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Benchmarking CMA-ES with Basic Integer Handling on a Mixed-Integer Test Problem Suite

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ABSTRACT

We compare the performances of one implementation of CMA-ES (pycma version 3.3.0) for optimizing functions with both continuous and integer variables. The implementation incorporates a lower bound on the variance along the integer coordinates to keep the optimization from stalling. This benchmark will serve as a baseline for further works on pycma. Results show substantial improvement since the last benchmarked version of pycma. Also this implementation is competitive with other mixed integer algorithms.

CCS CONCEPTS

•Computing methodologies → Continuous space search;

KEYWORDS

Benchmarking, Black-box optimization, Mixed-integer optimization

ACM Reference format:

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1 INTRODUCTION

Mixed optimization problems are of great importance in real-world applications. Typically, variables include real-valued degrees of freedom that correspond, directly or not, to physical measurements (e.g. angles, frequencies, forces, etc.) as well as discrete (integer or binary) settings that correspond to categorical choices (e.g. materials) or service activations (e.g. radar modes). Therefore, developing algorithmic variants that can handle several types of optimization variable at the same time without impairing the search process will be very useful in practice.

In the context of black box optimization for problems with continuous variables, evolutionary algorithms which update a covariance matrix, namely CMA-ES, have been studied for more than 20 years

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[10]. While the CMA-ES was originally not designed to handle integer variables, it can be employed with integer variables by using the integer part of a continuous variable in the fitness evaluation. This is however expected to lead to integer variables getting stuck in the resulting fitness plateaus, and several versions have been proposed to improve the algorithm in this situation [4, 5].

In order to study mixed integer problems within the COCO framework [9], the bbob-mixint testbed was proposed in [13]. This testbed is based on the 24 functions of the bbob testbed with 80% of the variables to be integer with an arity between 2 and 16.

In order to prevent variables getting stuck on the same integer level, for example in CMA-ES, a lower bound on the variance can be set such that there remains a reasonable probability for an integer variable to “jump” to another integer level, as for example in CMA-ES with margin (CMA-ESwM) [4]. The same principle is implemented in the pycma code with Integer Handling (cma-IH in the benchmark) with a more simplistic approach.

The purpose of this paper is to measure the performance of the current implementation of the widely distributed cma-IH code (version 3.3.0) [6] with different options and compare its performance with previous results and enhancements.

2 ALGORITHM PRESENTATION

The general idea behind cma-IH is to set a lower bound for the variance of the integer variables. It prevents integer variables from being trapped in one value. We formulate the bounding using the covariance matrix decomposition from the CMA-ES with diagonal decoding [1]. At each new iteration $t + 1$, new candidate solutions, $x^{(t+1)}$, are sampled according to a multivariate normal distribution.

$$\begin{aligned} x^{(t+1)} &\sim \mathcal{N}(m, \sigma^{(t)^2} C^{(t)}) \\ &\sim m + \sigma^{(t)} \sqrt{C^{(t)}} \mathcal{N}(0, \mathbf{I}), \end{aligned}$$

where C is a covariance matrix and σ is the step size. In order to bound the standard deviation of each integer variable, we introduce the diagonal scaling matrix D ,

$$x^{(t+1)} \sim m + \sigma^{(t)} D^{(t)} \sqrt{C^{(t)}} \mathcal{N}(0, \mathbf{I}),$$

where $D^{(0)}$ is the identity. The update of σ and C are done as in the original CMA-ES algorithm. Then, the diagonal matrix D is updated based on the current standard deviation in each coordinate. The standard deviation of the i^{th} -th coordinate of x , $\sigma_{\text{std}(i)}^{(t)}$, is computed with the diagonal elements of C and D :

```

import cocoex
import cma
suite = cocoex.Suite('bbob-mixint', '', '')
for problem in suite :
    up_bound = list(problem.upper_bounds[
        :problem.number_of_integer_variables]) +
        [None]
    lo_bound = list(problem.lower_bounds[
        :problem.number_of_integer_variables]) +
        [None]
    cma.fmin2(problem, problem.initial_solution, 1,
        {'bounds': [lo_bound, up_bound]
        'CMA_std': (problem.upper_bounds
        - problem.lower_bounds)/5,
        'integer_variables': list(range(
        problem.number_of_integer_variables)),
        restarts =9)})
    
```

Figure 1: Calling code to benchmark `cma.fmin2`.

$$\sigma_{std(i)}^{(t)} = \sigma^{(t)} D_{i,i}^{(t)} \sqrt{C_{i,i}^{(t)}}$$

This standard deviation has to be compared with a lower bound σ_{LB} . If the standard deviation in the i^{th} coordinate is smaller than the threshold value, $\sigma_{std(i)}^{(t)} < \sigma_{LB}$, then the D matrix is scaled up in this coordinate.

$$D_{i,i}^{(t+1)} \leftarrow \begin{cases} \frac{\sigma_{LB}}{\sigma^{(t)} \sqrt{C_{i,i}^{(t)}}} & \text{if } 1 \leq i \leq N_{\text{int}} \text{ and } \sigma_{std(i)}^{(t)} \leq \sigma_{LB} \\ D_{i,i}^{(t)} & \text{otherwise} \end{cases} \quad (1)$$

where N_{int} is the number of integer variables. In the version 3.3.0 of `pycma` with integer handling (`cma-IH`), the lower bound is set to:

$$\sigma_{LB} = \frac{1}{2N_{\text{int}} + 1} \quad (2)$$

3 EXPERIMENTAL PROCEDURE

Figure 1 shows the calling code and options used to run the benchmark for `cma-IH`. A maximum of nine restarts may be performed and each restart doubles the population size starting from the default (IPOP-CMA-ES) [2]. The initial step size is chosen to sample solutions mainly within the upper and the lower bound of the problem. The bounds are enforced on the integer variables only. The maximum number of function evaluations allowed per problem is set to 10^4 times the number of dimension of the problem.

This current implementation `cma-IH` is compared to performance data from the `bbob-mixint` COCO archive¹. We show results of the algorithms given in Table 1.

The experiments were performed and the plots were produced with COCO [9], version 2.6.3.

4 CPU TIMING

In order to evaluate the CPU timing of the algorithm, we have run the `cma-IH` algorithm with restarts on the `bbob-mixint` test

¹See <https://numbbo.github.io/data-archive>

Table 1: Compared algorithms

<code>cma-IH</code>	<code>pycma</code> version 3.3 (current) with the default integer handling option
<code>CMA-ES-pycma</code>	previous integer handling of <code>pycma</code> benchmarked in [13]
<code>CMA-ESwM</code>	CMA-ES with margin benchmarked in [3]
<code>cma-NoIH</code>	<code>pycma</code> version 3.3 (current) without any integer handling option
<code>cmaIH1e-1</code>	as <code>cma-IH</code> with a larger coordinate-wise lower bound on the sample standard deviation of $\sigma_{LB} = 10^{-1}$
<code>DE-scipy</code>	Differential Evolution implemented in <code>scipy</code> benchmarked in [13]
<code>RANDOMSEARCH</code>	Random Search algorithm for baseline

`suite` [13] with a maximum budget of $10^4 \times$ dimensions function evaluations according to [11].

The Python code was run on a Linux machine with 32 cores, Intel® Xeon® E7 to T3 v4 processor. The time per function evaluation averaged over all functions in the test bed for dimensions 5, 10, 20, 40, 80 and 160 equals 3.7, 4.9, 5.1, 5.6, 6.4 and 8.4×10^{-4} seconds respectively.

5 RESULTS

We show results from experiments according to [11] and [8] on the benchmark functions given in [13]. Figures 2 and 3 show summary results for the different function groups. Figure 4 shows the empirical distribution of function evaluations to reach 51 target values on the single functions [9]. Tables 2 and 3 present expected runtimes and statistical tests.²

The **expected runtime (ERT)**, used in the tables, depends on a given target precision, $I_{\text{target}} = f_{\text{opt}} + \Delta f$, 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 [11, 12]. **Statistical significance** is tested with the rank-sum test for a given target Δf_t using, for each trial, either the number of needed function evaluations to reach f_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.

Comparing two integer handling versions of `pycma`. We compare the performance of `cma-IH` (the current default implementation) versus `CMA-ES-pycma` (an older implementation). In comparison, the `cma-IH` performs increasingly better with increasing dimension and is overall about ten times faster than `CMA-ES-pycma` in dimension 80 (see Figure 3, lower right). The largest differences we observe on the ill-conditioned and multi-modal functions. The difference on the linear slope function is mainly due to the boundary handling which was applied also to the continuous variables in the `CMA-ES-pycma` experiment, as we confirmed in additional

²The entire data can be found at <https://trmarty.github.io/MixedIntegerData/>

experiments (not shown). The `cma-IH` performs statistically significantly better on 6, 8, 10, 16 and 15 functions in dimension 5, 10, 20, 40 and 80, respectively. The `CMA-ES-pycma` performs better on the separable ellipsoid function `f2` in dimension 20, 40 and 80.

Comparing pycma with and without the integer handling. The `cma-IH` and `cma-NoIH` perform very similar overall. The only statistically significant difference we observed is on the separable ellipsoid function `f2` in dimension 5 (not shown), where `cma-IH` is about three times faster than `cma-NoIH`, probably due to preventing additional restarts before to reach better targets. The default lower bound on the sample standard deviations for integer variables has overall little impact on the performance on this test suite.

A larger lower bound for the standard deviations. In order to understand the impact of the choice of the standard deviation lower bound value, we have run experiments with a few different bound values and show the results for the lower bound set to 10^{-1} . While in the smaller dimensions the effects are minor, in larger dimension the `cmaIH1e-1` performs overall best and is three times faster than `cma-IH` on the ill-conditioned functions in larger dimension for budgets above 100 times dimension. On the 80-dimensional *sphere* function, `cmaIH1e-1` solves the last target ten times quicker than `cma-IH` and also two times quicker than `CMA-ESwM`. The `cmaIH1e-1` also solves the *Ellipsoid separable* whereas `cma-IH` gets stuck at around 20% of targets. The `cmaIH1e-1` is slower than `CMA-ESwM` by a factor of approximately 3 on functions 5, 13 and 14, however it is significantly better than the current version `cma-IH` on functions 2, 5 or 12 while not being worse on all other functions. For this range of dimensions, bounding the standard deviation to 10^{-1} is a simple yet effective solution.

6 CONCLUSION

We have assessed the integer handling implemented in the current `pycma` module [7] (version 3.3.0). The performance with integer handling is overall superior to a previously benchmarked version, however it behaves quite similar to the version without integer handling. We attribute the latter observation to a suboptimal parameter setting: tests with a lower bound for the sample standard

deviations of $1/10$, which is considerably larger than the original setting, reveal a remarkably improved performance on a number of functions. In particular in larger dimension, this variant performs overall best.

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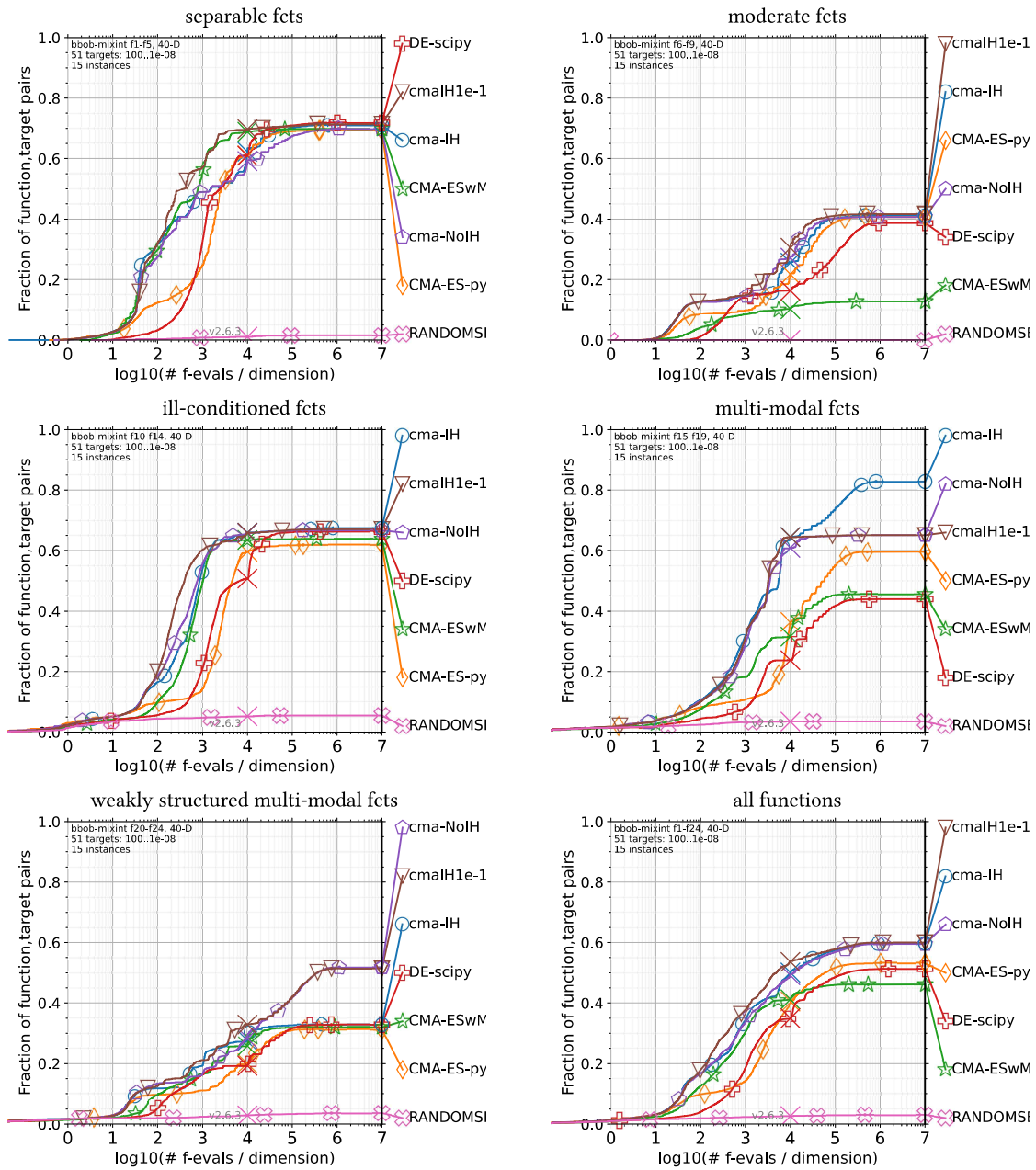


Figure 2: Bootstrapped empirical cumulative distribution of the number of f -evaluations divided by dimension (FEvals/DIM) for 51 targets with target precision in $10^{[-8..2]}$ for all functions and subgroups in 40-D.

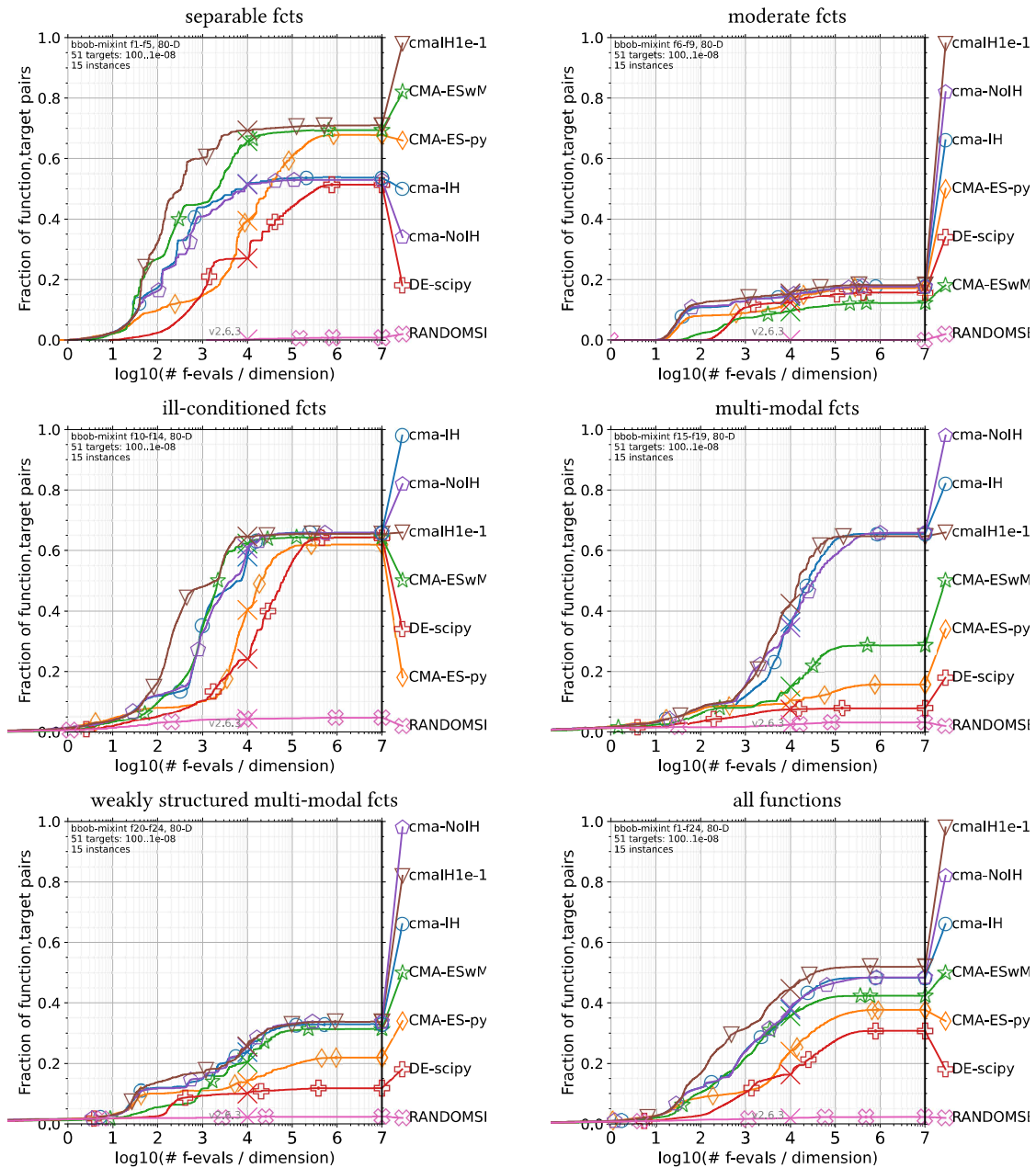


Figure 3: Bootstrapped empirical cumulative distribution of the number of f -evaluations divided by dimension (FEvals/DIM) for 51 targets with target precision in $10^{[-8..2]}$ for all functions and subgroups in 80-D.

