

Comparing Natural Evolution Strategies to BIPOP-CMA-ES on Noiseless and Noisy Black-box Optimization Testbeds

Tom Schaul

Courant Institute of Mathematical Sciences, New York University
Broadway 715, New York, USA
schaul@cims.nyu.edu

ABSTRACT

Natural Evolution Strategies (NES) are a recent member of the class of real-valued optimization algorithms that are based on adapting search distributions. Exponential NES (xNES) are the most common instantiation of NES, and particularly appropriate for the BBOB 2012 benchmarks, given that many are non-separable, and their relatively small problem dimensions. Here, we augment xNES with adaptation sampling, which adapts learning rates online, and compare the resulting performance directly to the BIPOP-CMA-ES algorithm, the winner of the 2009 black-box optimization benchmarking competition (BBOB). This report provides an extensive empirical comparison, both on the noise-free and noisy BBOB testbeds.

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

Keywords

Evolution Strategies, Natural Gradient, Benchmarking

1. INTRODUCTION

Evolution strategies (ES), in contrast to traditional evolutionary algorithms, aim at repeating the type of mutation that led to those good individuals. We can characterize those mutations by an explicitly parameterized *search distribution* from which new candidate samples are drawn, akin to estimation of distribution algorithms (EDA). Covariance matrix adaptation ES (CMA-ES [12]) innovated the field by

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. To copy otherwise, to republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee.

GECCO'12 Companion, July 7–11, 2012, Philadelphia, PA, USA.
Copyright 2012 ACM 978-1-4503-1178-6/12/07 ...\$10.00.

introducing a parameterization that includes the full covariance matrix, allowing them to solve highly non-separable problems.

A more recent variant, *natural evolution strategies* (NES [22, 6, 20, 21]) aims at a higher level of generality, providing a procedure to update the search distribution's parameters for any type of distribution, by ascending the gradient towards higher expected fitness. Further, it has been shown [17, 15] that following the *natural gradient* to adapt the search distribution is highly beneficial, because it appropriately normalizes the update step with respect to its uncertainty and makes the algorithm scale-invariant.

Exponential NES (xNES), the most common instantiation of NES, used a search distribution parameterized by a mean vector and a full covariance matrix, and is thus most similar to CMA-ES (in fact, the precise relation is described in [4] and [5]). Given the relatively small problem dimensions of the BBOB benchmarks, and the fact that many are non-separable, it is also among the most appropriate NES variants for the task. Adaptation sampling is a technique for the online adaptation of its learning rate, which is designed to speed up convergence. This may be beneficial to algorithms like xNES, because the optimization traverses qualitatively different phases, during which different learning rates may be optimal.

In this report, we retain the original formulation of xNES (including all parameter settings, except for an added stopping criterion), but augmented with adaptation sampling. We compare this algorithm (xNES-as) to the winning entry of the 2009 BBOB competition, namely BIPOP-CMA-ES, described in detail in [7, 8]. We describe the comparative empirical performance on all 54 benchmark functions (both noise-free and noisy) of the BBOB 2012 workshop.

2. NATURAL EVOLUTION STRATEGIES

Natural evolution strategies (NES) maintain a search distribution π and adapt the distribution parameters θ by following the *natural gradient* [1] of expected fitness J , that is, maximizing

$$J(\theta) = \mathbb{E}_\theta[f(\mathbf{z})] = \int f(\mathbf{z}) \pi(\mathbf{z}|\theta) d\mathbf{z}$$

Just like their close relative CMA-ES [12], NES algorithms are invariant under monotone transformations of the fitness function and linear transformations of the search space. Each iteration the algorithm produces n samples $\mathbf{z}_i \sim \pi(\mathbf{z}|\theta)$, $i \in \{1, \dots, n\}$, i.i.d. from its search distribution, which is parameterized by θ . The gradient w.r.t. the parameters θ can

be rewritten (see [22]) as

$$\nabla_{\theta} J(\theta) = \nabla_{\theta} \int f(\mathbf{z}) \pi(\mathbf{z} | \theta) d\mathbf{z} = \mathbb{E}_{\theta} [f(\mathbf{z}) \nabla_{\theta} \log \pi(\mathbf{z} | \theta)]$$

from which we obtain a Monte Carlo estimate

$$\nabla_{\theta} J(\theta) \approx \frac{1}{n} \sum_{i=1}^n f(\mathbf{z}_i) \nabla_{\theta} \log \pi(\mathbf{z}_i | \theta)$$

of the search gradient. The key step then consists in replacing this gradient by the natural gradient defined as $\mathbf{F}^{-1} \nabla_{\theta} J(\theta)$ where $\mathbf{F} = \mathbb{E} [\nabla_{\theta} \log \pi(\mathbf{z} | \theta) \nabla_{\theta} \log \pi(\mathbf{z} | \theta)^{\top}]$ is the Fisher information matrix. The search distribution is iteratively updated using natural gradient ascent

$$\theta \leftarrow \theta + \eta \mathbf{F}^{-1} \nabla_{\theta} J(\theta)$$

with learning rate parameter η .

2.1 Exponential NES

While the NES formulation is applicable to arbitrary parameterizable search distributions [22, 15], the most common variant employs multinormal search distributions. For that case, two helpful techniques were introduced in [6], namely an exponential parameterization of the covariance matrix, which guarantees positive-definiteness, and a novel method for changing the coordinate system into a ‘‘natural’’ one, which makes the algorithm computationally efficient. The resulting algorithm, NES with a multivariate Gaussian search distribution and using both these techniques is called *xNES*, and the pseudocode is given in Algorithm 1.

Algorithm 1: Exponential NES (xNES)

input: $f, \boldsymbol{\mu}_{\text{init}}, \eta_{\sigma}, \eta_{\mathbf{B}}, u_k$

initialize $\boldsymbol{\mu} \leftarrow \boldsymbol{\mu}_{\text{init}}$
 $\sigma \leftarrow 1$
 $\mathbf{B} \leftarrow \mathbb{I}$

repeat

for $k = 1 \dots n$ **do**

 draw sample $\mathbf{s}_k \sim \mathcal{N}(0, \mathbb{I})$

$\mathbf{z}_k \leftarrow \boldsymbol{\mu} + \sigma \mathbf{B}^{\top} \mathbf{s}_k$

 evaluate the fitness $f(\mathbf{z}_k)$

end

 sort $\{(\mathbf{s}_k, \mathbf{z}_k)\}$ with respect to $f(\mathbf{z}_k)$

 and assign utilities u_k to each sample

 compute gradients

$\nabla_{\delta} J \leftarrow \sum_{k=1}^n u_k \cdot \mathbf{s}_k$

$\nabla_{\mathbf{M}} J \leftarrow \sum_{k=1}^n u_k \cdot (\mathbf{s}_k \mathbf{s}_k^{\top} - \mathbb{I})$

$\nabla_{\sigma} J \leftarrow \text{tr}(\nabla_{\mathbf{M}} J) / d$

$\nabla_{\mathbf{B}} J \leftarrow \nabla_{\mathbf{M}} J - \nabla_{\sigma} J \cdot \mathbb{I}$

 update parameters

$\boldsymbol{\mu} \leftarrow \boldsymbol{\mu} + \sigma \mathbf{B} \cdot \nabla_{\delta} J$

$\sigma \leftarrow \sigma \cdot \exp(\eta_{\sigma} / 2 \cdot \nabla_{\sigma} J)$

$\mathbf{B} \leftarrow \mathbf{B} \cdot \exp(\eta_{\mathbf{B}} / 2 \cdot \nabla_{\mathbf{B}} J)$

until *stopping criterion is met*

2.2 Adaptation Sampling

First introduced in [15] (chapter 2, section 4.4), *adaptation sampling* is a new meta-learning technique [19] that can

adapt hyper-parameters online, in an economical way that is grounded on a measure statistical improvement.

Here, we apply it to the learning rate of the global step-size η_{σ} . The idea is to consider whether a larger learning-rate $\eta'_{\sigma} = \frac{3}{2} \eta_{\sigma}$ would have been more likely to generate the good samples in the current batch. For this we determine the (hypothetical) search distribution that would have resulted from such a larger update $\pi(\cdot | \theta')$. Then we compute importance weights

$$w'_k = \frac{\pi(\mathbf{z}_k | \theta')}{\pi(\mathbf{z}_k | \theta)}$$

for each of the n samples \mathbf{z}_k in our current population, generated from the actual search distribution $\pi(\cdot | \theta)$. We then conduct a *weighted* Mann-Whitney test [15] (appendix A) to determine if the set $\{\text{rank}(\mathbf{z}_k)\}$ is inferior to its reweighted counterpart $\{w'_k \cdot \text{rank}(\mathbf{z}_k)\}$ (corresponding to the larger learning rate), with statistical significance ρ . If so, we increase the learning rate by a factor of $1 + c'$, up to at most $\eta_{\sigma} = 1$ (where $c' = 0.1$). Otherwise it decays to its initial value:

$$\eta_{\sigma} \leftarrow (1 - c') \cdot \eta_{\sigma} + c' \cdot \eta_{\sigma, \text{init}}$$

The procedure is summarized in algorithm 2 (for details and derivations, see [15]). The combination of xNES with adaptation sampling is dubbed *xNES-as*.

One interpretation of why adaptation sampling is helpful is that half-way into the search, (after a local attractor has been found, e.g., towards the end of the valley on the Rosenbrock benchmarks f_8 or f_9), the convergence speed can be boosted by an increased learning rate. For such situations, an online adaptation of hyper-parameters is inherently well-suited.

Algorithm 2: Adaptation sampling

input : $\eta_{\sigma, t}, \eta_{\sigma, \text{init}}, \theta_t, \theta_{t-1}, \{(\mathbf{z}_k, f(\mathbf{z}_k))\}, c', \rho$

output: $\eta_{\sigma, t+1}$

compute hypothetical θ' , given θ_{t-1} and using $3/2 \eta_{\sigma, t}$

for $k = 1 \dots n$ **do**

$w'_k = \frac{\pi(\mathbf{z}_k | \theta')}{\pi(\mathbf{z}_k | \theta)}$

end

$S \leftarrow \{\text{rank}(\mathbf{z}_k)\}$

$S' \leftarrow \{w'_k \cdot \text{rank}(\mathbf{z}_k)\}$

if *weighted-Mann-Whitney*(S, S') $< \rho$ **then**

return $(1 - c') \cdot \eta_{\sigma} + c' \cdot \eta_{\sigma, \text{init}}$

else

return $\min((1 + c') \cdot \eta_{\sigma}, 1)$

end

3. EXPERIMENTAL SETTINGS

We use identical default hyper-parameter values for all benchmarks (both noisy and noise-free functions), which are taken from [6, 15]. Table 1 summarizes all the hyper-parameters used.

In addition, we make use of the provided target fitness f_{opt} to trigger *independent* algorithm restarts¹, using a simple

¹It turns out that this use of f_{opt} is technically not permitted by the BOB guidelines, so strictly speaking a different restart strategy should be employed, for example the one described in [15].

Table 1: Default parameter values for xNES (including the utility function and adaptation sampling) as a function of problem dimension d .

parameter	default value
n	$4 + \lceil 3 \log(d) \rceil$
$\eta_\sigma = \eta_B$	$\frac{3(3 + \log(d))}{5d\sqrt{d}}$
u_k	$\frac{\max(0, \log(\frac{n}{2} + 1) - \log(k))}{\sum_{j=1}^n \max(0, \log(\frac{n}{2} + 1) - \log(j))} - \frac{1}{n}$
ρ	$\frac{1}{2} - \frac{1}{3(d+1)}$
c'	$\frac{1}{10}$

ad-hoc procedure: If the log-progress during the past $1000d$ evaluations is too small, i.e., if

$$\log_{10} \left| \frac{f_{\text{opt}} - f_t}{f_{\text{opt}} - f_{t-1000d}} \right| < (r+2)^2 \cdot m^{3/2} \cdot [\log_{10} |f_{\text{opt}} - f_t| + 8]$$

where m is the remaining budget of evaluations divided by $1000d$, f_t is the best fitness encountered until evaluation t and r is the number of restarts so far. The total budget is $10^5 d^{3/2}$ evaluations.

Implementations of this and other NES algorithm variants are available in Python through the PyBrain machine learning library [18], as well as in other languages at www.idsia.ch/~tom/nas.html.

4. RESULTS

Results from experiments according to [9] on the benchmark functions given in [2, 10, 3, 11] are presented in Figures 1, 2 and 3 and in Tables 2, 3 and 4. The **expected running time (ERT)**, used in the figures and table, depends on a given target function value, $f_t = f_{\text{opt}} + \Delta f$, and is computed over all relevant trials 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 [9, 13]. **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.

Some of the result plots (like performance scaling with dimension on the noisy benchmarks), as well as the CPU-timing results were omitted here but are available in a stand-alone benchmarking report [16].

5. DISCUSSION

Figure 2 gives a good overview picture, showing that across all benchmarks taken together, both BIPOP-CMA-ES and xNES-as performs better than most of the BBOB 2009 contestants.

According to Tables 2, 3 and 4, BIPOP-CMA-ES is consistently outperforming xNES-as (in dimensions 5 and 20)

on functions 1, 5, 6, 15, 20, 23, 101, 102, 103, 105, 107, 108, 109, 114, 120, 122, 123 and 127, and it additionally does so in dimension 20 on functions 8, 9, 12, 16, 24 104, 113 and 116.

On the other hand, xNES-as is consistently outperforming BIPOP-CMA-ES (in dimensions 5 and 20) on functions 4, 10, 11, 18, 115 and 118, and additionally does so on dimension 20 on function 2.

In conclusion, we find that xNES-as is close in performance to BIPOP-CMA-ES, across a large fraction of the benchmark functions; but there is some diversity as well, with xNES-as being significantly better on 6 of the functions and significantly worse on 18 of them. Clearly, xNES-as underperforms on multi-modal functions, a weakness that could be addressed through larger population sizes, or better even, *adaptive* population sizes – possibly using a similar scheme than the one presented here for making learning rates adaptive.

Acknowledgements

The author wants to thank the organizers of the BBOB workshop for providing such a well-designed benchmark setup, and especially such high-quality post-processing utilities.

This work was funded in part through AFR postdoc grant number 2915104, of the National Research Fund Luxembourg.

6. REFERENCES

- [1] S. I. Amari. Natural Gradient Works Efficiently in Learning. *Neural Computation*, 10:251–276, 1998.
- [2] S. Finck, N. Hansen, R. Ros, and A. Auger. Real-parameter black-box optimization benchmarking 2009: Presentation of the noiseless functions. Technical Report 2009/20, Research Center PPE, 2009. Updated February 2010.
- [3] S. Finck, N. Hansen, R. Ros, and A. Auger. Real-parameter black-box optimization benchmarking 2010: Presentation of the noisy functions. Technical Report 2009/21, Research Center PPE, 2010.
- [4] N. Fukushima, Y. Nagata, S. Kobayashi, and I. Ono. Proposal of distance-weighted exponential natural evolution strategies. In *2011 IEEE Congress of Evolutionary Computation*, pages 164–171. IEEE, 2011.
- [5] T. Glasmachers, T. Schaul, and J. Schmidhuber. A Natural Evolution Strategy for Multi-Objective Optimization. In *Parallel Problem Solving from Nature (PPSN)*, 2010.
- [6] T. Glasmachers, T. Schaul, Y. Sun, D. Wierstra, and J. Schmidhuber. Exponential Natural Evolution Strategies. In *Genetic and Evolutionary Computation Conference (GECCO)*, Portland, OR, 2010.
- [7] N. Hansen. Benchmarking a BI-population CMA-ES on the BBOB-2009 function testbed. In Rothlauf [14], pages 2389–2396.
- [8] N. Hansen. Benchmarking a BI-population CMA-ES on the BBOB-2009 noisy testbed. In Rothlauf [14], pages 2397–2402.
- [9] N. Hansen, A. Auger, S. Finck, and R. Ros. Real-parameter black-box optimization benchmarking 2012: Experimental setup. Technical report, INRIA, 2012.

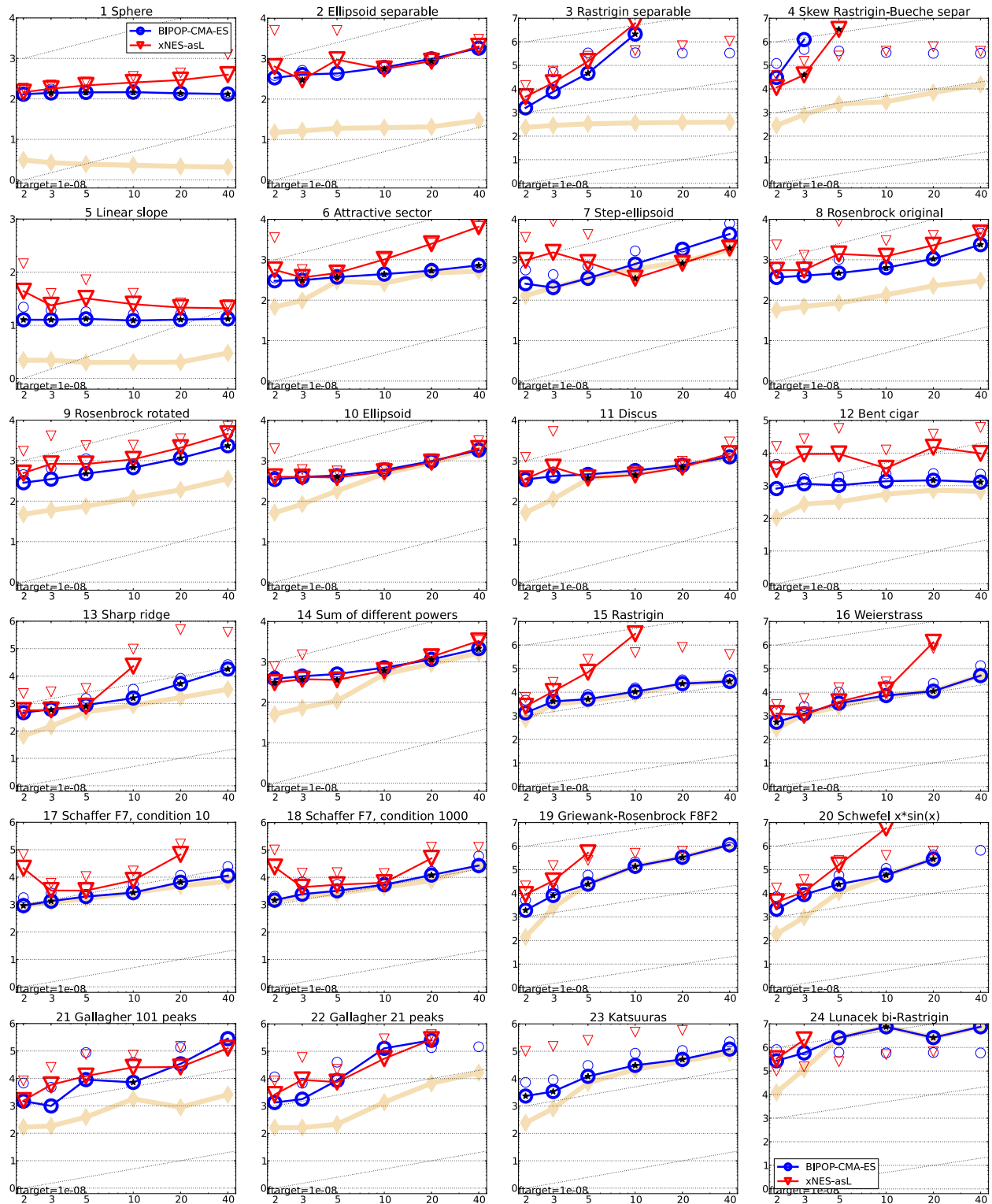


Figure 1: Expected running time (ERT in number of f -evaluations) divided by dimension for target function value 10^{-8} as \log_{10} values versus dimension. Different symbols correspond to different algorithms given in the legend of f_1 and f_{24} . Light symbols give the maximum number of function 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-CMA-ES, ∇ :xNES-as.

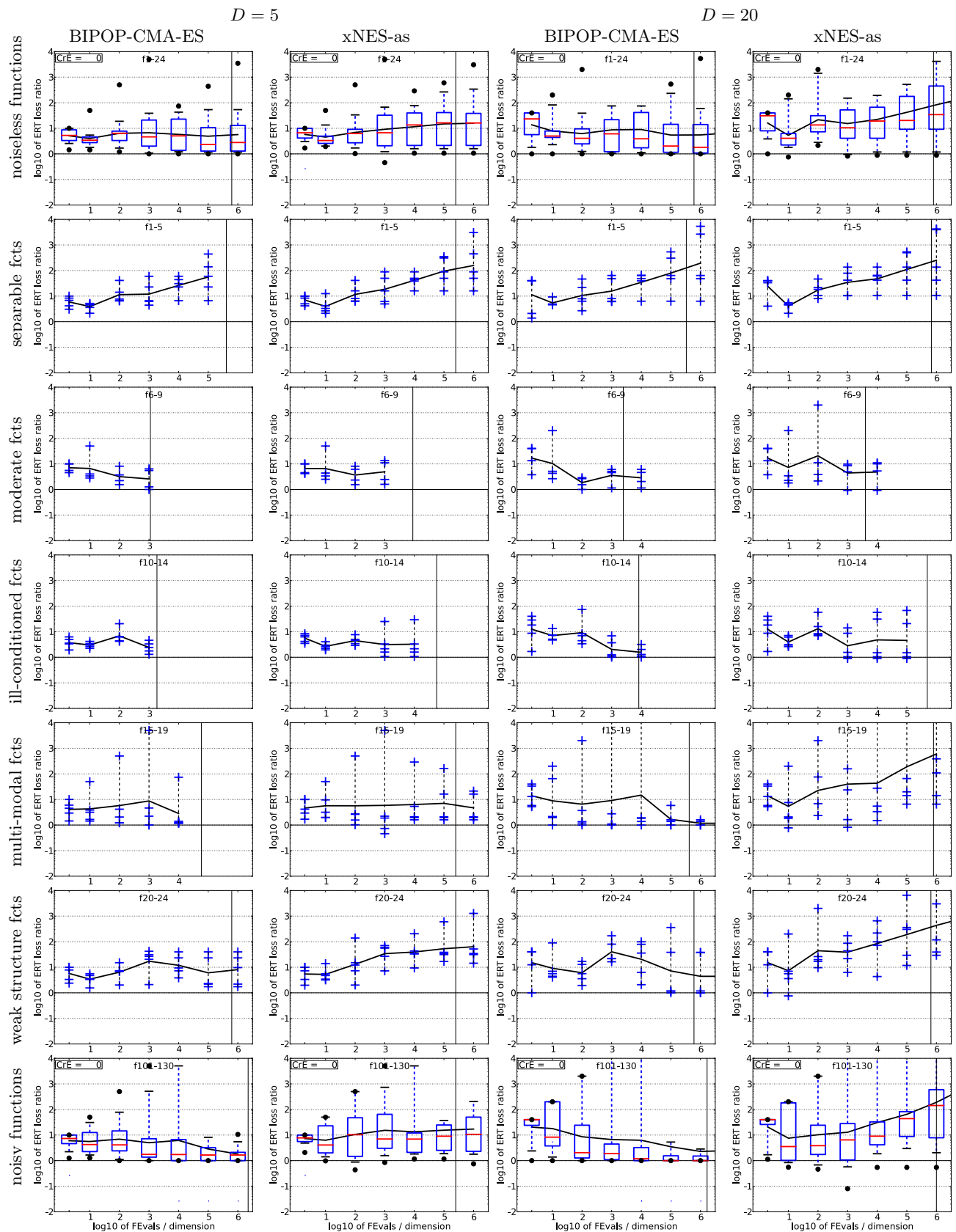


Figure 3: ERT loss ratio vs. a given budget FEvals. Each cross (+) represents a single function. The target value f_t used for a given FEvals is the smallest (best) recorded function value such that $ERT(f_t) \leq FEvals$ for the presented algorithm. Shown is FEvals divided by the respective best $ERT(f_t)$ from BBOB-2009 for functions f_1 – f_{24} in 5-D and 20-D. Line: geometric mean. Box-Whisker error bar: 25-75%-ile with median (box), 10-90%-ile (caps), and minimum and maximum ERT loss ratio (points). The vertical line gives the maximal number of function evaluations in a single trial in this function subset.

