Black-Box Optimization for Machine Learning: the Scale and the Chaining

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Abstract

Inspired by observations in neuro-control and various reproducibility issues in machine learning black-box optimization papers, we analyze the effect of scaling in black-box optimization with discrete and with continuous decision variables, where scale refers to the unknown distance from the origin to the optimum. In particular, we (i) propose new artificial benchmarks including properties observed in the real world and in particular in neural reinforcement learning (ii) observe the good performance of quasi-opposite sampling and of particle-swarm optimization in some problems for which the scale is critical (iii) observe a robust performance of discrete optimization methods focusing on an optimized decreasing schedule of the mutation scale (iv) design more efficient black-box optimization algorithms that combine, sequentially, optimization algorithms with good scaling properties in a first phase, then robust optimization algorithms for the middle phase, followed by fast convergence techniques for the final optimization phase. All methods are included in a public optimization wizard.

1 Introduction

Black-box optimization is the optimization of functions on discrete or continuous domains without any gradient or white-box information. Inspired by the Dagstuhl seminar 23251 *Challenges in Benchmarking Optimization Heuristics* (July 2023), we develop additional benchmarks in a black-box optimization platform, namely Nevergrad, which contains a large family of problems including reinforcement learning, tuning for machine learning, planning and others.

The contributions of this paper are twofold. First, we analyze benchmarks. Following Meunier et al. (2022), we observe that one can significantly modify the results of a benchmark by changing the distribution of the optima, in particular by scaling its variables (e.g., by placing them closer to zero or closer to the boundary of the domain). The distribution of the optima, typically induced by the random shifts used in benchmarking platforms, importantly impacts the experimental results. We therefore include a set of different benchmarks with different scaling, ensuring that the tested algorithms cannot be re-parametrized for each specific benchmark. Likewise, we introduce multi-scale and parametric benchmarks for investigating such scaling issues (Section 3.2.2) with the results described in Section 4.1. We also highlight that real-world benchmarks bring new insights, including elements related to budget pointed out by (Ungredda et al., 2022; Dagstuhl participants, 2023) , and showed by the results in the (non-Nevergrad) real-world cases (Section 6) and in the real-world part of the benchmarking suite of Nevergrad (Section 4.2). The diversity of benchmarks is important for making results transferable to other problems (Section 3.1), so we increase the diversity of the distributions of optima over many benchmarks, with a multi-scale approach, and the diversity of the budget/dimension ratio. In particular, we observe results in these problems with increased diversity of the distribution of the optima similar to those observed in real-world benchmarks.

Second, in Section 3.3, we focus on algorithms which perform well in a context of unknown scale, both in discrete and continuous domains. These contributions are integrated into a state-of-the-art wizard for black-box optimization which improves the state of the art on average on many benchmarks (Section 4 and later).

2 State of the art

Black-box optimization is an important part of AI, with applications, among many others, in reinforcement learning and planning. The scale, in the sense of the distance to the optimum, has been identified as a key issue in many papers. After Rechenberg (1973) focusing on the adaptation of the scale, Rahnamayan et al. (2007) focuses on initializing population-based methods for robustness to the scale in the continuous context, and in the discrete case, Doerr et al. (2019); Einarsson et al. (2019); Doerr et al. (2017); Dang & Lehre (2016) are entirely based on scheduling the scale of mutations. Methods focusing on a fixed schedule are particularly robust in the discrete setting. In particular, our results confirm their robustness compared to adaptive methods such as (Kruisselbrink et al., 2011). In terms of continuous black-box optimization methods, Differential Evolution (DE) (Storn & Price, 1997) and Particle Swarm Optimization (PSO) (Kennedy & Eberhart, 1995) are well-known. Compared to CMA (Hansen & Ostermeier, 2003), their focus on quickly approximating the right scale are compatible with very high dimensional settings, where CMA is mainly robust to conditioning/rotation issues. Bayesian methods (Jones et al., 1998) and methods based on machine learning are another branch of the state-of-the-art: among them, SMAC3 (Lindauer et al., 2022) and HyperOpt (Bergstra et al., 2015) perform particularly well. Cobyla (Powell, 1994) comes from the mathematical programming community, and it frequently performs remarkably well in low budget cases (Raponi et al., 2023). Sequential Quadratic Programming is another well known approach with an excellent local convergence rate. Recently, wizards (inspired by other areas such as (Xu et al., 2008)) have become usual. These tools combine various base algorithms, for being immediately (without tuning) reasonably effective on many benchmarks, independently of noise, parallelism, budget, type of variables, and number of objectives. They typically use a lot of static portfolio choices (Liu et al., 2020; Meunier et al., 2022) and of bet-and-run (Weise et al., 2019). We use chaining more intensively than existing wizards. We note that the best performing method in the BBO challenge (AX-team, 2021) is a wizard termed Squirrel (Awad et al., 2020) combining, among others, DE and SMAC3.

In terms of platforms, many libraries exist (e.g., (Johnson, 1994; FacebookResearch, 2020; Virtanen et al., 2020)). Nevergrad (Rapin & Teytaud, 2018) imports these libraries and others. In terms of benchmarks/applications, the BBO Challenge (AX-team, 2021), Keras (Chollet et al., 2015), Scikit-LearnPedregosa et al. (2011), COCO/BBOB (Hansen et al., 2009a), LSGO (Li et al., 2013), IOH (Doerr et al., 2018), OpenAI Gym (Brockman et al., 2016) are well known. Nevergrad includes them or some of their variants and many others.

3 Experimental Setup

Motivated by recent warnings such as (Kapoor & Narayanan, 2023; Li & Talwalkar, 2019), we first take a moment in Section 3.1 to reflect on reproducibility, before we present selected benchmark suites (Section 3.2) and algorithms (Section 3.3). Concerning the suites and algorithms, we cannot provide here an exhaustive presentation of all methods. Hence, we present the most relevant ones and refer interested readers to (Rapin & Teytaud, 2018). Implemented in Python programming language, the Nevergrad platform can be considered human-readable.

3.1 Reproducibility

Reproducibility matters (López-Ibáñez et al., 2021). All our code is hence available in open access. It is now part of the Nevergrad codebase (Rapin & Teytaud, 2018). A PDF with all experimental results is available at `tinyurl.com/dagstuhloid`. Though our focus is on the *ability to rerun everything*, the entire data are available at `tinyurl.com/bigdagstuhloid`[1]. As these URLs are automatically updated, they might differ thanks to additional work by contributors and re-runs. Upon acceptance of this submission, we will make a "frozen" version of code and data and store them into a permanent storage facilities such as Zenodo. In the same vein, the version of (e.g., Pypi) packages can have an impact, but maybe results which are valid only for a specific version of some packages might not be that valuable. As most platforms, Nevergrad requires

[1]Warning: $>$ 300MB, representing data from more than 20 million runs.

a minimum version number for each package, and not a fixed version number. Our modifications do not change this. Details about reproducibility are mentioned in Appendix A.

3.2 Benchmark Suites (a.k.a. Problem Collections)

We seek to have a diverse set of benchmark suites, covering large ranges of problem settings encountered in practice. This includes, for instance diversity with respect to budget, performance measure, distribution of the optima. Table 1 summarizes the diversity of our benchmarks and their parameters. For each benchmark suite, the detailed setup is described at `github.com/facebookresearch/nevergrad/blob/main/nevergrad/benchmark/experiments.py`.

3.2.1 Budgets

Ungredda et al. (2022); Dagstuhl participants (2023) showed that cases with budget with more than 100 times the dimension might be the exception rather than the norm. In real-world applications, we may even face settings in which the total number of function evaluations may not exceed a fraction of the dimension. We therefore consider a large variety of different scalings of the budget, including cases with budget far lower than the dimension.

3.2.2 Scaling and Distribution of Optima

Throughout the discussion, we assume that the center of the domain is zero. This is not the case in all benchmarks: this is just a simplification for shortening equations, so that we can use $-x$ for symmetries instead of $c - (x - c)$ with c being the center, and $||x||$ instead of $||x - c||$. We observe that scaling is an important issue in benchmarks. Typically in real-world scenarios, we do not know in advance the norm of the optimum. Assuming that the optimum has all coordinates randomly independently drawn with center zero implies that the squared norm of the optimum is, nearly always, close to the sum of variances: this is the case in many artificial benchmarks. Consequently, it reduces the generality of the conclusions.

Different distributions of the optimum: MS-BBOB. MS-BBOB is quite similar to BBOB (Hansen et al., 2009b) or YABBOB (Rapin & Teytaud, 2018). However, MS-BBOB (multi-scale black-box optimization benchmark), has different scales for the distribution of optima. This is done by introducing a scaling factor τ which varies in $\{0.01, 0.1, 1.0, 10.0\}$. This scaling factor is used as a factor for the random drawing of optima. For example, in some benchmarks, Nevergrad uses a normal random variable for choosing the optimum: we multiply this random variable by τ.

Zero-penalization: ZP-MS-BBOB. Many benchmarks, including our benchmarks in MS-BBOB are symmetrical w.r.t. zero. The optimum might be translated, but that translation has zero mean. This special role of the center might imply that the neighborhood of zero provides too much information. Actually, many real-world problems have misleading values close to zero, in particular in control or neuro-control (e.g., for neuro-control the control is just zero if all weights in a layer are zero). Therefore we consider zero-penalized problems, with a heavy penalty for candidates much closer to zero than the optimum. We call this variant ZP-MS-BBOB (zero-penalized MS-BBOB).We note that PSO variants perform quite well in these benchmarks, which coincides with the results described in Raponi et al. (2023).

Real-world benchmarks. "(RW)" means that the benchmark is a real-world problem. Note that the definition of "real-world" is not so simple. We are entirely in silico, and in some cases the model has been simplified. This just means that we consider this as sufficiently real-world for being tagged that way. Our experiments include neuro-control with OpenAI Gym (Brockman et al., 2016), policy optimization with Aquacrop (Raes et al., 2009), PCSE (de Wit, 2021), and hyperparameter tuning with Keras (Chollet et al., 2015) and scikit-learn (Pedregosa et al., 2011).

3.3 Key Algorithms for scaling issues

We highlight here only a few selected approaches. All details and all implementations, of the algorithms discussed here and many more, are available at `github.com/facebookresearch/nevergrad`.

3.3.1 Opposite and quasi-opposite sampling

Rahnamayan et al. (2007) propose to initialize the population in DE as follows: (i) randomly draw half the population as usual and (ii) for each point p in this half population, also add $-p$ (opposite sampling) or $-r \times p$ (quasi-opposite sampling, where r is chosen i.i.d. uniformly at random in the interval $[0, 1]$). A key advantage of the quasi-opposite method is that the resulting population includes points with all norms, which is beneficial for settings with unknown scaling. We use quasi-opposite sampling in DE and PSO, with variants termed QODE, QNDE, SPQODE, LQODE, SODE, QOTPDE, QOPSO, SQOPSO, fully described in Appendix B. We observe good results, overall, for SQOPSO and various quasi-opposite tools (Section 5), in particular in the real-world context (Section 4.2).

3.3.2 Other algorithms focusing on scaling in the continuous case

Cobyla is good when the scale of the optimum is unknown as shown by later results, and quasi-opposite sampling helps DE in the same context. Another solution for guessing the scaling of the optimum is to assume that the scaling of the optimum x for different variables might be similar, i.e., $\log |x_i| \simeq \log |x_j|$ for $i \neq j$. Inspired by this observation, we propose RotatedTwoPointsDE, a variant of DE using a 2-point crossover (Holland, 1975), with the possibility of moving the cut part to other variables. Thus, more precisely, DE typically mixes the ith variable of an individual and the ith variable of another individual and the child

Algorithm 1 Three variants of Carola. MetaModel refers to the MetaModel implementation in (Rapin & Teytaud, 2018), based on quadratic approximations built on the best points so far.

Carola1:	Carola2:	Carola3:
Require: Budget b Apply Cobyla with budget $b/2$. Apply CMA with MetaModel with budget $b/2$ and initial point the best point so far.	**Require:** Budget b ***Fast approximation:*** apply Cobyla with budget $b/3$. ***Robust local search:*** Apply CMA with MetaModel with budget $b/3$ and initial point the best point so far. ***Fast local search:*** Apply SQP (Sequential Quadratic Programming) with initial point the best point so far and budget $b/3$.	**Require:** Budget b, number w of workers Apply w copies of Carola2 in parallel, with budget b/w

gets the result at the ith position. This happens for several indices i, but the ith variable has no impact on the jth variable if $j \neq i$. TwoPointsDE uses the two-points crossover, which has a similar property: the difference with the classical DE is that the impacted variables are in a segment of consecutive variables. Both DE and TwoPointsDE find scales by working somehow separately on variables. RotatedTwoPointsDE can move this segment of consecutive variables, and therefore it might combine the ith variable of an individual and the ith variable of another individual and the child gets the result at the jth position where $j = i + k$ (modulo the number of variables) for some $k \neq 0$. The assumption behind RotatedTwoPointsDE is that the scale is not totally different, at least in terms of order of magnitude, for different variables: we can carry variables from a position to another. GeneticDE, then, uses RotatedTwoPointsDE during 200 candidate generations (for finding the correct scale) before switching to TwoPointsDE. We observe an excellent performance of GeneticDE on some problems, though this requires further investigation as opposed to quasi-opposite sampling which performs very well on most real-world problems, or as opposed to Carola2 and its integration in the NgIoh4 wizard which performs excellently on many benchmarks as discussed later.

3.3.3 The scaling of mutations in the context of discrete optimization

In discrete optimization, the good old $1/d$ mutation consists in randomly mutating each variable with probability $1/d$ in dimension d. Typically, a single variable is mutated; and it rarely includes more than two variables. Some algorithms, in particular after the good results in (Dang & Lehre, 2016), use a fixed random distribution of mutation rates. The adaptation of FastGA (Doerr et al., 2017) in Nevergrad consists in randomly drawing a probability p (instead of using $p = 1/d$) in $[0, \frac{1}{2}]$ (in $[0, 1]$, if the arity is greater than two).

DiscreteLenglerOnePlusOne, inspired by Einarsson et al. (2019), consists in using a schedule. In this case, the probability p decreases during the optimization run. We observe good results for DiscreteLenglerOnePlusOne: for example for the Bonnans benchmark (Bonnans et al., 2023), which is completely different from the functions used for testing and designing DiscreteLenglerOnePlusOne that is mathematically derived on simpler functions. The results are presented in Figure 1. Results of DiscreteLenglerOnePlusOne are also

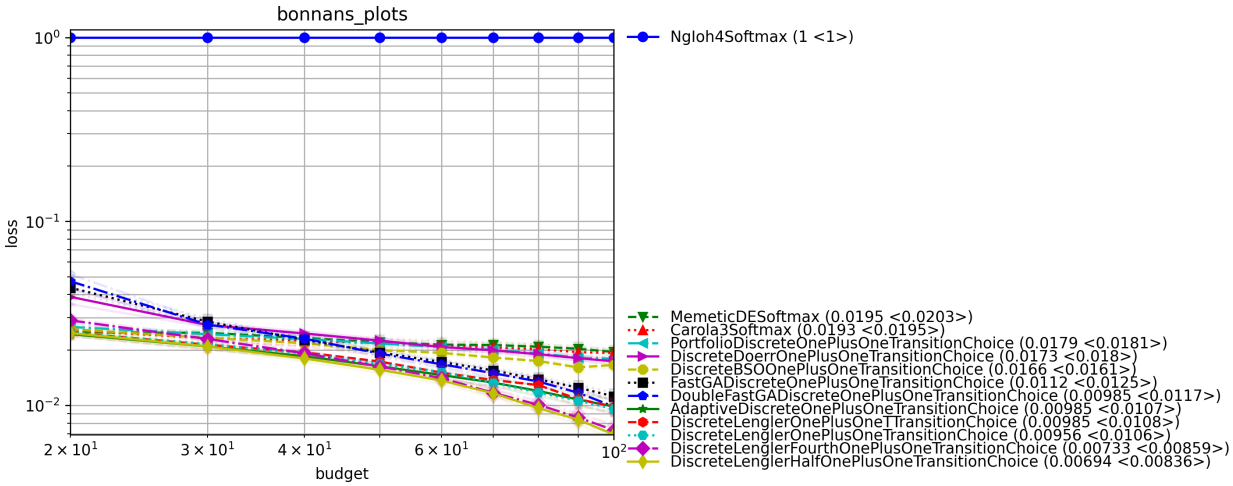

Figure 1: Various methods (only the best 12 ones are presented, and the single worst) on the Bonnans (discrete) function. The Softmax representation (converting the problem to a continuous one as optiinally proposed in (Rapin & Teytaud, 2018)) performs poorly here compared to the standard TransitionChoice. The DiscreteLenglerOnePlusOne method (and its variant with modified parameters, with similar names) performs well on Bonnans functions (Bonnans et al., 2023).

good on InstrumDiscrete, SequentialInstrumDiscrete, and PBOReduced problems. In terms of ablation, most of the variants with perturbed hyperparameters also perform well.

3.3.4 Chaining: Carola algorithms.

From observations on IOH (Doerr et al., 2018), we propose two new principles for the design of black-box optimization wizards. First, whereas it is classical (e.g., Memetic algorithms (Moscato, 1989)) to run evolution strategies first and local methods afterwards (as Nevergrad's NGOpt frequently does), we observe that Cobyla is excellent for low budget. We therefore consider Carola (Cost-effective Asymptotic Randomized Optimization with Limited Access), a method running Cobyla first and then other methods, as presented in Algorithm 1. Second, our insights are gathered in a new black-box optimization wizard, which we dub NgIoh. We demonstrate in this work that this wizard performs well, on average, on many benchmarks. Overall, including the many benchmarks on which NgIoh does not differ too much from NGOpt, NgIoh slightly outperforms the existing wizard NGOpt from Nevergrad, with a clear gap specifically for problems such that the scale of the optimum cannot be known in advance (Section 4.1). We build several variants, which perform similarly. NgIoh4 performs slightly better overall. NgIoh4 is basically the same as NGOpt (Nevergrad's wizard), except that it switches to Carola2 depending on rules that prefer the Carola2 algorithm in case of moderate budget (Algorithm 2). The constants in the rules were chosen based on the observations described in Doerr et al. (2018). We actually tested several variants of NgIoh, all of them performing quite well and being available in Rapin & Teytaud (2018). NgIoh4 is seemingly the best one.

Ablation: Carola3 is an adaptation of Carola2 for the parallel case, so let us focus on the comparison between Carola1, Carola2, and algorithms on which they are based, namely Cobyla, CMA and MetaModel. We observe in Figure 2 better results for Carola2. MetaModel and several CMA variants are absent of the figure because we keep only the 25 best of the 57 tested methods: CMA, OldCMA (before some tuning), LargeCMA (with larger population) and MetaModel (CMA plus the MetaModel, as used as a component of Carola2) are ranked 43, 29, 40 and 33 respectively (vs 3 for Carola2).

Algorithm 2 The NgIoh4 pseudocode, combining NGOpt and ideas extracted from results in IOH(Doerr et al., 2018).

Require: Budget b, dimension d, domain D, number w of workers.
  if $w = 1$ and D is continuous and ($d < 100$ and $20d \leq b \leq 1000d$) or ($d < 50$ and $b < 1000d$). **then**
    Apply Carola2
  else
    Apply NGOpt
  end if

3.4 Performance Criteria

For each benchmark we consider two figures. First, the **Frequency of winning figure.** A heatmap, showing the frequency at which a method (row) outperforms on average another method (column). Averages are computed over all instances and all budgets. Methods are ordered by the average such frequency, over all other methods. The columns show the names of the methods, appended with the number of settings they were able to tackle (for example, some methods have no parallel version and therefore do not run on all settings).

Second, the **Normalized simple regret figure.** A convergence curve, with the budget on the x-axis and the average (over all budgets) normalized (linearly, to $[0, 1]$) loss. Note that some benchmarks do not have the same functions for the different values of the budget. Therefore we might have a rugged curve, not monotonous. This is even more the case for wizards such as NGOpt or NGOptRW which make decisions based on the budget. They might make a bad choice for some values of the budget, leading to irregular curves.

The complete archive (see Appendix A) shows many competence maps. Given the hyperparameters of a benchmark (e.g., dimension, budget, level of noise, among others), the competence maps in the full archive show, for a given pair of hyperparameter values, which algorithms performs the best on average.

4 Selected benchmarks

We cannot include here all benchmarks from the Nevergrad platform, including our additions. We present only some of them. First, multiple scales benchmarks, because we believe that Section 3.2.2 points out an important issue for improving black-box optimization benchmarks. Second, real-world benchmarks, because we need more benchmarks rooted in real-world problems. We refer to the automatically generated `tinyurl.com/dagstuhloid` for further details and Section 5 for an aggregated view of all the results. In Section 6, we present external applications, so that more independent results are included.

4.1 Multi-scale black-box optimization benchmarks: dealing with the scaling issues

In the case of continuous optimization, we present new benchmarks, adapted from YABBOB (Rapin & Teytaud, 2018) using comments from Section 3.2.2. While CMA variants dominate in BBOB (small scale, large budget, focus on frequency of solving with a given precision) and DE variants dominate in LSGO (Li et al., 2013) (larger scale, groups of variables), we propose a benchmark close to BBOB or YABBOB, but with a specific effort to not make the scale of the norm of the optimum to be known in advance (Section 3.2.2).

An important hyperparameter for the optimization methods, in particular when the budget is moderate, is the scale. Sometimes the optimum is close to the center, sometimes it is far. The principle of our proposed and open-sourced multi-scale BBOB (MS-BBOB) benchmark is that it contains four different scales, and the algorithms are not informed of which scale is used for each instance. We also apply the zero-penalization, as discussed in Section 3.2.2. The resulting benchmark is termed ZP-MS-BBOB, and experiments are presented in Figure 2. It is an artificial benchmark, but it is inspired by various existing benchmarks (Cotton, 2020a;b; Raponi et al., 2023). The best methods are all based on Carola (Section 3.3.4) or NgIoh (which uses Carola inside NGOpt), or on quasi-opposite sampling. We conclude that the Carola method (using Cobyla first) and

quasi-opposite samplings are both good for adapting a method to the right scaling of variables. Figures 7 and 8 present the results on the variants of BBOB in Nevergrad, showing that results are not deteriorated, compared to NGOpt, on these other benchmarks. Section 5 also shows that, on the wide family of benchmarks in Nevergrad, NgIoh4 outperforms NGOpt.

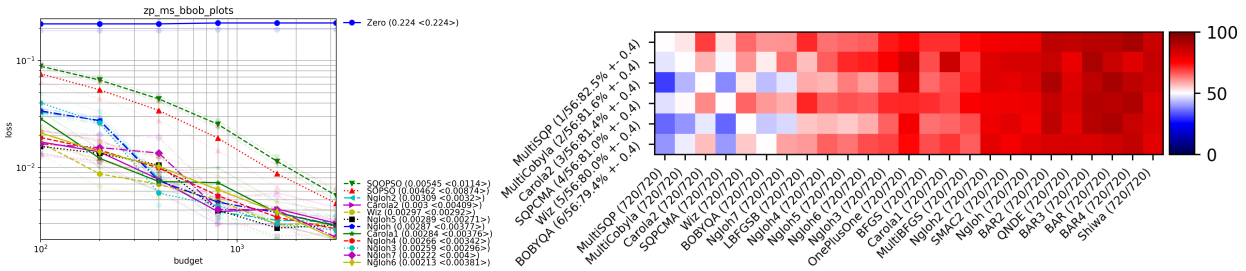

Figure 2: The best performing methods for ZP-MS-BBOB for normalized regret (left, lower is better, includes the 12 best methods and the worst) and frequency of winning (right, best on the left, includes the 26 best): the right-hand side takes into account all budgets, hence the different rankings, and presents much more algorithms: 26 best methods, on average over all budgets of the experiment, are presented on the right, out of 58 methods, whereas the 12 best for the average normalized loss at maximum budget of the experiment are presented on the left. The good performances of Carola and NgIoh variants (including Wiz, also based on Carola2) are visible in both. The quasi-opposite variant of PSO is also good. Carola2 is the best of the Carola variants for most budgets (see detailed curve on the left, or the ranking for the average frequency of winning on the right). We note on the right that many mathematical programming methods (using SQP, BFGS with finite differences, BOBYQA or Cobyla) are excellent for low budget (so that they get a good ranking on the right), which corroborates the idea of using Cobyla as a first step in Carola2. Right: 58 algorithms are ran (the 26 best are presented), and the previous wizard, NGOpt, is ranked 22 and CMA is ranked 38. Left: NGOpt is ranked 15th and CMA is ranked 49th (12 best are presented).

4.2 Real world benchmarking in Nevergrad

We note, in the real-world benchmarks of Nevergrad, that PSO and DE variants, in particular with quasi-opposite sampling, perform better than in artificial benchmarks. The rankings below are obtained for a different number of problems for which each algorithm is best in terms of normalized simple regret. We also note that NGOptRW, designed by adapting NGOpt for real-world instances by bet-and-run (Weise et al., 2019) PSO/DE/NGOpt, performs very well. NGOptRW runs these three algorithms during one third of the budget, and keep the best of them for the rest. It vastly outperforms NGOpt and all others, though Carola3 (the possibly parallel adaptation of Carola2) is not bad.

- 5 times best: NGOptRW
- 3 times best: Carola3
- 2 : SODE (Special-Opposite DE, with a non-uniform rule for r)
- 2 : BAR (bet-and-run of the (1+1) evolution strategiy and DiagonalCMA and OpoDE. OpoDE runs the $(1+1)$ strategy with one-fifth rule followed by differential evolution).
- 1 : pysot
- 1 : SQOPSO (quasi-opposite PSO)
- 1 : QOTPDE (quasi-opposite TwoPointsDE)
- 1 : QOPSO (quasi-opposite PSO, quasi-opposition for positions only and not speed)
- 1 : QODE (quasi-opposite DE)
- 1 : NgIoh3
- 1 : MetaRecentering (Meunier et al., 2021)
- 1 : LargeCMA (CMA with greater initial variance)
- 1 : HyperOpt

5 Statistics over all benchmarks

For short, we include below only the number of times each method was ranked first. NgIoh4 is the best with 10 times the first position. It is also the best for the number of times it is ranked the second or the third one.

- 10 NgIoh4
- 9 SQPCMA
- 7 NgIoh6
- 6 NGOptRW
- 6 NGOpt
- 6 Carola3
- 5 Wiz
- 5 NgIoh5

The full details are reported in Appendix D. NgIoh4 performs even better if we remove the variants NgIoh6 and NgIoh5 (documented in Rapin & Teytaud (2018)) from the statistics, because they are quite similar.

6 Other authors: application to external real-world problems

Finally, we include a few use cases by Nevergrad users. The benchmarks and setups have been developed independently of the benchmarking platform included in Nevergrad. The plotting tools, functions, and criteria, are frequently different from the rest of the paper. They, on purpose, quantify the robustness of the conclusions drawn on our update of the Nevergrad benchmark, specifically for the real-world cases.

6.1 Infrastructure: optimizing a caching policy

In this application, Nevergrad is used to optimize a caching strategy. The problem comprises 84 decision variables for the optimization. These variables encode the cache strategy. We run each method in several variants, with random parameters a, b, and c so that constraints are penalized by $a \times constraintViolation^b \times i^c$, with i being the iteration index. With this dynamical constraint penalization scheme, constraints violations are increasingly penalized so that eventually solutions without any violations are found. Compared to artificial benchmarks above, the setting has been influenced by the computational cost. All methods including GeneticDE, PSO, DE, TwoPointsDE, DiagonalCMA were run the same number of times, and the 11 best results are presented. We observe (Figure 6, left) that GeneticDE performs best and in general, DE variants perform well. One of the conclusions from this experiment is how much most Bayesian methods cannot be used for large budgets and dimension 84 (none of the methods available in Nevergrad was usable here), and computing gradients by finite differences (introducing a factor 85 in the computational cost) is also unfeasible. The results are consistent with the effectiveness, in our benchmarking suite, of DE variants for real-world problems with similar size/budget (Section 4.2). However, we would not have guessed the good performance of GeneticDE for this specific problem. Another observation is that we get a strong improvement compared to the handcrafted heuristic implemented before using standard algorithm (+70%) and also better than the manually designed solution (initial point). The problem is repeated: there are frequently new versions to be solved, so that doing this experiment is useful for doing a choice of algorithm for the future. We note (unpresented experiments) that Inoculation (adding in the population 8 points obtained in previous optimization runs) roughly reduces the computational cost by a factor five: we get roughly the same performance with 20% of the budget.

6.2 Crop optimization

This application combines Nevergrad, PCSE(de Wit, 2021), and NASA data(Sparks, 2018) for optimizing the choice of crops in many countries. Figure 3 presents a specialization of the code to Kenya, including choosing crops and their varieties, depending on climate. Compared to the original code in Nevergrad, there are additional variables, for choosing the crop and the variety. After the present performance check (confirming the good behavior of NGOptRW), a forthcoming publication is under work for various crops and continents.

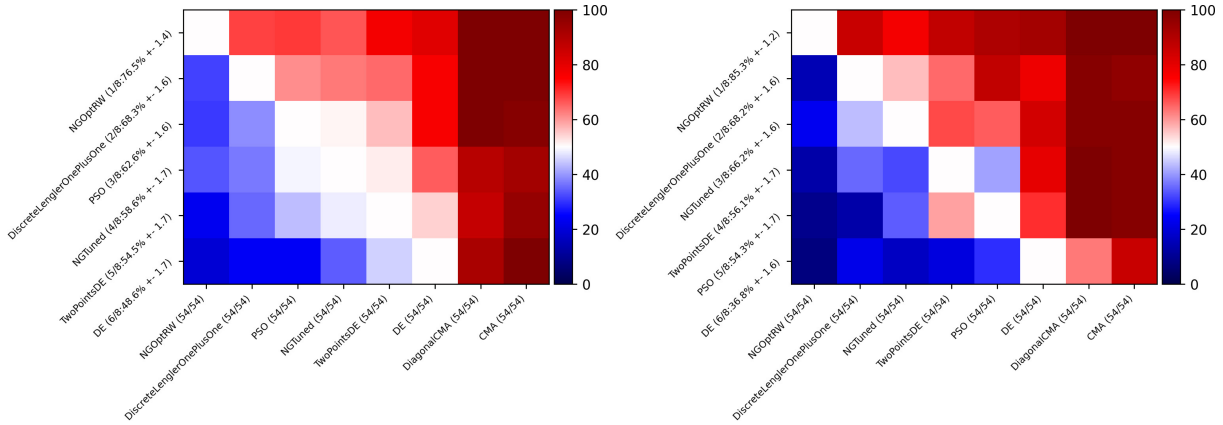

Figure 3: Comparison between optimization methods for crop optimization in the case of Kenya (left: 2011, corresponding to a particularly dry year; right: 2006). Setup as in Section 3.4: the heatmap shows the frequency at which method X (row) outperforms method Y (col). Rows and cols are ranked by average frequency against all other methods: top/left is best. As in many real-world cases NGOptRW is excellent.

6.3 Mobile Network Base Station Placement Optimization

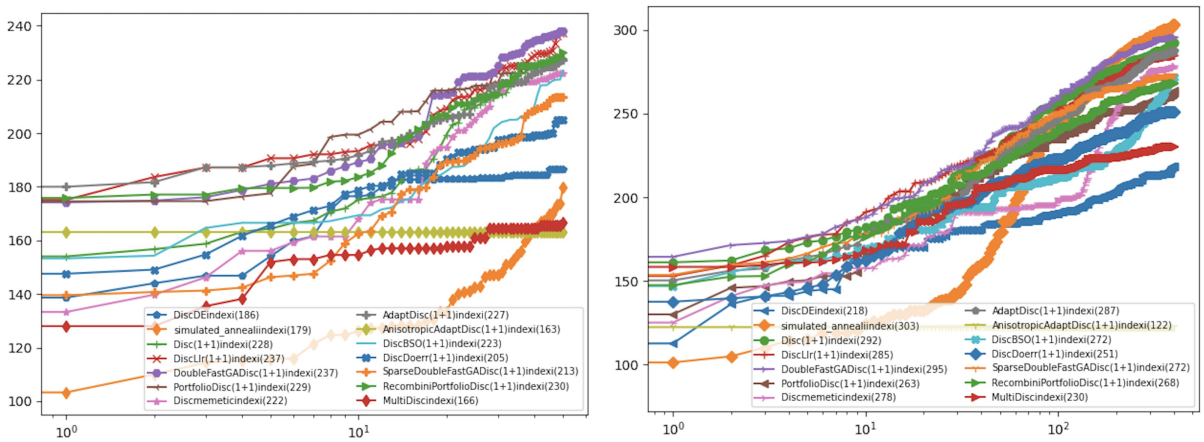

Figure 4: Placement of base stations of a mobile network: optimization with budget 50 (left) and 400 (right): the greater the better, average best score between parentheses. We observe that Nevergrad methods performed quite well for the low budget case but the specific method (Simulated Annealing with ad hoc mutation operator, in orange) developed for the problem at hand is the best for budget 400. Between parenthesis, the best obtained value. Llr is short for Lengler (Doerr et al., 2019; Einarsson et al., 2019).

Figure 4 presents experimental results regarding the optimization of the placement of base stations for a mobile network. An original ad hoc implementation already existed before testing Nevergrad on this problem. The method which typically performs best in our discrete benchmarks, namely Lengler (Doerr et al., 2019; Einarsson et al., 2019) (which uses a fixed, predefined mutation schedule), as well as FastGA (Doerr et al., 2017) (also a method with fixed mutation schedule, but here the schedule is a stationary stochastic random variable), is also good here. We observe that while methods in Nevergrad perform well for low budget and outperform the original method by far, the original method performs best for greater budgets. Seemingly, the key point is that it uses specific mutation operators, whereas Nevergrad focuses on lists of variables with generic operators. Nevergrad improves results only when the ratio size/budget is not too low.

6.4 Robust topology optimization

Figure 5 presents the results for the optimization of mirrors smaller than a micron aimed at reflecting light at wavelength between 400nm and 650nm using only two materials.

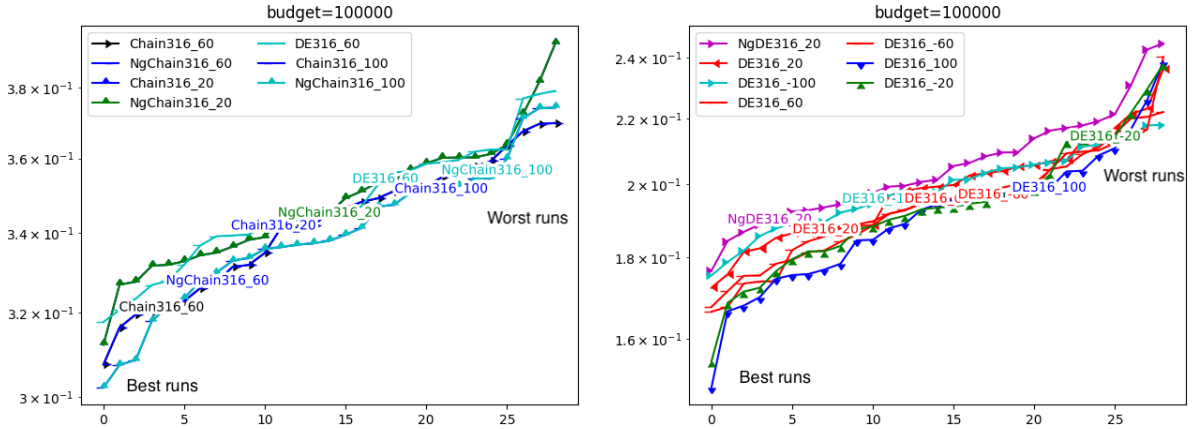

Figure 5: We perform photonics optimization (mirrors for various wavelengths) for 40, 50, 60, 70, 80 layers respectively: we keep only 40 and 80 for short and refer to the appendix for more. For each algorithm we plot the results of 30 runs (best on the left, worst on the right): a horizontal curve means constant results whereas a sharp increase means variable results. Methods are ranked by median value. Only the few best are presented for readability (legend: best at the end, i.e. bottom of the right column): extended version with more algorithms in the ranking in appendix, Figure 9. For moderate numbers of layers, the ranking is unclear (with Chaining of DE and BFGS frequently good), whereas for large-scale versions DE dominates (for 80 layers, the 6 codes based on DE corresponding to the 6 values of the sampling parameter dominate all other combinations algorithm/sampling). The impact of the sampling parameter (suffix of the algorithm name) is unclear.

Only the 7 best performing methods are presented, but actually 30 methods are run: There are 5 algorithms: DE, BFGS, Chain (a chaining of DE during half budget, followed by BFGS) from Nevergrad, and the DE and Chain from Pymoosh (Langevin et al., 2023). For differentiating methods from Nevergrad, we add a prefix Ng for those methods. Each of them is run with a sampling parameter in $\{-100, -60, -20, 20, 60, 100\}$, hence 30 methods. This parameter specifies how robustness to wavelength is taken into account and has little impact here: the detailed description is beyond the scope of the present paper. Another sampling parameter is fixed at 316 (the square root of the budget) after preliminary experiments: it is actually the most important choice in the optimization design, other values are removed from plots as this is not the point in the present paper.

We observe that all strong methods, in the highest dimensional cases, are DE (either the one from Nevergrad, which is quite standard, or the one in PyMoosh which has been optimized for the problem at hand). This limited comparison validates the choice of DE in PyMoosh, though testing more algorithms could be possible. In lower dimension, adding BFGS after DE looks good: the chaining of DE and BFGS frequently performs best.

6.5 Gym

Nevergrad contains OpenAI Gym problems, which were deprecated after the issues of Gym v0.24.0, so that Gym was not included in recent exports of the Nevergrad benchmarks. We update the code importing Gym and rerun the experiments. Our code is merged in the codebase. Results are presented in Fig. 6 (right): SQOPSO performs well.

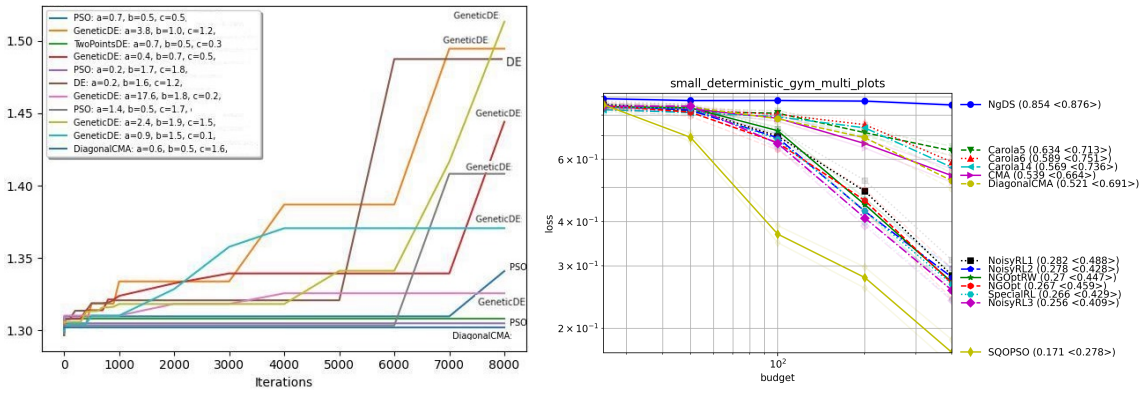

Figure 6: Left: Comparison of various methods on the infrastructure problem. The upper the better, only the 11 best results are presented: GeneticDE is frequently among the 11 best whereas all methods were run the same number of times. Right: Experiments on Gym, confirming the good performance of SQOPSO (and existing wizards dedicated to reinforcement learning, with RL in the name Rapin & Teytaud (2018)) for neurocontrol.

7 Conclusions

Scale is all you need. We note that both in continuous and discrete benchmarks, the scale is important, specifically in the black-box case. **In the discrete case**, the best methods are frequently based on Lengler (Einarsson et al., 2019), which is based on a predefined schedule of mutation scales. This schedule differs from the classical $1/d$ mutation in particular in early stages. We note that the mathematically derived Lengler method outperforms some handcrafted methods based on the same principle of a decreasing rate, and many methods with adaptive mutation rates. It also outperforms mathematically derived methods such as (Doerr et al., 2017; Dang & Lehre, 2016), which use a fixed probability distribution of the mutation rates. We see the chaining of methods with different regimes in continuous domains as analogous to the predetermined schedule of Einarsson et al. (2019) in the discrete case. In any case, both approaches perform well. This is also a reminder that conclusions raised from benchmarks have little reproducibility if the scale of the early sampling of the different optimization methods is completely different, as in many benchmarks written specifically for one specific paper about one algorithm.

Quasi-opposite sampling. An unexpected result is the good performance of quasi-opposite sampling (Rahnamayan et al., 2007) (see QODE, QNDE, QOPSO, SQOPSO in Section 5). We adapted it from DE to PSO, with SQOPSO using, for each particle p with speed v, another particle with position $-r \times p$ and speed $-r \times v$ (see Section 3.3.1). Equipped with quasi-opposite sampling, DE and PSO perform quite well in the real-world part of our benchmarking suite (Sections 4.2 and 6), with particularly good results of SQOPSO in the case of neurocontrollers for OpenAI Gym. A posteriori, this is consistent with the importance of scale.

In spite of (actually, even because of) the random shift method, many benchmarks have roughly the same norm of the optimum for all instances. If we define the position of optima by e.g., a multivariate normal distribution with mean zero and identity covariance matrix (or more generally, independent coordinates with all roughly the same variance, so that variants of the central limit theorem can be applied), then in large dimension the optimum has, almost always, a norm close to $\sqrt{dimension}$ (see Section 3.2.2). This is not observed in real-world benchmarks, hence the great real-world performance of the methods above (quasi-opposite sampling) tackling such issues. We advocate MS-BBOB or ZP-MS-BBOB for designing artificial benchmarks close to scaling issues found in the real-world.

Optimization wizards. As in SAT competitions and as discussed in the Dagstuhl seminar (Hoos, 2023), we observe excellent results for wizards. All methods performing well on a wide range of benchmarks (without tuning for each benchmark separately) are wizards. NgIoh4 is based on NGOpt, a complex handcrafted wizard based on experimental data, and adds insights from the present paper. It performs well on many benchmarks (Section 5). NgIoh4 aggregates many base algorithms. We see in the detailed logs that it uses

CMA, DE, PSO, Holland crossover, bandit methods for handling noise, discrete (1+1) methods with mutation rates schedules, meta-models, Cobyla, multi-objective adaptations of DE, the simple (1+1) evolution strategy with one-fifth rule (Rechenberg, 1973) in some high-dimensional contexts, bet-and-run, and others. Our guess is that it could still be improved by ideas from NGOptRW or quasi-opposite sampling, or by tuning its rules in favor of Carola2 or Carola3 in more general cases.

Low-budget optimization, and first part of a chaining in continuous domains. SMAC3 got better results than other Bayesian Optimization methods. Bayesian Optimization methods are limited to low budget / dimension contexts, and a strong competitor for continuous optimization with low budget is Cobyla. We propose to use Cobyla as a first step before other methods, because it is good at understanding the global shape of a problem (Sections 3.3.4 and 4.1). Carola2 is a chaining of 3 stages: Cobyla for a fast first approximation, CMA with MetaModel for a robust optimization, and SQP for a final fast local search. It performs very well as a component of NgIoh4, and its counterpart Carola3 (compatible with parallel settings) performs very well in many real-world benchmarks (Section 4.2). Chaining was already present in Rapin & Teytaud (2018), with the classical fast local convergence at the end in many cases, and also for noisy optimization, with a classical algorithm (not taking care of noise) as a first step before switching to a real noisy optimization method in the wizard of Meunier et al. (2022).

Reality gap. The gap between real world and artificial benchmarks is still large, as shown by the different best algorithms in real-world vs artificial contexts. In particular in the continuous context, NGOpt/NgIoh dominates the artificial benchmarks whereas a bet-and-run (termed NGOptRW) of DE, PSO, and NGOpt is better in the real-world. Also quasi-opposite sampling seems to be great for the real-world context, more than for artificial benchmarks based on random shifts (random shifts with all components of the shift being independent; or other distributions than random shifts, provided that many coordinates are independent and have roughly the same variance) which lead to nearly the same norm of the optimum for all replicas. Our zero-penalized and multi-scale variants of black-box optimization benchmarks (Section 4.1: due to the random factor applied to all coordinates, the central limit theorem does not apply) are a step in this direction and we plan to add more of such benchmarks. Another element in terms of reality gap is that in the present paper (and in most works on wizards), we did not use in the wizard information such that "is a real world problem" or "is a weight of a neural net", but such wizards are under development. We note that in (AX-team, 2021; Awad et al., 2020), the best performing method was using the names of variables for choosing between different options. We merge MS-BBOB, ZP-MS-BBOB and our updated Gym in the public Nevergrad platform, as well as all new codes mentioned above. Another important point is that including cases with budget far lower than the dimension is also essential (Ungredda et al., 2022).

Good benchmarks exist, they should be used, in particular in machine learning papers. Reproducibility is a growing concern in machine learning (Kapoor & Narayanan, 2022), specifically in black-box optimization (Markov, 2023). In spite of efforts in the 2000s for creating better benchmarks, benchmarks with optimum at zero, or ad-hoc experiments with a heavily tuned method *with parameters optimized for each benchmark separately* are still published in many conferences. A related and slightly more subtle effect is that the scaling of the initialization can easily make baselines pointless and create non-reproducible results.

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A Reproducibility

A.1 Reproducing results

How to reproduce the results in the present paper:

- Install Nevergrad by cloning the git repository (see details at (Rapin & Teytaud, 2018)).
- Running:
  - Without cluster: `python -m nevergrad.benchmark yabbob --num\_workers=67` if you want to run YABBOB on 67 cores.
  - With cluster equipped with Slurm: Run "sbatch scripts/dagstuhloid.sh" script for launching experiments with Slurm. It is written assuming that Slurm is installed: it should be feasible to adapt it to other job scheduling tools. Running this script several times will increase the number of replicas and increase precision.
- For plotting results, run "scripts/dagstuhloid_plot.sh". Of course, some data might be missing if not enough runs are complete.
- To modify the parallelism, dimension, budget, list of tested algorithms, you might edit `nevergrad_repository/nevergrad/benchmark/experiments.py`.

The present paper in LaTeX is automatically generated by the commands above. Then, the authors have edited the corresponding file for the text and rearranged sections, in particular moving to the appendix or to an URL many of the individual results on specific benchmarks. An example of the huge original PDF file can be found at `tinyurl.com/dagstuhloid`. We emphasize that reproducibility is not limited to the possibility of reproducing the exact same numbers. We consider results that can only be obtained by certain random seeds uninteresting. We therefore do not fix the seeds.

A.2 What if your computational power is insufficient?

We want everything to be easy to rerun entirely from scratch. This requires important computational power. However, it is possible to run manually and separately some benchmarks. In this case, one can easily edit the main script and reduce the number of benchmarks, possibly up to a single benchmark at a time. At the time of writing, and probably in the years to come, we periodically rerun all the benchmarks and accept pull requests so that a limited computational power should not be an obstacle to reproducibility. Likewise, we take care of running all merged codes. Please note that creating a pull request and pinging us at `facebook.com/groups/nevergradusers` is a simple solution to get heavy computations done, we are more than happy to run what you need if the computational cost is reasonable.

B Additional information on algorithms

We use quasi-opposite DE, in several flavors:

- QODE, the classical quasi-opposite DE.
- QNDE, which is QODE during half the budget and then BFGS with finite differences.
- SPQODE (SPecial QODE), which is QODE with population size $1 + \sqrt{\log(d+3)}$ in dimension d.
- LQODE (Large QODE), which is QODE with initialization range multiplied by 10 (each individual is multiplied by 10).
- SODE (Special Opposite DE), in which r is $\exp(-5 \times U(0,1))$ instead of $U(0,1)$ (with $U(0,1)$ uniform in $[0,1]$).

- QOTPDE combines TwoPointsDE (DE with Holland 2-points crossover) and QODE.

We also consider quasi-opposite sampling for PSO:

- Randomly draw half the population as usual.
- QOPSO (Quasi-Opposite PSO): for each point p with velocity v in this half population, also add $-r \times p$ with a randomly drawn velocity, with r randomly drawn uniformly in $[0, 1]$.
- SQOPSO (Special Quasi-Opposite PSO): for each point p with velocity v in this half population, also add $-r \times p$ with velocity $-r \times v$, with r randomly drawn uniformly in $[0, 1]$.

C Additional information on benchmarks

Table 1: Diversity of our benchmarking platform and of our automatic report.

(a)

	Min	Max
Dimension	1	20×10^3
Budget	10	3×10^6
# objectives	1	6
Noise dissymetries	False	True
Noise	False	True*
# blocks of variables$^\sharp$	1	16
# of workers	1	500

*many different levels of noise
$^\sharp$with independent rotations

(b)

Category	Benchmarks
Real-world, ML tuning	Keras, Scikit-learn (SVM, Decision Trees, Neural nets)
Real-world, not ML tuning	Crops, rockets, energy, fishing, photonics, game
Discrete	PBO, Bonnans, others (includes: unordered variables)

D Statistics over all benchmarks: full details

We point out that NGOpt and its variants are wizards (automatic algorithm selectors and combinators) created by the same authors as Nevergrad, and their (good) results might therefore be biased: we recognize that common authorship for benchmarks and algorithms implies a bias, and, given that our tools are based on NGOpt and other tools in Nevergrad, this applies to us as well. Another issue is that statistics based on frequencies of performing in the top k are a risky thing: when two codes are very close to each other, they are both penalized by each other: we must be careful with interpretations. Nonetheless, we provide aggregated results for convenience.

D.1 NGOpt versus Base algorithms: validating wizards

Here base algorithms have no metamodel and no complex combinations: wizards are excluded, except NGOpt. NGOpt is the only sophisticated combination: this is an analysis of NGOpt, and this validates that NGOpt performs better than the base algorithms it is built on. We consider statistics on the top k methods, for $k = 1$, $k = 2$, $k = 3$.

D.1.1 Number of times each algorithm was ranked first: NGOpt and base algorithms

- 29 NGOpt
- 8 HyperOpt
- 8 Cobyla
- 7 QODE
- 6 OnePlusOne
- 5 SODE
- 4 SPQODE
- 4 QOTPDE

D.1.2 Number of times each algorithm was ranked among the 2 first: NGOpt and base algorithms

- 45 NGOpt
- 16 QODE
- 16 OnePlusOne
- 16 Cobyla
- 12 HyperOpt
- 10 QORealSpacePSO
- 9 SQOPSO
- 8 QOPSO

D.1.3 Number of times each algorithm was ranked among the 3 first: NGOpt and base algorithms

- 51 NGOpt
- 23 Cobyla
- 20 QODE
- 20 OnePlusOne
- 19 SQOPSO
- 15 HyperOpt
- 14 QORealSpacePSO
- 12 SODE

D.2 Comparing simple algorithms only: wizards, multilevels, specific standard deviations, and combinations excluded

Simple algorithms might be less overfitted, more robust: we consider the same experiments, but with only "simple" algorithms: no chaining, no metamodel, no tuned parameters, no bet-and-run, no wizard. The success (robustness) of quasi-opposite sampling (for PSO or DE) is visible. in results below. We also note the excellent performance of Cobyla, thanks to great results for moderate budget.

D.2.1 Number of times each algorithm was ranked first: no wizard, no combination

- 14 Cobyla
- 9 QODE
- 8 OnePlusOne
- 8 HyperOpt
- 6 QORealSpacePSO
- 5 SODE
- 5 QNDE
- 4 SPQODE

D.2.2 Number of times each algorithm was ranked among the 2 first: no wizard, no combination

- 17 QODE
- 17 OnePlusOne
- 17 Cobyla
- 13 QORealSpacePSO
- 12 SQOPSO
- 12 HyperOpt
- 10 GeneticDE
- 10 DiscreteLenglerOnePlusOneT

D.2.3 Number of times each algorithm was ranked among the 3 first: no wizard, no combination

- 23 QODE
- 23 Cobyla
- 20 SQOPSO
- 20 OnePlusOne
- 16 QORealSpacePSO
- 15 HyperOpt
- 15 DiagonalCMA
- 13 OldCMA

D.3 Everything included

For the results of this section, we include all codes, wizards as well as base algorithms. All strong methods are wizards, except tools based on quasi-opposite samplings. The only algorithms making it to the top are (i) wizards (ii) bet and run / aggregations (such as SQPCMA) (iii) HyperOpt (iv) quasi-opposite tools (v) Carola variants.

D.3.1 Number of times each algorithm was ranked first: everything included

- 10 NgIoh4
- 9 SQPCMA
- 7 NgIoh6
- 6 NGOptRW
- 6 NGOpt
- 6 Carola3
- 5 Wiz
- 5 NgIoh5

D.3.2 Number of times each algorithm was ranked among the two first: everything included

- 22 NgIoh4
- 14 NgIoh5
- 12 NgIoh6
- 11 SQPCMA
- 11 NGOpt
- 10 Shiwa (an old wizard, anterior to NGOpt, designed in Liu et al. (2020))
- 8 QODE
- 8 NgIoh2

D.3.3 Number of times each algorithm was ranked among the three first: everything included

- 29 NgIoh4
- 27 NgIoh5
- 21 NgIoh6
- 16 Shiwa
- 14 NGOpt
- 12 HyperOpt
- 11 SQPCMA
- 11 QODE

E Additional experimental figures

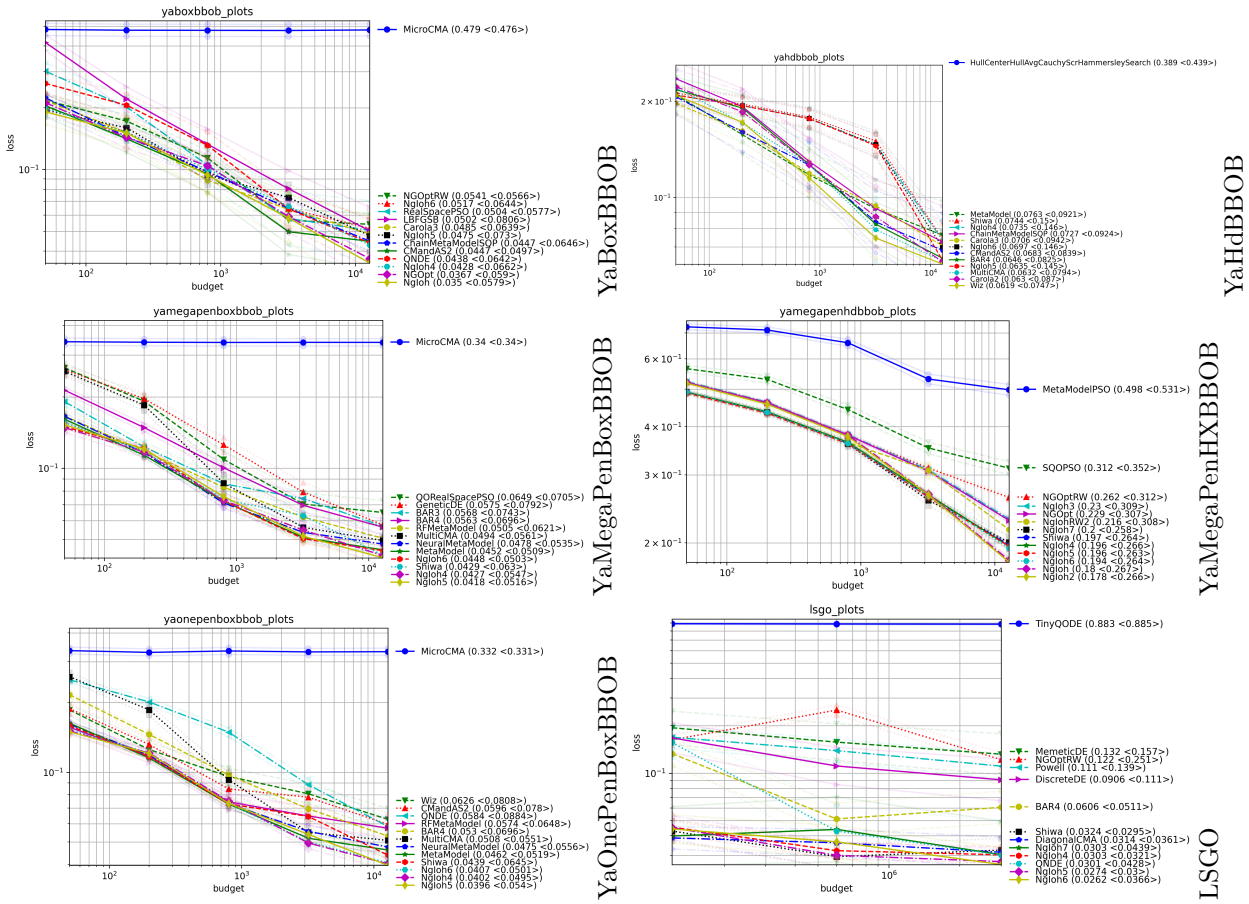

Figure 7: Variants of YABBOB with small ratio budget/dimension and LSGO. Other variants of BBOB in Fig. 8. This is average normalized loss (see details in Section 3.4, with only the best methods (NgIoh4 is always there) and the single worst; see Fig. 10, 11 and 12 for more methods in the frequency of winning figures.

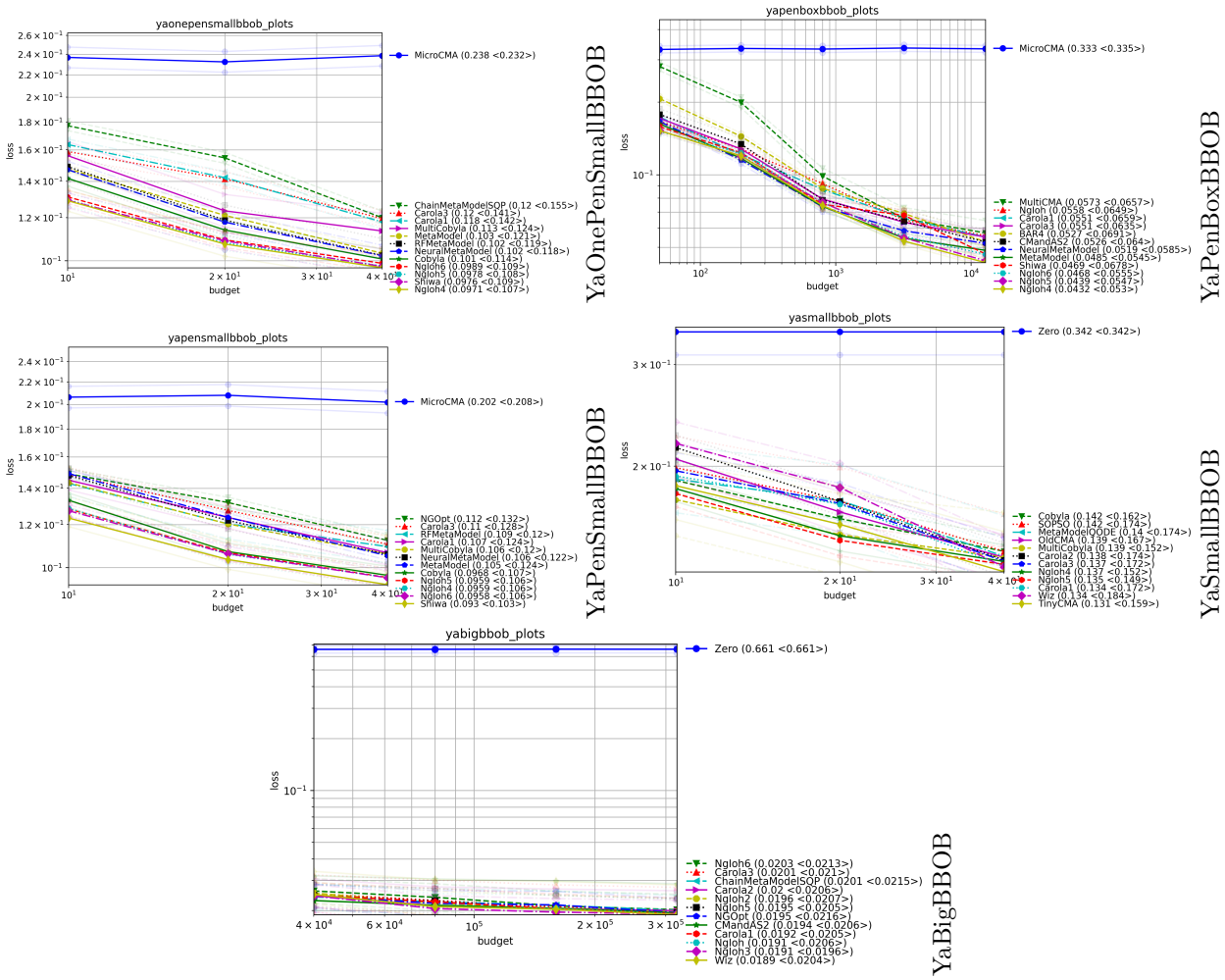

Figure 8: Variants of YABBOB with small ratio budget/dimension. The last one, YaBigBBOB, is the opposite, with a large ratio budget/dimension. Only the 12 best methods and the worst are presented, all benchmarks include several variants of CMA, DE, PSO and others (see referenced URLs or Fig. 12 for all details and more algorithms). Overall, NgIoh variants are excellent.

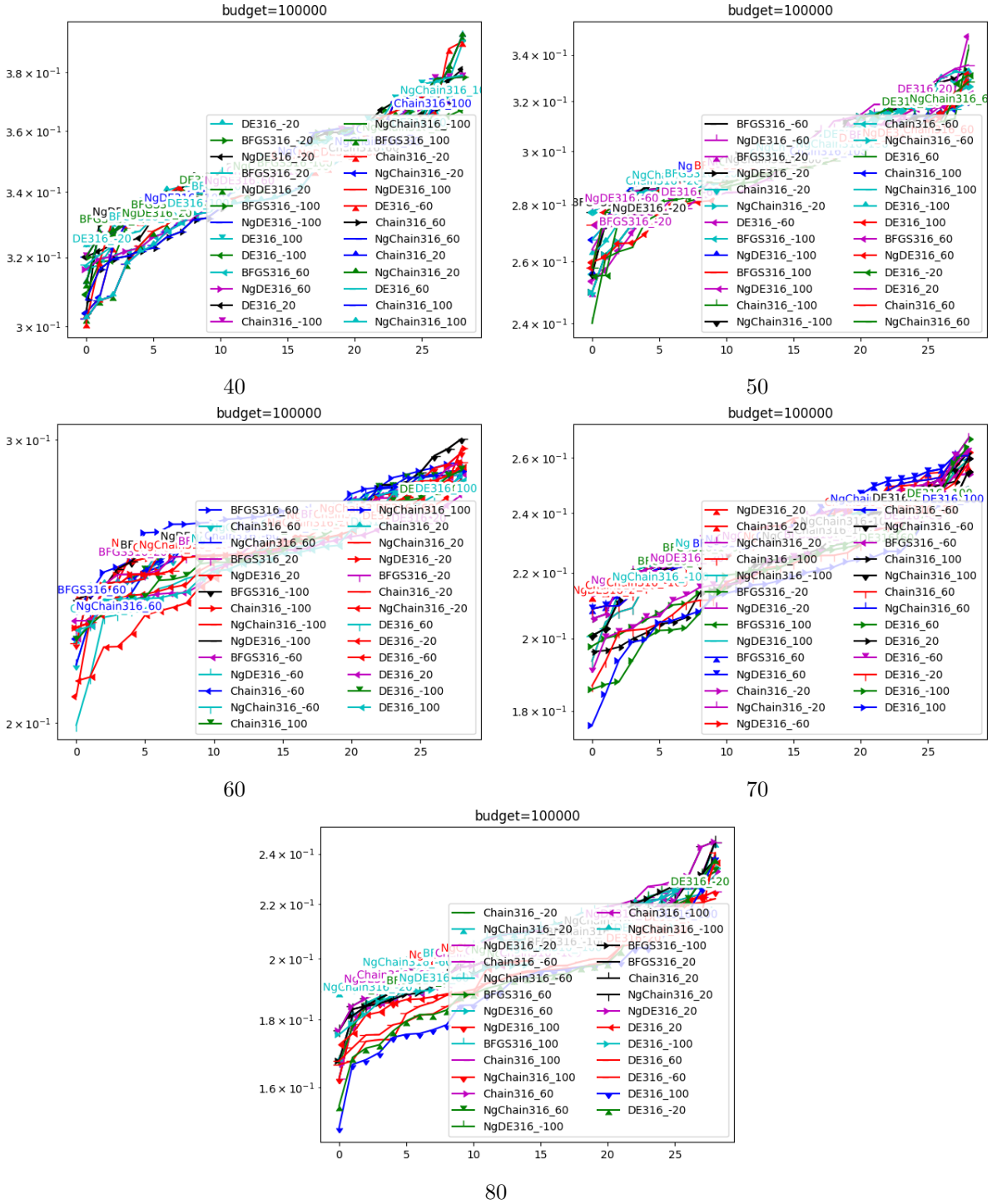

Figure 9: Photonics optimization (mirrors for various wavelengths) for 40, 50,60,70,80 layers respectively: sorted result of the 30 runs of each method (best run on the left and worst run on the right). The 27 best (for the median) are presented (best at the end, right column, bottom), this extends Fig. 5. For moderate numbers of layers, comparisons are unclear, whereas for large-scale versions DE dominates.

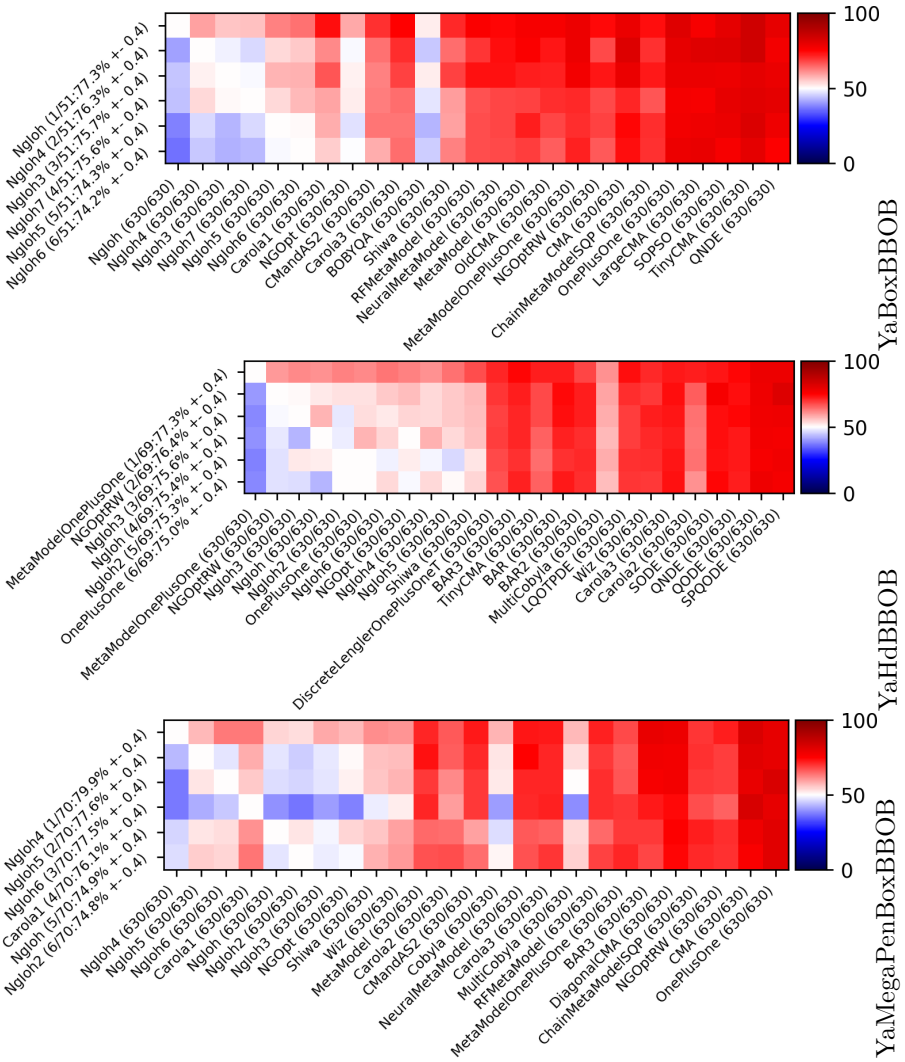

Figure 10: Variants of YABBOB with small ratio budget/dimension. Other variants of YABBOB in Fig. 11 and 12. This is the frequency of winning figure (see details in Section 3.4, with the best methods on the left. NgIoh variants dominate.

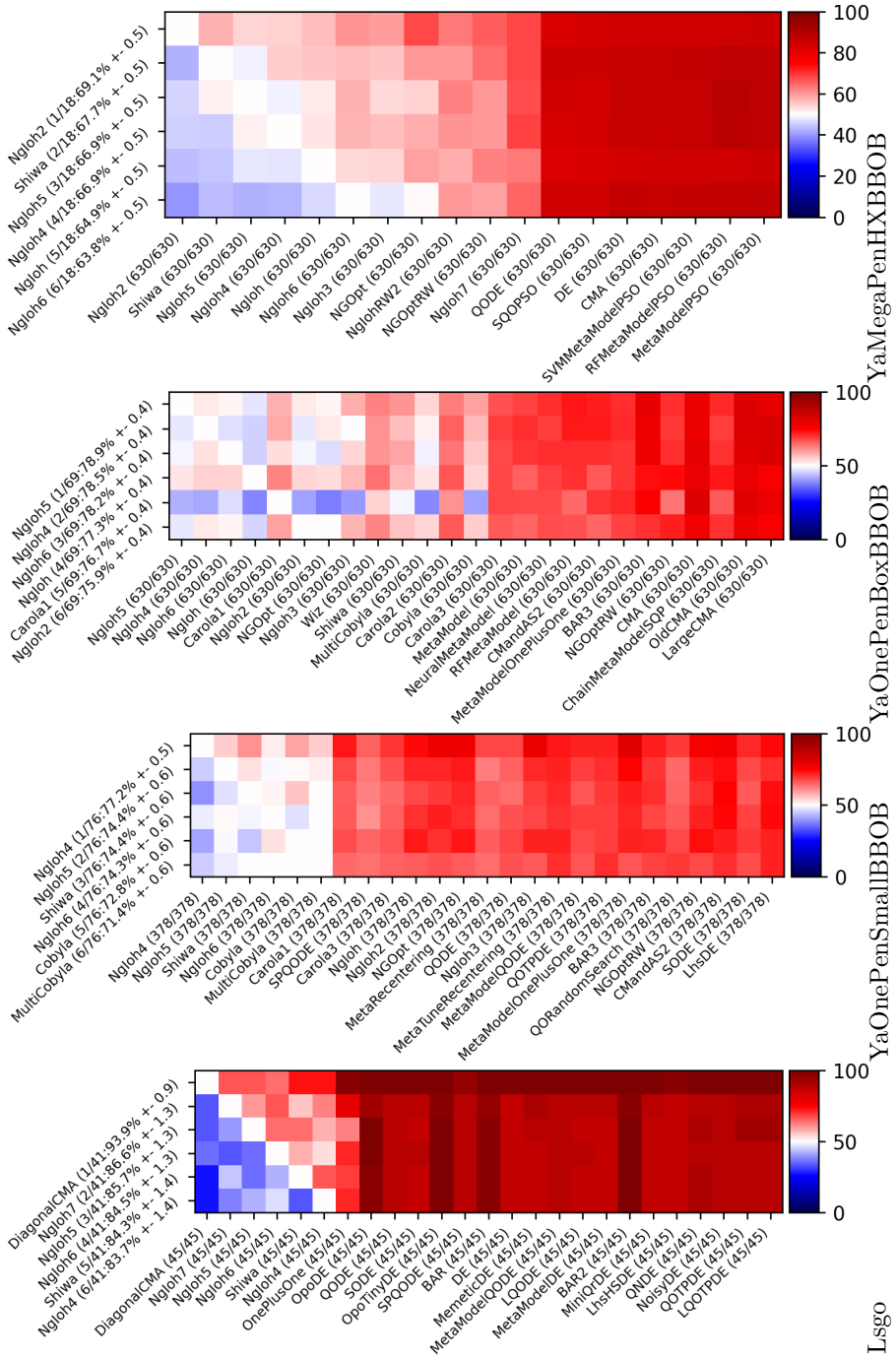

Figure 11: Variants of YABBOB with small ratio budget/dimension and LSGO(Li et al., 2013). Other variants of YABBOB in Fig. 10 and 12. This is the frequency of winning figure (see details in Section 3.4, with the best methods on the left.

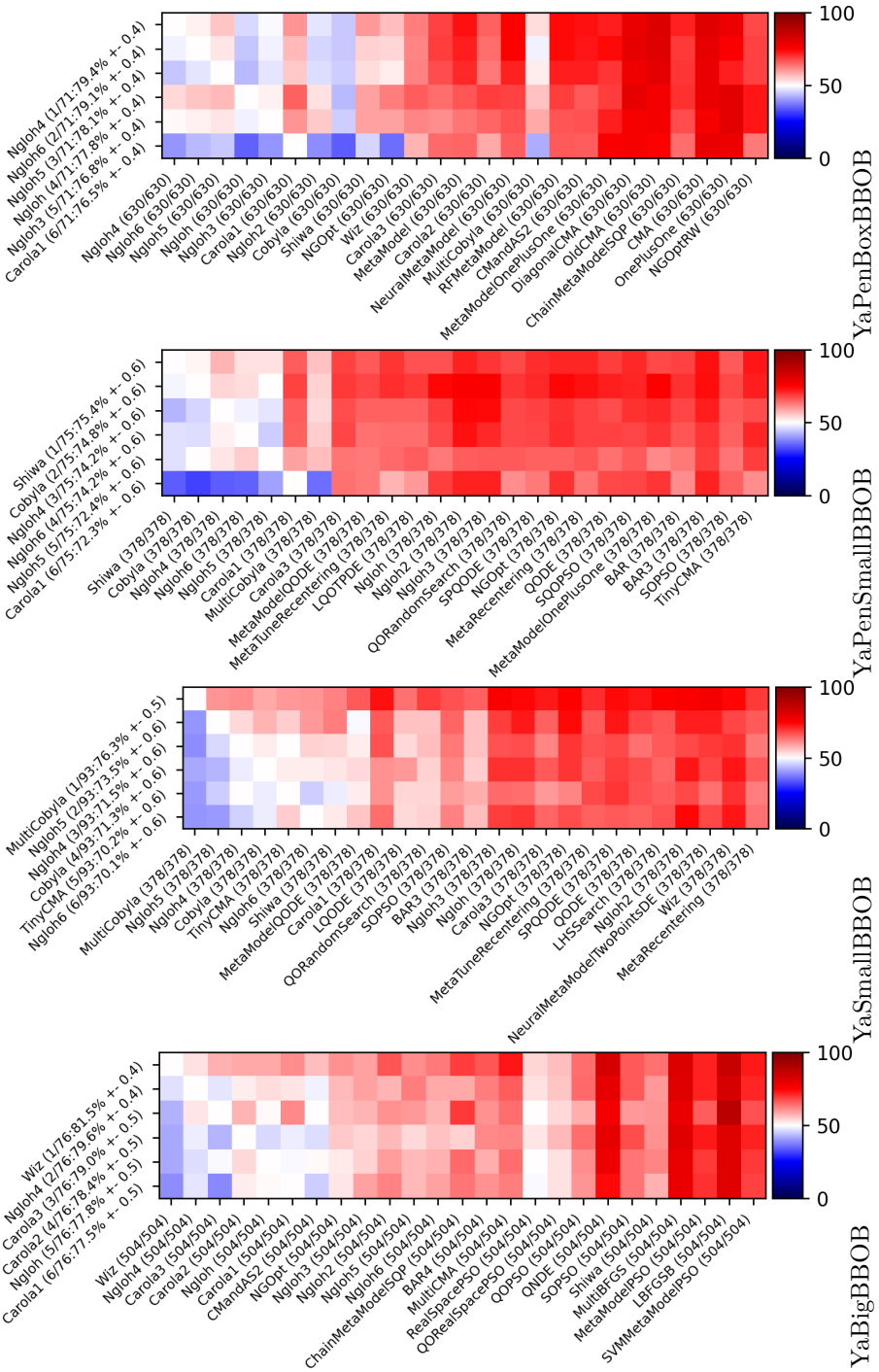

Figure 12: Top: 3 variants of YABBOB with small ratio budget/dimension. Bottom: YaBigBBOB, is the opposite, with a large ratio budget/dimension. Frequency of winning figure as detailed in Section 3.4, with the best methods on the left. NgIoh variants and (except for the last) Cobyla dominate.