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BI-population CMA-ES Algorithms with Surrogate Models and Line Searches

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ABSTRACT

In this paper, three extensions of the BI-population Covariance Matrix Adaptation Evolution Strategy with weighted active covariance matrix update (BIPOP-aCMA-ES) are investigated. First, to address expensive optimization, we benchmark a recently proposed extension of the self-adaptive surrogate-assisted CMA-ES which benefits from more intensive surrogate model exploitation (BIPOP-saACM-k). Second, to address separable optimization, we propose a hybrid of BIPOP-aCMA-ES and STEP algorithm with coordinate-wise line search (BIPOP-aCMA-STEP). Third, we propose HCMA, a hybrid of BIPOP-saACM-k, STEP and NEWUOA to benefit both from surrogate models and line searches. All algorithms were tested on the noiseless BBOB testbed using restarts till a total number of function evaluations of $10^6 n$ was reached, where n is the dimension of the function search space.

The comparison shows that BIPOP-saACM-k outperforms its predecessor BIPOP-saACM up to a factor of 2 on ill-conditioned problems, while BIPOP-aCMA-STEP outperforms the original BIPOP-based algorithms on separable functions. The hybrid HCMA algorithm demonstrates the best overall performance compared to the best algorithms of the BBOB-2009, BBOB-2010 and BBOB-2012 when running for more than $100n$ function evaluations.

Categories and Subject Descriptors

G.1.6 [Numerical Analysis]: Optimization—*global optimization, unconstrained optimization*; F.2.1 [Analysis of Algorithms and Problem Complexity]: Numerical Algorithms and Problems

General Terms

Algorithms

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Keywords

Benchmarking, black-box optimization, evolution strategy, CMA-ES, self-adaptation, surrogate models, surrogate-assisted optimization, separable optimization

1. INTRODUCTION

The Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [5] has become a popular tool for continuous black-box optimization. However, CMA-ES is a rather local optimization algorithm and can be ineffective when dealing with multi-modal optimization problems. In order to avoid premature convergence to local optima, several restart strategies for CMA-ES have been proposed [1, 3, 14]. These strategies, typically based on restarting and increasing (more generally, on varying) the population size and initial mutation step-size each time at least one stopping criterion of CMA-ES is met, implement the simplest niching approach but rather in the time than in space [21]. Thanks to its population-based nature, the CMA-ES benefits from using larger population sizes on multi-modal functions with some global structure and, thus, typically outperforms quasi-Newton methods such as BFGS [23]. The latter, however, often outperforms CMA-ES on a special but quite popular class of noiseless unimodal functions, when gradient information is useful. This drawback of CMA-ES becomes especially undesirable when dealing with expensive optimization, where each function evaluation takes some time and/or costs some money.

A common way to reduce the cost of optimization within Evolutionary Algorithms is to periodically learn a surrogate model of the expensive function and exploit it during the search by pre-filtering promising solutions and/or by optimizing the surrogate directly instead of the expensive function. These approaches have been adopted within Evolution Strategies and CMA-ES by using different surrogate learning approaches: Radial Basis Functions network [7], Gaussian Processes [25], Artificial Neural Network [10], Support Vector Regression [12], Local-Weighted Regression [11, 2], Ranking Support Vector Machine (Ranking SVM) [11, 13, 8]. More recently it has been shown [17] that key invariance properties of CMA-ES can be preserved even in surrogate-assisted scenario by using Ranking SVM approach. Moreover, hyper-parameters used to build surrogate models can be also adapted during the search allowing the user to define only the range of these hyper-parameters, while their actual values will be adapted by the ^{s*}aACM-ES algorithm [17].

In this paper, we benchmark the recently proposed extension of ** aACM-ES, referred to as ** aACM-ES-k, where the surrogate model is more intensively exploited by increasing the population size used for its optimization. This extension further improves the performance of the surrogate-assisted CMA-ES on uni-modal functions, however, almost does not improve the performance of multi-modal functions. This is especially true for separable multi-modal functions, where CMA-ES is outperformed by Evolutionary Algorithms which explicitly or implicitly exploit separability. In order to investigate that would be the effect of such an exploitation by CMA-ES, we present a hybrid version of CMA-ES algorithm and *select the easiest point* (STEP) [24, 19] algorithm, which performs coordinate-wise search and is quite efficient on separable functions [24, 19]. Finally, to benefit both from surrogate models and line searches, we propose a hybrid CMA (HCMA) which combines ** aACM-ES-k, STEP and NEWUOA algorithm [20].

2. THE ALGORITHMS

2.1 The $(\mu/\mu_w, \lambda)$ -CMA-ES

In each iteration t , $(\mu/\mu_w, \lambda)$ -CMA-ES [5] samples λ new solutions $x_i \in \mathbb{R}^n$, where $i = 1, \dots, \lambda$, and selects the best μ among them. These μ points update the distribution of parameters of the algorithm to increase the probability of successful steps in iteration $t + 1$. The sampling is defined by a multi-variate normal distribution, $\mathcal{N}(m^t, \sigma^t C^t)$, with current mean of distribution m^t , $n \times n$ covariance matrix C^t and step-size σ^t . Most of algorithms which will be benchmarked in this paper are based on an active version of the CMA-ES (in short, aCMA-ES) with negative covariance matrix update [9, 6].

2.2 The BIPOP-aCMA-ES

In BIPOP-CMA-ES [3] after the first single run (when at least one of stopping criteria is met) with default population size, the CMA-ES is restarted in one of two possible regimes by taking into account the budget of function evaluations spent in the corresponding regime. Each time the algorithm is restarted, the regime with smallest budget used so far is used.

Under the first regime the population size is doubled as $\lambda_{large} = 2^{i_{restart}} \lambda_{default}$ in each restart $i_{restart}$ and uses some fixed initial step-size $\sigma_{large}^0 = \sigma_{default}^0$.

Under the second regime the CMA-ES is restarted with some small population size λ_{small} and step-size σ_{small}^0 , where λ_{small} is set to

$$\lambda_{small} = \left\lceil \lambda_{default} \left(\frac{1}{2} \frac{\lambda_{large}}{\lambda_{default}} \right)^{U[0,1]^2} \right\rceil, \quad (1)$$

Here $U[0, 1]$ denotes independent uniformly distributed numbers in $[0, 1]$ and $\lambda_{small} \in [\lambda_{default}, \lambda/2]$. The initial step-size is set to $\sigma_{small}^0 = \sigma_{default}^0 \times 10^{-2U[0,1]}$.

The active version of BIPOP-CMA-ES (BIPOP-aCMA-ES) has been proposed in [14].

2.3 The BIPOP- ** ACM-ES

The ** ACM-ES [17] is the surrogate-assisted version of the $(\mu/\mu_w, \lambda)$ -CMA-ES, where Ranking SVM-based surrogate model is used periodically instead of the expensive function

for direct optimization. The use of Ranking SVM allows to preserve invariance properties of CMA-ES w.r.t. rank-preserving transformations of the objective function and orthogonal transformations of the search space. The main loop of ** ACM-ES: the surrogate model \hat{f} is optimized for \hat{n} generations by the CMA-ES, then the expensive function f is optimized for one generation. To adjust the number of generations \hat{n} for the next time, the model error is computed as a fraction of incorrectly predicted comparison relations that is observed after ranking the last λ evaluated points according to f and \hat{f} . The ** ACM-ES performs an online optimization of the surrogate model hyper-parameters during the optimization of the objective function by performing a search in a space of model hyper-parameters, and by generating λ_{hyp} surrogate models in each iteration. The information about the fittest models with the smaller prediction error on the last λ evaluated solutions is used to adjust the surrogate hyper-parameters for the next iteration. The detailed description of ** ACM-ES is given in [17].

2.4 The BIPOP- ** ACM-ES-k

A more intensive exploitation of a surrogate model can be useful if the model is sufficiently precise. An extension of ** ACM-ES, based on this idea, referred to as ** ACM-ES-k, has been proposed in [18]. In ** ACM-ES-k, \hat{f} is optimized for \hat{n} generations by CMA-ES with population size $\lambda = k_\lambda \lambda_{default}$ and number of parents $\mu = k_\mu \mu_{default}$, where $k_\lambda \geq 1$ and $k_\mu \geq 1$. Then, f is optimized for 1 generation by CMA-ES with population size $\lambda = \lambda_{default}$ and number of parents $\mu = \mu_{default}$. The original ** ACM-ES corresponds to ** ACM-ES-k with $k_\lambda = 1$ and $k_\mu = 1$. Thus, larger values of k_λ and k_μ lead to a more intensive exploitation of \hat{f} . To prevent the algorithm from a potential divergence when \hat{n} oscillates around 0 and 1, $k_\lambda > 1$ is used only if $\hat{n} \geq \hat{n}_{k_\lambda}$, where \hat{n}_{k_λ} is the number of generations which corresponds to an "accurate enough" model to be intensively exploited.

2.5 The BIPOP-aCMA-STEP

The *select the easiest point* (STEP) [24, 19] is a simple line search method which is based on iterative interval division. The STEP determines the next point to evaluate by analyzing the usefulness of evaluation the function at the middle of an interval $[x_i, x_{i-1}]$ with respect to the interval *difficulty* computed as [24]

$$D = \frac{4\hat{y} - 2\Delta y + 4\sqrt{\hat{y}^2 - \hat{y}\Delta y}}{\Delta x^2}, \quad (2)$$

where $\Delta x = x_i - x_{i-1}$, $\Delta y = f(x_i) - f(x_{i-1})$, $\hat{y} = f^* - f(x_{i-1}) + l$, f^* is the best solution found so far by the STEP and l is the tolerance (i.e., the precision required for the value of the optimum).

The STEP can be applied to n -dimensional optimization problem by performing n coordinate-wise iterative or parallel searches. A variant of iterative search: optimize f along the coordinate i for N_{STEP} function evaluations or until a stopping criterion is met, then fix the best x_i , increment i and repeat the procedure again while $i \leq n$. This approach is quite straightforward but requires N_{STEP} to be set a priori. However, N_{STEP} can be initialized by a small value and then incremented (e.g., doubled) in a similar way as the population size in BIPOP-aCMA-ES each time STEP finishes the search on n coordinates. This approach might lead to a

loss of a factor of about 2 in terms of number of function evaluations compared to an optimal setting of N_{STEP} . Moreover, some step function-like improvement of the objective function can be observed due to switch between variables, this also means that objective values of tested solutions are far away in the objective space during the coordinate-wise search on all but n -th coordinate.

We propose a parallel STEP search where at each iteration one step per coordinate is performed, then x_i^* which corresponds to the best solution so far *along* the coordinate i is used to construct a recommended solution x^* combined of $x_i^*, i = 1, \dots, n$. The objective value of this solution is estimated and is used for two purposes. First, if the value of this solution is worse (up to some precision p) than the one of a solution recommended in the previous iteration, then f is non-separable or/and noisy. In this case, it is not recommended to use the STEP. Second, the new recommended solution can be of the same quality as the previous one even if the problem is separable. In this case, the STEP still can run while its best recommended solution is better than the one found by its competitor algorithm running in parallel with, e.g., the same budget of function evaluations.

In BIPOP-aCMA-STEP algorithm, a fraction ρ_{STEP} of function evaluations is allocated to the STEP, while $1-\rho_{STEP}$ is allocated to the BIPOP-aCMA-ES. At each iteration after the first $n_{MinIterSTEP}$ iterations, the best solutions of two algorithms are compared and the STEP is stopped if its best solution is worse or if its current solution is worse than its previously recommended solution.

2.6 The HCMA

The HCMA algorithm is a hybrid of BIPOP-^{s*}aACM-ES-k and STEP algorithms coupled as described in the previous section. Additionally, the NEWUOA algorithm [20] is used for the first $10n$ function evaluations to insure good convergence of the HCMA on simple functions which can be efficiently approximated by quadratic surrogate models. All solutions generated by STEP and NEWUOA are not used by BIPOP-^{s*}aACM-ES-k for surrogate learning since the sampling/test distribution of CMA-ES might not correspond to the training distribution defined by these solutions.

2.7 The Benchmarked Algorithms

For benchmarking we consider five CMA-ES algorithms in BIPOP restart scenario [3]: BIPOP-aCMA-ES [16, 3], BIPOP-^{s*}aACM-ES [17], BIPOP-^{s*}aACM-ES-k [18], BIPOP-aCMA-STEP and HCMA¹. For all but BIPOP-^{s*}aACM-ES-k [18] and BIPOP-aCMA-STEP algorithms the BBOB results are taken from the literature. The setting of parameters of BIPOP-^{s*}aACM-ES-k is given in [18], the maximum number of function evaluations is set to 10^6n . However, surrogate models are used only for the first $2 \cdot 10^5$ (10^4n for $n = 20$) function evaluations for $n = 2, 3, 5, 10, 20$ and $2 \cdot 10^3n$ evaluations for $n = 40$ in order to reduce the overall running time and to fit to the BBOB-2013 focus on expensive optimization with the budget of up to 10^3n function evaluations. The value of k_λ is set to 1, 1, 1, 10, 100, 1000 for $n = 2, 3, 5, 10, 20, 40$, respectively; $k_\mu = 1$ for all dimensions; $\hat{n}_{k_\lambda} = 4$. The value of l (respectively, p) of the STEP is set to 10^{-10} (respectively, 10^{-8}), $n_{MinIterSTEP} = 10$ and $\rho_{STEP} = 0.5$. The following parameters of NEWUOA are

¹For the sake of reproducibility the source code is available at <http://sites.google.com/site/bbobgecco2013/>

used [22]: $m = 2n + 1$ interpolation points, the initial radius ρ_{beg} of the search region is set to 10, the final radius ρ_{end} is set to 10^{-16} , the maximum number of function evaluations is set to $10n$.

3. RESULTS

Results from experiments according to [4] on the benchmark functions given in [4] are presented in Figures 1 and 2 and in Table 1. The **expected running time (ERT)**, used in the figures and table, depends on a given target function value, $f_t = f_{opt} + \Delta f$, and is computed over all relevant trials (on the first 15 instances) as the number of function evaluations executed during each trial while the best function value did not reach f_t , summed over all trials and divided by the number of trials that actually reached f_t [4]. **Statistical significance** is tested with the rank-sum test for a given target Δf_t (10^{-8} as in Figure 1) using, for each trial, either the number of needed function evaluations to reach Δf_t (inverted and multiplied by -1), or, if the target was not reached, the best Δf -value achieved, measured only up to the smallest number of overall function evaluations for any unsuccessful trial under consideration.

The BIPOP-^{s*}aACM-ES and BIPOP-^{s*}aACM-ES-k perform similarly for $n = 2, 3, 5$ and before 10^4n function evaluations because $k_\lambda = 1$ is used, after 10^4n evaluations BIPOP-^{s*}aACM-ES-k represents BIPOP-aCMA-ES. For larger n , BIPOP-^{s*}aACM-ES-k outperforms BIPOP-^{s*}aACM-ES on unimodal ill-conditioned problems, e.g., for 20-dimensional ones the target function values 10^{-8} can be reached faster (see Figure 1, Table 1): by a factor of 1.8 on f_2 Separable Ellipsoid and f_{10} Rotated Ellipsoid functions, by a factor of 1.5 on f_{11} Discus, by a factor of 1.1 on f_{12} Bent cigar, by a factor of 1.8 on f_{13} Sharp ridge and by a factor of 1.2 on f_{14} Sum of different powers. On f_8 and f_9 Rosenbrock's function the speedup of a factor of about 1.3 is obtained.

A relative loss of performance (compared to BIPOP-^{s*}aACM-ES) on multi-modal functions can be explained by not using surrogate models after 10^4n and thus using the original BIPOP-aCMA-ES which usually is outperformed by BIPOP-^{s*}aACM-ES. A loss of performance is observed on f_6 Attractive sector (by a factor of 1.2), f_{17} Schaffer (by a factor of 1.2) and f_{23} Katsuuras (by a factor of 1.5). However, the reason of this loss remains unclear for f_{17} and f_{23} functions because a similar loss of performance is also observed on the same problems in dimension 5 where $k_\lambda = 1$ for both algorithms (i.e., there is no intensive surrogate model exploitation). This difference might be explained by the stochasticity of multi-modal optimization or by fact of adapting an additional hyper-parameter - a stopping criterion of SVM surrogate learning procedure in BIPOP-^{s*}aACM-ES-k [18], whose values were fixed in BIPOP-^{s*}aACM-ES [17]. The adaptation of this hyper-parameter probably is not efficient enough compared to the offline tuned value, but this adaptation makes the algorithm more parameter-free. While there is no data to assess the effect of more intensive surrogate model exploitation for budgets larger than 10^4n , the loss of performance on f_6 is clearly due to $k_\lambda > 1$. A simple way to reduce this loss would be to increment \hat{n}_{k_λ} , but this might decrease the speedup on ill-conditioned problems back toward the level of BIPOP-^{s*}aACM-ES.

The results shown in Figure 2 suggest that separable multi-modal functions such as f_3 Separable Rastrigin and f_4 Separable Skew Rastrigin-Bueche can be easily solved by BIPOP-

aCMA-STEP and HCMA thanks to its STEP part. Thus, this kind of hybridization is beneficial if the main target is to solve the maximum number of problems within a relatively large budget of function evaluations.

The HCMA demonstrates the best performance among the tested algorithms after $100n$ function evaluations. The hybridization with STEP allows to exploit the separability when it is detected, i.e., when STEP generates better solutions than BIPOP-^{s*}aACM-ES-k. In a few cases when separability was not detected successfully 3-dimensional f_3 Rastigin and 3-, 5-dimensional f_4 Skew Rastrigin-Bueche separable functions, it seems that $10n$ function evaluations ($n_{MinIterSTEP} = 10$) sometimes is not sufficient to see the difference between STEP and BIPOP-^{s*}aACM-ES-k on these problems.

4. CPU TIMING EXPERIMENT

The time complexity of BIPOP-aCMA-STEP is essentially the same as the one of BIPOP-aCMA-ES since the STEP has linear time complexity and its relatively small "constant factor" (see Eq.(2)) depends only on a particular implementation. The time complexity of BIPOP-^{s*}aACM-ES-k was measured after 15 runs on 20-dimensional f_8 , the cost per function evaluation is about 0.45 seconds (runs were performed on different machines with 2.2 and 2.4 GHz cores under Ubuntu 10.04 using Octave 3.2.3). These results are similar to the ones of [15], the time complexity can be reduced by a factor of $\lambda_{hyp} = 20$ by switching off the adaptation of surrogate hyper-parameters.

5. CONCLUSION

In this paper, we have compared the recently proposed self-adaptive surrogate-assisted BIPOP-^{s*}aACM-ES-k with intensive surrogate model exploitation and its predecessor BIPOP-^{s*}aACM-ES with the BIPOP-aCMA-ES. The comparison shows that the performance of surrogate-assisted CMA-ES can be further improved on ill-conditioned functions, e.g., on 20-dimensional f_{10} Rotated Ellipsoid the BIPOP-^{s*}aACM-ES-k algorithm is about 6 times faster than BIPOP-aCMA-ES and about 1.8 times faster than BIPOP-^{s*}aACM-ES. However, the performance on multi-modal functions should be further analyzed for a larger maximum number of function evaluations.

The proposed BIPOP-aCMA-STEP as expected shows good results on separable multi-modal functions by exploitation when it is detected (when STEP performs better than BIPOP-aCMA-ES). The proposed hybrid HCMA algorithm demonstrates the best overall performance when running for more than $100n$ function evaluations on 10-, 20- and 40-dimensional problems, its overall performance for this budget of function evaluations and for these dimensions is better than of all algorithms tested during the BBOB-2009, BBOB-2010 and BBOB-2012.

It would be interesting to further develop HCMA and BIPOP-aCMA-STEP and make these algorithms better suited to partially-separable functions and/or adjust the algorithm to work in a sampling space of CMA-ES defined by its covariance matrix. A natural perspective is to improve the results of HCMA on multi-modal function by applying the recently proposed alternative restart strategies for CMA-ES [16].

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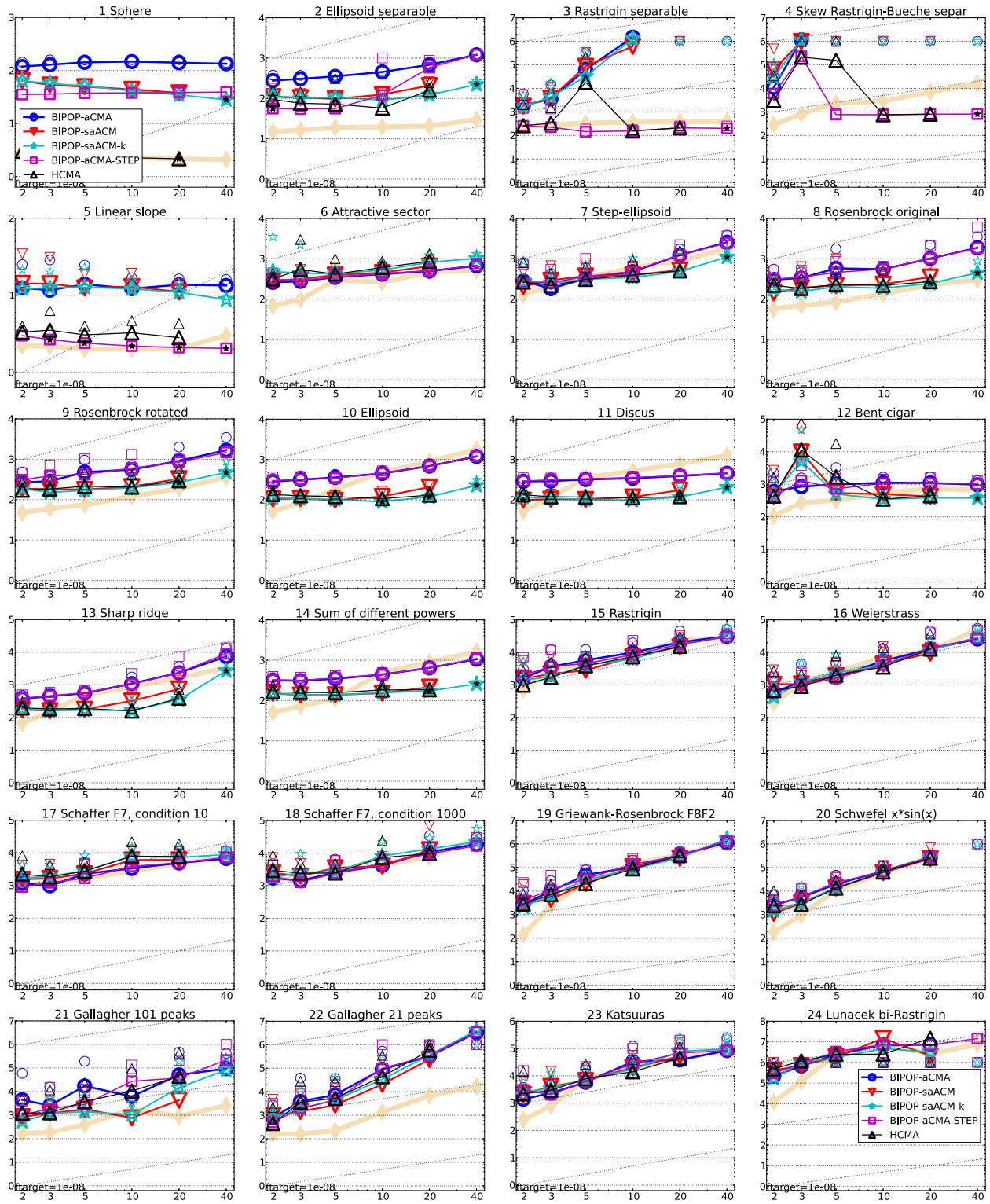


Figure 1: Expected running time (ERT in number of f -evaluations) divided by dimension for target function value 10^{-8} as \log_{10} values versus dimension. Different symbols correspond to different algorithms given in the legend of f_1 and f_{24} . Light symbols give the maximum number of function evaluations from the longest trial divided by dimension. Horizontal lines give linear scaling, slanted dotted lines give quadratic scaling. Black stars indicate statistically better result compared to all other algorithms with $p < 0.01$ and Bonferroni correction number of dimensions (six). Legend: \circ :BIPOP-aCMA, ∇ :BIPOP-saACM, \star :BIPOP-saACM-k, \square :BIPOP-aCMA-STEP, \triangle :HCMA.

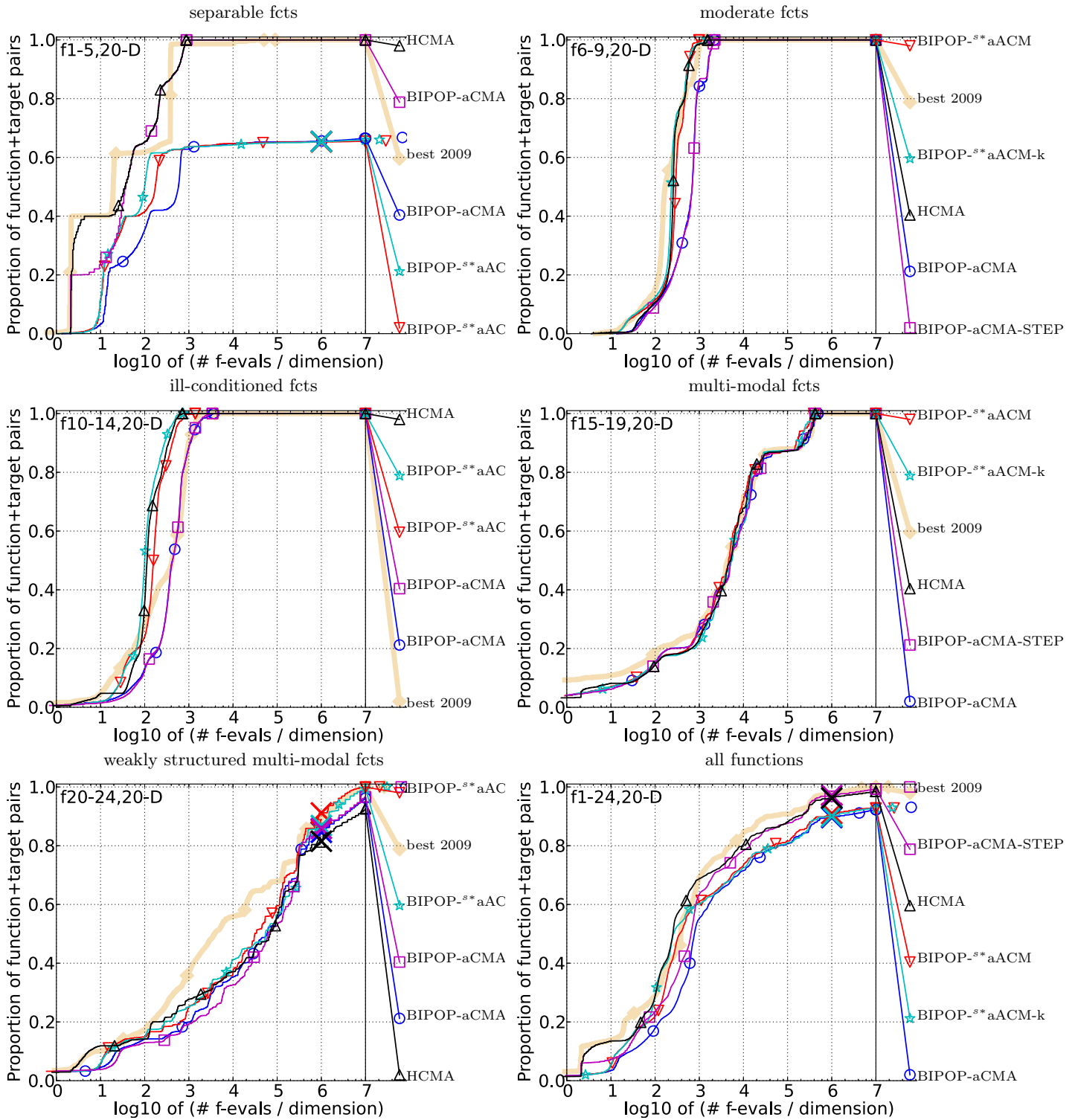


Figure 2: Bootstrapped empirical cumulative distribution of the number of objective function evaluations divided by dimension (FEvals/D) for 50 targets in $10^{[-8..2]}$ for all functions and subgroups in 20-D. The “best 2009” line corresponds to the best ERT observed during BBOB 2009 for each single target.

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