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A note on using performance and data profiles for training algorithms

M. Porcelli* and Ph. L. Toint†

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Abstract

It is shown how to use the performance and data profile benchmarking tools to improve algorithms' performance. An illustration for the BFO derivative-free optimizer suggests that the obtained gains are potentially significant.

Keywords: algorithmic design, algorithms' training, trainable codes, derivative-free optimization.

Mathematics Subject Classification: 65K05, 90C56, 90C90.

1 Introduction

Making algorithms efficient and reliable is obviously desirable for both their designers and their users. Since most algorithms involve parameters, it is therefore important to choose them well. In an attempt to do so, the authors [9] proposed BFO, a derivative-free optimization algorithm which is trainable, in the sense that it contains an internal procedure to select its algorithmic parameters to improve algorithmic performance, both from the point of view of the designer (using a large collection of diverse benchmarking cases) and of the user (focusing on a possibly more specific class of applications). Moreover BFO is also designed so that it can be used to train other codes. Obviously, improving performance requires a workable definition of this concept. As in [9], we assume that performance of an algorithm on a given problem can be measured by a number and that better performance corresponds to smaller such numbers. To make things concrete, and since we will be concerned below with derivative-free optimization, we shall consider from now on that performance is given by the number of objective function evaluations required by a solver to solve a given optimization problem¹ Given a vector of algorithmic parameters q and a collection of benchmarking problems \mathcal{P} , algorithmic performance was then measured using one of two classical techniques. The first is the 'average' performance over all test problems, the second, inspired by robust optimization, is the average of the worst performance obtained for a slight variation of q . In the first case, one then attempts to improve algorithmic performance by approximately minimizing the *average training function* [3, 1, 2]

$$\min_q \phi_{\mathcal{P}}^A(q) \tag{1}$$

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¹In other contexts, possible measures involve error on the result, computing time, memory usage, etc.

where $\phi_{\mathcal{P}}^A(q)$ counts the total number of evaluations of the problem objective function to solve all the problems in \mathcal{P} . In the second case, improvement is sought by approximately minimizing the *robust training function*

$$\min_q \phi_{\mathcal{P}}^R(q) \quad \text{where} \quad \phi_{\mathcal{P}}^R(q) \stackrel{\text{def}}{=} \max_{\hat{q} \in \mathcal{B}(q)} \phi_{\mathcal{P}}^A(\hat{q}) \quad (2)$$

with $\mathcal{B}(q)$ being a local box centered at q allowing perturbations of each algorithmic parameter. In both cases, the minimization of the training function also typically involves bound constraints on the admissible range of each algorithmic parameter. It was shown in [9] that an approximate local minimization of either of these training functions can bring substantial improvements in efficiency and reliability. The final comparison (and that with other derivative-free approaches) was then reported using the now widely accepted performance and data profile techniques (see [5] for the first and [8] for the second).

The purpose of the present short note is to explain how it is possible to use these two latter benchmarking measures directly for training, instead of merely for comparison. As in [9], we focus on the BFO derivative-free solver because it directly implements the relevant tools, but we stress that the approach is not limited to this particular case.

The paper is organized as follows. We first briefly recall, in Section 2, the definition of performance and data profiles given in [5, 8] and then derive the new training measures and associated training procedures in Section 3. A numerical illustration is reported in Section 4.

2 Performance and data profiles

Let \mathcal{S} be a set of solvers (or solver variants) and let \mathcal{P} be a set of benchmarking problems of cardinality $|\mathcal{P}|$. *Performance profiles* are defined in terms of a performance measure $t_{p,s} > 0$ obtained for each $p \in \mathcal{P}$ and $s \in \mathcal{S}$. As above, we will consider here that $t_{p,s} > 0$ is the number of function evaluations required to satisfy a user-defined convergence test. For each $p \in \mathcal{P}$, let $\hat{t}_{p,s} = \min_{s \in \mathcal{S}} t_{p,s}$ and define $r_{p,s} = t_{p,s}/\hat{t}_{p,s}$ to be the performance ratio, so that the best solver s for a particular problem p attains the lower bound $r_{p,s} = 1$. We set $r_{p,s} = \infty$ when solver s fails to satisfy the convergence test on problem p . For $\tau \geq 1$, each solver $s \in \mathcal{S}$ and each problem $p \in \mathcal{P}$, one then defines

$$k(r_{p,s}, \tau) = \begin{cases} 1 & \text{if } r_{p,s} \leq \tau, \\ 0 & \text{otherwise.} \end{cases}$$

The performance profile for solver s is then given by the function

$$p_s(\tau) = \frac{1}{|\mathcal{P}|} \sum_{p \in \mathcal{P}} k(r_{p,s}, \tau), \quad \tau \geq 1.$$

By definition of $t_{p,s}$, $p_s(1)$ is the fraction of problems for which solver s performs the best, $p_s(2)$ gives the fraction of problems for which the solver's performance is within a factor of 2 of the best, and that for τ sufficiently large, $p_s(\tau)$ is the fraction of problems solved by s . More generally, $p_s(\tau)$ can be interpreted as the probability for solver $s \in \mathcal{S}$ that the performance ratio $r_{p,s}$ is within a factor τ of the best possible ratio. Therefore, $p_s(1)$ measures efficiency of the solver while its robustness (high probability of success on the set \mathcal{P}) is measured in terms of $p_s(\infty)$. A key feature of performance profiles is that they give information on the *relative* performance of several solvers [4, 8], which therefore strongly depends of the considered set \mathcal{S} of competing solvers or algorithmic variants [7].

In order to provide a benchmarking tool that gives the behaviour of a solver independently of the other solvers in \mathcal{S} , Moré and Wild [8] proposed the *data profile* measure motivated by

the user interest in the percentage of problems that can be solved with a certain computational “budget”. For $\nu > 0$ and each $s \in \mathcal{S}, p \in \mathcal{P}$, one defines

$$g(t_{p,s}, \tau) = \begin{cases} 1 & \text{if } t_{p,s} \leq \nu(n_p + 1), \\ 0 & \text{otherwise,} \end{cases}$$

where n_p is the number of variables in $p \in \mathcal{P}$. The scaling by $n_p + 1$ is intended to consider the computational budget as in “simplex gradient” evaluations, rather than directly in function evaluations. The data profile for solver $s \in \mathcal{S}$ is then given by

$$d_s(\nu) = \frac{1}{|\mathcal{P}|} \sum_{p \in \mathcal{P}} g(t_{p,s}, \nu), \quad \nu > 0,$$

and measures the percentage of problems that can be solved with ν “simplex gradient” evaluations.

3 New training measures and how to use them

We observe that, by definition, the plots of the performance and data profiles are staircase graphs and that, by the above discussion, the higher the curve corresponding to a solver, the better is its performance. This trivial observation suggests two new training strategies that simply consists in finding the parameter configuration that maximize the area under the staircase graph generated by the performance or data profiles, respectively.

Let \mathcal{Q} be the set of acceptable algorithmic parameters, $q \in \mathcal{Q}$ be a parameter configuration and let s_q be the solver variant with parameter configuration q . Consider data profiles first. We can define for each $q \in \mathcal{Q}$ the *data profile training function*

$$\phi_{\mathcal{P}}^D(q) \stackrel{\text{def}}{=} \int_{\nu_{\min}}^{\nu_{\max}} d_{s_q}(\nu) d\nu,$$

where $0 \leq \nu_{\min} < \nu_{\max}$ are user-specified values identifying a ‘range of computational budgets’ of interest, and then consider the corresponding data profile training problem

$$\max_{s \in \mathcal{Q}} \phi_{\mathcal{P}}^D(q). \tag{3}$$

The analogous problem for performance profiles is less obvious since, as discussed above, the computation of $p_{s_q}(\tau)$ depends on the behaviour of more than one solver, that is, in our case, on the performance of the trained solver with respect to different values of its algorithmic parameters q . We therefore propose to proceed sequentially from an initial parameter configuration indexed by $i = 0$ and to evaluate the performance for a particular q by always comparing it to that obtained for q_0 . Given the profile window $[\tau_{\min}, \tau_{\max}]$ for some $1 \leq \tau_{\min} < \tau_{\max}$ and the initial algorithmic configuration $q_0 \in \mathcal{Q}$, we define the *performance profile training function* $\phi_{\mathcal{P}}^P$ by

$$\phi_{\mathcal{P}}^P(q) \stackrel{\text{def}}{=} \int_{\tau_{\min}}^{\tau_{\max}} [p_{s_q}(\tau) - p_{s_{q_0}}(\tau)] d\tau. \tag{4}$$

Training then corresponds to solving (possibly very approximately) the performance profile training problem

$$\max_{q \in \mathcal{Q}} \phi_{\mathcal{P}}^P(q). \tag{5}$$

In order to evaluate $\phi_{\mathcal{P}}^P$ and $\phi_{\mathcal{P}}^D$ in (3)-(5) respectively, one has to provide enough information to compute the profiles $p_s(\tau)$ and $d_s(\nu)$ during the training optimization process.

Let $q \in \mathcal{Q}$ be a parameter configuration and let s_q be the (BFO) algorithmic variant using parameters q . Let the profiles windows $[\tau_{min}, \tau_{max}]$ and $[\nu_{min}, \nu_{max}]$ be given. We compare different parameter configurations declaring that the problem p with objective function f_p is solved by the variant s_q as soon as it produces an approximate solution x_q such that

$$f_p(x_q) \leq f_p^* + \chi(f_p(\bar{x}) - f_p^*) \stackrel{\text{def}}{=} c_p \quad (6)$$

where \bar{x} is the starting point for the problem p , f_p^* is an approximation of the smallest obtainable value of f_p and $\chi \in [0, 1]$ is a tolerance. The test (6) therefore compares the function value reduction $f(\bar{x}) - f(x_q)$ achieved by x_q relative to the best possible reduction $f(\bar{x}) - f^*$ [8]. We say that c_p , as defined in (6), is the *cut-off value* for problem p .

Given an initial parameter configuration q_0 , a starting point \bar{x} and a tolerance $\chi > 0$, the training strategy proceed as follows. First, starting from \bar{x} , the solver variant s_{q_0} is run over the set \mathcal{P} with high accuracy in order to evaluate the best objective found f_p^* for each $p \in \mathcal{P}$ and the resulting cut-off value c_p . Then, the number of function evaluations needed to the solver variant s_{q_0} to reach c_p , that is the value $t_{p,s_{q_0}}$, is retrieved. If data-profile training is considered, this enough to compute the corresponding value of the objective $\phi_{\mathcal{P}}^D(q_0)$. The initial objective function value for performance-profile training is initialized to zero (see (4)). Optimizing the relevant objective function (i.e. (3) or (5)) can then be conducted (using BFO with its default parameters and its standard termination test in our case), in the course of which the solver variant is run again with better and better values of the algorithmic parameters q , the performance measures t_{p,s_q} being always computed with respect to the initial cut-off value c_p .

4 Numerical illustration

We now illustrate the above proposals by reporting some results obtained when training the BFO derivative-free optimization package by modifying its internal algorithmic parameters.

4.1 Experimental setup

The inner details of the BFO method are of little interest here (we refer the interested reader to [9] for a full description). It is enough for our present purposes to describe it as a direct-search optimizer evaluating the relevant objective function at points on a randomly oriented variable meshsize grid (in a process called the poll-step) and accepting an improved function value whenever it satisfies a 'sufficient decrease' condition relative to the current grid meshsize. So-called 'inertia direction' are also computed using a number of past iterates and are privileged when constructing the grid. The minimization is terminated when the grid meshsize becomes smaller than a user-supplied threshold ϵ . The BFO algorithmic parameters considered for training in our present experiments are presented in Table 1.

We define \mathcal{P} to be the set of benchmarking problems used in [9] and consisting in 55 bound-constrained problems with continuous variables of small dimensions extracted from the CUTEst library [6]. The list of problem names with their dimension is given in Table 2. The solution of each test problem is attempted setting $\epsilon = 10^{-12}$ in the BFO convergence test and allowing 10000 function evaluations at most.

Starting from the initial parameter configuration q_0 in Table 3, the four optimization problems (1)-(2)-(3)-(5) are approximately solved imposing bound constraints on the parameters with bounds l and u reported in Table 3. The local box $\mathcal{B}(q)$ in (2) is defined for continuous parameters

Parameters	Type	Description
α	c	The grid expansion factor
β	c	The grid shrinking factor
γ	c	The maximum grid expansion factor
δ	c	The initial stepsize vector
η	c	The sufficient decrease fraction in the poll step
inertia	i	The number of iterations for the inertia direction

Table 1: BFO parameters selected for training.

Name	n	Name	n	Name	n	Name	n	Name	n
ALLINIT	4	HADAMALS	4	HS38	4	MDHOLE	2	PENTDI	5
BDEXP	10	HARKERP2	10	HS3	2	NCVXBQP1	10	POWELLBC	6
BIGGSB1	10	HART6	6	HS3MOD	2	NCVXBQP2	10	PROBPENL	10
CAMEL6	2	HATFLDA	4	HS45	5	NCVXBQP3	10	PSPDOC	4
CHARDIS0	10	HATFLDB	4	HS4	2	NONSCOMP	10	QUDLIN	12
CHEBYQAD	4	HATFLDC	9	HS5	2	OSLBQP	8	S368	8
CVXBQP1	10	HIMMELP1	2	KOEBHEL	4	PALMER1A	6	SIMBQP	2
EG1	3	HS110	10	LINVERSE	9	PALMER2B	4	SINEALI	4
EXPLIN	12	HS1	2	LOGROS	2	PALMER3E	8	SPECAN	9
EXPLIN2	12	HS25	3	MAXLIKA	8	PALMER4A	6	WEEDS	3
EXPQUAD	12	HS2	2	MCCORMCK	10	PALMER4	4	YFIT	3

Table 2: The benchmark problem set \mathcal{P} : name and dimension n .

as the Cartesian product of the intervals $[0.95q, 1.05q]$ for continuous parameters and $\{q\}$ for discrete ones, allowing perturbations of each continuous algorithmic parameter by at most 5%.

	α	β	γ	δ	η	inertia
q_0	1.5	1/3	5	1	10^{-1}	10
l	1	0.01	1	0.25	10^{-4}	5
u	2	0.95	10	10	0.5	30

Table 3: Starting parameter configuration q_0 and lower/upper bounds in the training optimization problems.

As in [9], we set the BFO termination threshold $\epsilon = 10^{-2}$ when solving the training minimization problems (1)-(2)-(3)-(5), and $\epsilon = 10^{-1}$ for the approximate solution of the inner minimization problem in (2). We also set an upper bound of 200 parameter configuration trials. Finally, the cut-of values used for data and performance profile strategies are obtained by solving each problem with $\epsilon = 10^{-12}$ and default parameters given in Table 3 and the training is run using $\chi = 10^{-4}$ in (6). Experiments were carried out using Matlab R2016b on Intel Core i7 CPU 920 @ 2.67GHz x 8 12GB RAM.

Even if the training process using approximate minimizations of the relevant objective function guarantees improvements on the initial guess q_0 , it is important to remember that there is absolutely no guarantee of reaching a local solution of the training problem, not to mention a global one.

4.2 Results

We report in Table 4 the values of the trained BFO parameters obtained using the four training strategies. Values of parameters using the profile training strategies are obtained setting the profile windows $[\nu_{\min}, \nu_{\max}] = [0, 2000]$ and $[\tau_{\min}, \tau_{\max}] = [1, 20]$, for the objectives in (3) and

(5), respectively. Table 4 also reports the gain (in percentage and as measured with the relevant objective function) in the number of problem function evaluations achieved by the training process.

	α	β	γ	δ	η	inertia	gain
q_A	1.2	1/3	9.7	0.25	10^{-4}	10	17%
q_R	2	0.25	8.5	0.25	10^{-4}	10	7%
q_P	1.5	1/3	5.9	1	10^{-4}	11	1%
q_D	1.6	0.32	4.8	0.25	10^{-4}	11	7%

Table 4: Values of the trained parameters using different training strategies.

These results show that potentially large gains in average number of function evaluations may be obtained by training with the average strategy (and to a lesser extent with the robust strategy), which is coherent with the findings of [9]. Of course, this says little about the distribution of these improvements across test problems, as is suggested by the fact that the improvements are more modest in terms of performance and data profiles.

Figure 1 shows that, despite the lack of guarantee of global optimality, BFO with q_P gives the best performance in terms of performance profile, while BFO with q_D is best in terms of data profiles. Figure 2 indicates that the performance improvements are also clear when using performance or data profiles, and thus, unsurprisingly, that the measure of improvement reported in Table 4 for these strategies might be misleading.

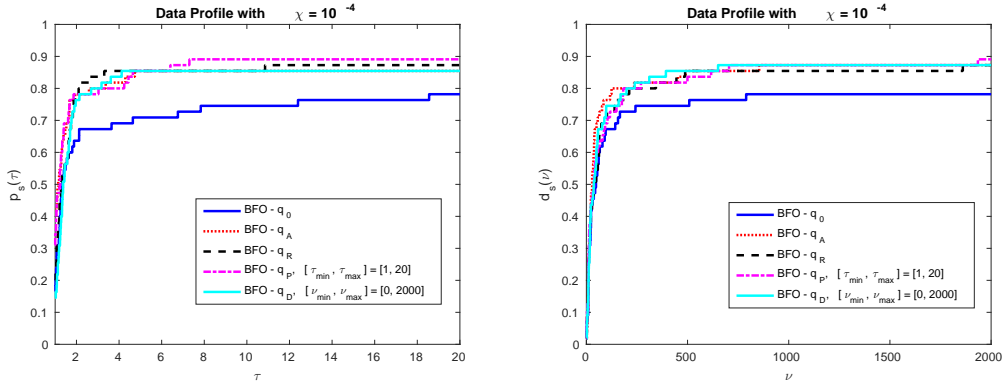


Figure 1: Performance (left) and data (right) profiles for BFO with different algorithmic parameters. Parameters q_P and q_D are trained in the intervals $[1, 20]$ and $[0, 2000]$, respectively.

We now focus on the behaviour of BFO trained by the new profile strategies and discuss the effect on performance of varying the training windows. From the definitions, we would expect a profile window with small values (i.e. τ_{\max} relatively modest) to boost performance, while a window with larger values (substantial τ_{\min}) to result in better reliability. Because the performance profile result shows little room for improvement either in efficiency or reliability (as shown by Figure 2), we illustrate these effects (and their limits) with using data-profile training.

We therefore repeated the training using the data-profile objective function (3) from the same initial parameter configuration q_0 , but using windows $[0, 300]$ and $[1500, 2000]$ instead of $[0, 2000]$. The resulting profiles are presented in Figures 3 and 4. While the expected improvement in efficiency using $[0, 300]$ is clearly visible in the first of these figures, the second shows that the procedure fails to produce an improved reliability when using the window $[1500, 2000]$, illustrating

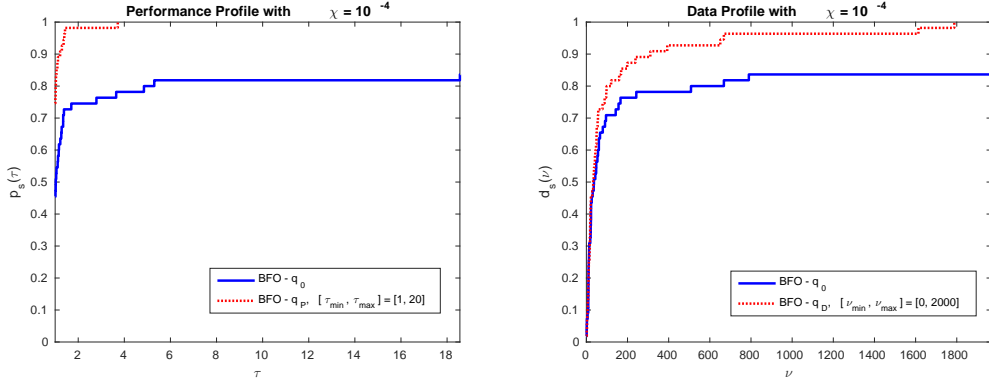


Figure 2: Performance profile for BFO with default parameters q_0 against BFO with q_P (left), and data profiles of BFO with default parameters q_0 against BFO with parameters q_D (right). Parameters q_P and q_D are trained in the default intervals $[1, 20]$ and $[0, 2000]$, respectively.

that approximately and locally minimizing the training function ($\phi_{\mathcal{P}}^D$ in this case) does indeed sometimes produce sub-optimal solutions.

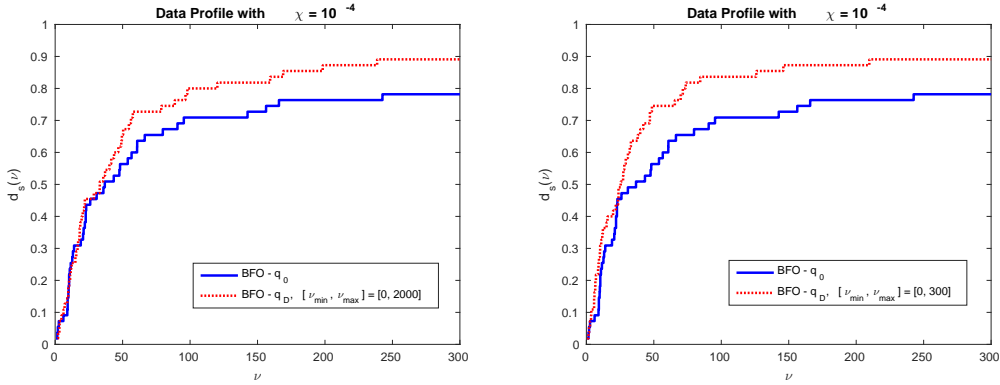


Figure 3: Zoom in the interval $[0, 300]$ of the data profiles obtained using BFO with q_0 and q_D trained in the default interval $[0, 2000]$ (left) and in the reduced interval $[0, 300]$ (right).

5 Conclusion

We have suggested how performance profiles and data profiles can be used to train algorithms and have illustrated our proposal by an application to the BFO package for derivative-free optimization. As expected, the results obtained show that significant gains in performance are possible but not guaranteed. The potential for improvement however suggests that the (careful) use of the proposed techniques is a useful tool in algorithmic design.

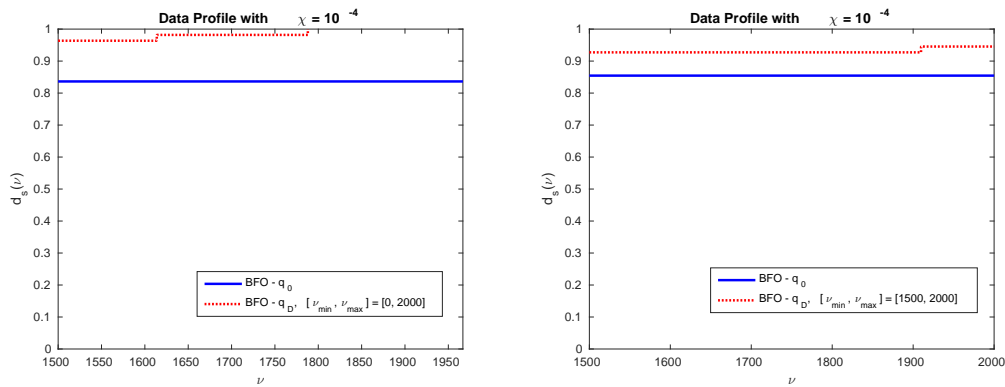


Figure 4: Zoom in the interval $[1500, 2000]$ of the data profiles obtained using BFO with q_0 and q_D trained in the default interval $[0, 2000]$ (left) and in the reduced interval $[1500, 2000]$ (right).

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