As their names suggest, they aim at solving unconstrained, bound-constrained and linearly-constrained problems respectively, using quadratic models of the objective function of the form (3.6). All three use the underdetermined interpolation technique described above to build the quadratic models, so that NEWUOA is more suitable than UOBYQA for solving problems with a relatively high dimension. They all set Ω_k in the trust-region subproblem (3.2) to be Ω, corresponding the whole space for NEWUOA, a box for BOBYQA and a polyhedron for LINCOA. A subtlety of BOBYQA is that the constraints are always respected, for each iterate and each point in $\mathcal{Y}_k$. Therefore, the geometry-improvement subproblem (3.4) should be adapted to incorporate the bound constraints, which makes its resolution more difficult. Moreover, as we already mentioned, at most one point of the interpolation set is altered at each iteration, which leads to an at-most rank-2 update of the Karush-Kuhn-Tucker (KKT) matrix of the variational problem (3.5). This remark suggests that it can be much more efficient to update such KKT matrix instead of computing it from scratch at each iteration. Powell derived an updating formula in [60] that requires only $\mathcal{O}(N^2)$ operations instead of $\mathcal{O}(N^3)$ if the computation was made from scratch with no loss of accuracy, where N denotes the number of interpolation points. When it comes to solving the trust-region subproblems (3.2), NEWUOA employs the Steihaug-Toint truncated conjugate gradient algorithm [70, 72], and BOBYQA and LINCOA use an active-set variation of it. However, the trust-region subproblem solver of BOBYQA always respects the bounds, while the solver of LINCOA may visit point lying outside of the polyhedron of the constraints, and may even return points that are slightly infeasible.

3.4 Geometry steps

We focus however our attention on polynomial models of the form

$$\widehat{f}_k(x) \stackrel{\text{def}}{=} g_k^\mathsf{T}(x - x_k) + (x - x_k)^\mathsf{T} B_k(x - x_k), \tag{3.6}$$

with $g_k \in \mathrm{R}^n$ and $B_k \in \mathrm{R}^{n\times n}$ being symmetric and may be zero for linear models, diagonal or general depending on the considered method. Such models admit respectively $n+1$, $2n+1$ and $(n+1)(n+2)/2$ coefficients, determined so that they satisfy the interpolation conditions (3.1). Whenever the models are defined by underdetermined interpolations, the freedom bequeathed by the interpolation conditions is usually taken up by a variational problem whose constraints are the conditions (3.1). Examples of such variational problems are the minimization of the Hessian of the models in Frobenius norm [16, 74], or the minimization of a term involving g_k and B_k in (3.6) [21]. Powell employed another example of such variational problem, namely the symmetric Broyden formula [54, 59], which will be studied later in this paper in Section 3.

4 An interface for the Powell's derivative-free solvers

Powell implemented all five methods in Fortran, in a very robust and efficient manner. However, less and less people are using Fortran in our present-day world, and Fortran has quite old standards. The authors developed therefore PDFO[3], named after "Powell's derivative-free optimization solvers". It is cross-platform package providing MATLAB® and Python interfaces for using all five Powell's DFO solvers, available for Linux, macOS and Windows. PDFO does not reimplement Powell's solvers, but rather links the modern languages MATLAB® and Python with the Fortran source code. At a low-level, it uses F2PY [50] to interface Python with Fortran and MEX to interface it with MATLAB®.

[3] Available at `https://www.pdfo.net/`.

4.1 Main structure of the package

The philosophy of PDFO is simple: providing to users a single function to solve a DFO problem. It takes for input an optimization problem of the form

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

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

$$A_{\mathcal{I}} x \leq b_{\mathcal{I}}, \quad A_{\mathcal{E}} x = b_{\mathcal{E}}, \tag{4.1c}$$

$$c_{\mathcal{I}}(x) \leq 0, \quad c_{\mathcal{E}}(x) = 0, \tag{4.1d}$$

where $l, u \in (\mathrm{R} \cup \{\pm\infty\})^n$, $A_{\mathcal{E}}$ and $A_{\mathcal{I}}$ are real matrices, $b_{\mathcal{E}}$ and $b_{\mathcal{I}}$ are real vectors, and $c_{\mathcal{E}}$ and $c_{\mathcal{I}}$ are multivariate functions. The problem (4.1) covers every possible case, since all matrices, vectors and functions can be set to zero from a mathematical viewpoint and PDFO does not require the constraints (4.1b), (4.1c), and (4.1d) to be provided. A broad example of use in MATLAB® is shown in Listing 1, where variable names have clear correspondances with the problem (4.1). The value returned by PDFO is the best point calculated, evaluated via a merit function. PDFO for MATLAB® also returns the corresponding optimal value, together with different fields describing the backend calculations and their behaviors.

Listing 1: An elementary example of PDFO in MATLAB®.

The package PDFO preprocesses the arguments provided by the user, detects the type of the problem and then invokes the Powell's solver that match the best the given problem. The initial preprocessing of the arguments includes a handling of their internal types together with some programming-related procedures to allow as much freedom in the problem definition as possible, to make the use of PDFO as easy as possible. More importantly, PDFO preprocesses the constraints provided, to generate a problem as simple as possible. For instance, all linear constraints in (4.1c) that are satisfied for every point in R^n are removed and obvious infeasibility in the constraints (4.1b) and (4.1c) are detected. 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, they define a subspace of R^n of lower dimension, and PDFO takes into account this property to generate a new $(n - \operatorname{rank} A_{\mathcal{E}})$-dimensional problem that is exactly equivalent to (4.1), using the QR factorization of $A_{\mathcal{E}}$.

A crucial point of BOBYQA and LINCOA is that they require the initial guess to be feasible, so that PDFO attempts to project the provided initial guess onto the feasible set (LINCOA would otherwise increase the coefficients of the right-hand side of the linear constraints to make the initial guess feasible). Another main feature of PDFO is its solver selection mechanism. When a constrained problem is received, the selected solver is the one corresponding to the most general constraint provided. For example, when PDFO receives a problem that admits both bound constraints (4.1b) and linear constraints (4.1c), LINCOA will be chosen. It is possible on some examples that LINCOA gives better results than BOBYQA on bound-constrained problems. This is likely because BOBYQA is a feasible method, while LINCOA may visit infeasible points (but on an engineering problem, these points may be unassessable). At last, when PDFO receives an unconstrained problem, it will attempt to solve it with UOBYQA when its size is reasonable ($2 \le n \le 8$, say), and with NEWUOA otherwise. We note that UOBYQA cannot handle problem with univariate objective function.

The authors wanted to keep the source code of all solvers in its original states, but introduced some minor revisions and corrections. A new parameter has been added to allow each solver to exit whenever a target value has been reached, and a flag of termination has been included in the returned values. A revision has also been made to the source code of COBYLA. In the original version, trial points may be discarded prematurely, before the update of the penalty coefficient of the merit function. This has been revised in PDFO. The authors also detected some minor bugs on failure exits, for which some returned values might not have been updated. Although very rarely, LINCOA might moreover encounter infinite cycling, even on well-conditioned problems. These bugs have been patched. PDFO also handle more carefully ill-conditioned problems, for which NaN values (resulting, e.g., from a division by zero) may occur. These values might cause infinite cycling or segmentation faults in the original code. In the early stage of PDFO, such errors occurred on the CUTEst problems [30] DANWOODLS or GAUSS1LS for example. NaN values detected in the objective or constraint functions are managed using extreme barriers, but NaN values encountered in the variables internal to the Fortran code result in early exit. Besides, when interfacing Fortran with MATLAB® and Python, rounding errors occur in the problem's variables, which led in extreme cases to failures. For example, when using PDFO, the user may provided initial and final trust-region radii Δ_0 and Δ_∞ (respectively set to 1 and 10^{-6} by default). If these values are chosen to be very close, although the condition $\Delta_0 \le \Delta_\infty$ is satisfied in the MATLAB® or Python code, the Fortran code may receive perturbed values with $\Delta_0 > \Delta_\infty$, leading to failure exit in the original code. Therefore, the conditions required by Powell are ensured in the Fortran code directly.

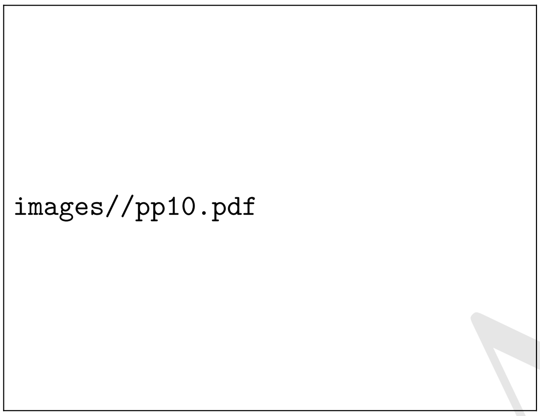
4.2 Some numerical results

4.2.1 Comparison on the CUTEst library

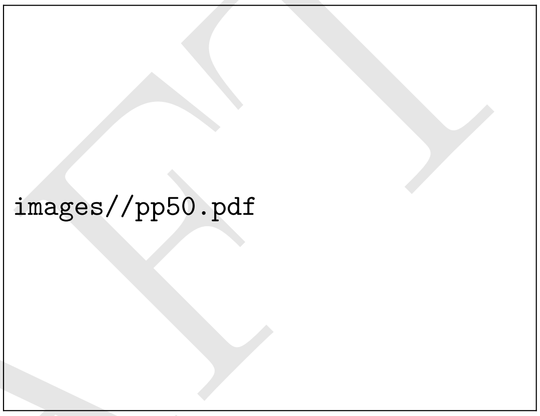
We first make a comparison of the PDFO's solvers on different problems from the CUTEst library [30]. Performance profiles [24, 47] on unconstrained problem of dimensions at most 10 and 50 are provided respectively in Figures 1a and 1b. Broadly speaking, a performance profile plots the proportion of problem solved with respect to the number of function evaluations required to achieve convergence, in logarithmic scale. The optimal value f_* of a given problem is considered to be the least value reached by each solver, and an execution is considered convergent up to a tolerance $\tau \geq 0$ whenever

$$f(x_0) - f(x_k) \geq (1 - \tau)[f(x_0) - f_*]. \tag{4.2}$$

We can observe an expected behavior; UOBYQA performs better on small problems than all the others, as it is based on quadratic models obtained by fully-determined interpolation, and the performances of COBYLA decrease with the dimension rise, as it uses only linear models to approximate locally the problem.



(a) Dimension at most 10.



(b) Dimension at most 10.

Figure 1: Performance profile on unconstrained problems with a precision $\tau = 10^{-4}$.

Consider however the following experiment. Given a smooth objective function f, assume that the value received by the solvers is

$$F_\sigma(x) = [1 + \sigma e(x)]f(x),$$

where $e(x)$ is a random variable that follows a standard normal distribution $\mathcal{N}(0, 1)$, and $\sigma \geq 0$ is a given noise level. Figure 2 presents the performance profiles on the same unconstrained problems of dimension at most 50 from the CUTEst library as the previous experiment by randomizing the objective functions as F_σ with $\sigma = 10^{-2}$. Because of the stochastic behavior of the experiment, the convergence test (4.2) needs to be adapted. Each problem is solved 10 times by each solver, the objective value considered at each iteration is the average value for all runs, and the optimal value f_* of a given problem is decided as follows. It is the least value reached by the solvers for every run on the noised variation of the problem and by all the solvers on the noise-free original problem. In doing so, one should expect a decrease of the proportion of problems solved when compared with the previous experiment.

images//pp50-noisy.pdf

Figure 2: Performance profile on noised variations of unconstrained problems of dimension at most 50 with a precision $\tau = 10^{-1}$.

We observe however a peculiar behavior of COBYLA on this experiment, as it defeats all other solvers on unconstrained problems even though it is not defined for such kind of problem, and uses the simplest models. It seems that the linear models of COBYLA are, in some sense, less sensitive to Gaussian noise, but the authors did not derive a theory for this behavior as of today.

4.2.2 An example of hyperparameter tuning problem

We consider now the more practical problem of the hyperparameter tuning of a support vector machine (SVM). The model we consider is a C-SVM [13] for binary classification problems with an RBF kernel, admitting two hyperparameters: a regularization parameter $C > 0$ and a kernel parameter $\gamma > 0$. We want to compare the performance of PDFO with a prominent Bayesian optimization method and random search (RS). To this end, we use the Python package `hyperopt` [9] for solving the optimization problems, which provides both tree of Parzen estimators (TPE) and RS methods. Our experiments are based on binary classifications problems from the LIBSVM datasets[4]. A description of the datasets employed is provided in Table 1.

The problem we consider is as follows. A dataset $\mathcal{P} \subseteq [-1, 1]^d$ from Table 1 is randomly split into a training dataset $\mathcal{L}$, admitting approximately 70% of the data, and a testing dataset $\mathcal{T}$, with $\mathcal{P} = \mathcal{L} \cup \mathcal{T}$. We want to maximize the 5-fold area under the curve (AUC) validation score of the SVM trained on $\mathcal{L}$ with respect to the hyperparameters C and γ. The AUC score, a real number in $[0, 1]$, measures the area underneath the receiver operating characteristic (ROC) curve, a graph representing the performance of a binary classification model. This curve plots the true positive classification rate with respect

[4] Available at `https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/`.

Table 1: Considered LIBSVM datasets description

Dataset $\mathcal{P}$	Attribute characteristic	Dimension d	Dataset size
splice	$[-1, 1]$, scaled	60	1000
svmguide1	$[-1, 1]$, scaled	4	3088
svmguide3	$[-1, 1]$, scaled	21	1242
ijcnn1	$[-1, 1]$	22	49 990

to the false positive classification rate at different classification thresholds. The 5-fold AUC validation score corresponds to the following. The set $\mathcal{L}$ is split into 5 folds, and the model is trained 5 times, on each union of 4 distinct folds. After each training, the AUC score is calculated on the last fold, which was not involved in the training process, giving rise to 5 AUC scores, the average of which corresponds to the 5-fold AUC validation score. It is then clear that such an experiment lies in the DFO context.

The numerical results for this experiment are provided in Appendix A. The AUC scores and accuracies presented in the tables correspond to the ones computed on $\mathcal{T}$ with an SVM trained on $\mathcal{L}$, with the tuned parameters C and γ. In a nutshell, it globally shows that the numerical performances of PDFO against the two classical approaches are very similar, but the computations requires much fewer AUC evaluations, and hence, much less computation time. This behavior is particularly visible on the dataset "ijcnn1" in Table 5, as the size of this dataset is much larger than the others. Thus, we can conclude that PDFO performed better than the package `hyperopt` on these problems, even though the final numerical results are mostly similar.

5 Conclusions

We have presented the package PDFO for MATLAB® and Python, which aims at simplifying the use of the Powell's DFO solvers. A more complete presentation of the package itself can be found on the PDFO website, together with different examples of use. The scope of PDFO in the future is not limited only to the Powell's DFO solvers. The authors are currently working on a new solver for nonlinearly-constrained optimization, which is aimed to be added to PDFO, and other DFO solvers may be included in the future to PDFO.

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A Hyperparameter tuning experiment results

Table 2: Hyperparameter tuning problem on the dataset "splice".

Solver	No. evaluations	AUC Score (10^{-1})	Accuracy (10^{-1})	Execution time (s)
PDFO	65	9.568	9.933	3.697
RS	100	6.409	5.300	4.635
RS	200	7.880	5.300	9.244
RS	300	7.880	5.300	13.763
TPE	100	5.000	5.033	4.889
TPE	300	7.736	5.300	15.726

Table 3: Hyperparameter tuning problem on the dataset "svmguide1".

Solver	No. evaluations	AUC Score (10^{-1})	Accuracy (10^{-1})	Execution time (s)
PDFO	68	9.966	9.730	4.906
RS	100	9.966	9.676	16.178
RS	200	9.966	9.676	32.914
RS	300	9.966	9.676	48.404
TPE	100	9.966	9.720	13.057
TPE	300	9.966	9.720	33.392

Table 4: Hyperparameter tuning problem on the dataset "svmguide3".

Solver	No. evaluations	AUC Score (10^{-1})	Accuracy (10^{-1})	Execution time (s)
PDFO	68	8.241	8.016	2.793
RS	100	8.025	7.882	4.233
RS	200	8.141	7.775	8.308
RS	300	8.141	7.775	12.414
TPE	100	7.774	7.453	4.197
TPE	300	8.106	7.989	12.912

Table 5: Hyperparameter tuning problem on the dataset "ijcnn1".

Solver	No. evaluations	AUC Score (10^{-1})	Accuracy (10^{-1})	Execution time (10^3s)
PDFO	59	9.940	9.819	1.892
RS	100	9.886	9.773	4.435
RS	200	9.886	9.773	9.146
RS	300	9.886	9.773	13.251
TPE	100	9.891	9.791	4.426
TPE	300	9.896	9.786	12.552

B Fake section

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