Derivative-Free Optimization Benchmarking and Performance Assessment

December 15, 2023 M2 Optimization, Université Paris-Saclay







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Practical Group Project

What do we want to achieve?

- understand some (new or not so new) algorithms
- learn how to conduct scientific testing, how to assess performance, and how to draw scientific conclusions from benchmarking data

How does it work?

- Today:
 - introduction to benchmarking
 - installation of COCO on your machines
 - first exercise to interpret (existing) benchmarking data
- In groups of 3
 - please use this to organize yourself: http://tinyurl.com/cocoproject2023

Practical Group Project

- We propose some possible algorithms (max. 1 group/algo)
 - but you can take others (e.g. your own)
 - benchmark this algorithm with the help of COCO (or other benchmarking software)
- 27th of January:
 - report (PDF) sent by email, 8 pages, template given by COCO
- 2nd of February:
 - 12 minutes presentation per group
 - + 10 minutes questions
 - about the algorithm
 - about its performance (compared to other algos)
 - order of the talks to be decided early next year
- 12th of January:
 - send a short progress statement by email (<10 lines)

Ideas for Algorithms/Papers

1) HypE: hypervolume estimation algorithm for multiobj. opt.

(C implementation available at https://sop.tik.ee.ethz.ch/download/supplementary/hype/)

- 2) ParEGO (multiobj. Efficient Global Optimization variant)
- 3) Gurobi (mixed-integer solver, academic license for free)
- 4) Nelder-Mead (on bbob-mixint)
- 5) Multiobjective NOMAD (https://www.gerad.ca/en/software/nomad/)
- 6a) Algorithms from PRIMA (https://github.com/libprima/prima)
- 6b) Algorithms from PDFO (https://pdfo.net)
- 7) TUrbO (https://github.com/uber-research/TuRBO)
- 8) derivative-free Newton method
- 9) SLSQP (from scipy.optimize) for constrained problems

[you will see more information/links in the Google document]

Ideas for Algorithms/Papers

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Note: for none of those algorithms, benchmarking data is available with COCO → additional (workshop) paper project possible afterwards

Benchmarking Optimization Algorithms

or: critical performance assessment







challenging optimization problems appear in many scientific, technological and industrial domains









Practical (Numerical) Blackbox Optimization



derivatives not available or not useful

Not clear:

which of the many algorithms should I use on my problem?

visualizing the raw data (single runs)

Displaying 3 runs (3 trials)



Displaying 51 runs

Don't hesitate to display all data (the appendix is your friend)



Displaying 51 runs



Which Statistics?



More Problems with Averages/Expectations

- to reliably estimate an expectation (from the *average*) we need to make *assumptions on the tail* of the underlying distribution
 - $\cdot \,$ these can not be implied from the observed data
 - AKA: the average is well-known to be (highly) sensitive to outliers (extreme events)
- rare events can only be analyzed by collecting a *large enough* number of data

from Hansen GECCO 2019 Experimentation tutorial

Which Statistics?



- unique for uneven number of data
- independent of log-scale, offset...

median(log(data))=log(median(data))

same when taken over x- or y-direction

• use the median as summary datum

unless there are good reasons for a different statistics out of practicality: use an odd number of repetitions

• more general: use quantiles as summary data

for example out of 15 data: 2nd, 8th, and 14th value represent the 10%, 50%, and 90%-tile

from Hansen GECCO 2019 Experimentation tutorial

Benchmarking =

evaluate the performance of optimization algorithms compare the performance of different algorithms

understand strengths and weaknesses of algorithms help in design of new algorithms

How Do We Measure Performance?

Meaningful quantitative measure

- quantitative on the ratio scale (highest possible)
 "algo A is two *times* better than algo B" is a meaningful statement
- assume a wide range of values
- meaningful (interpretable) with regard to the real world

possible to transfer from benchmarking to real world

How Do We Measure Performance?

Meaningful quantitative measure

- quantitative on the ratio scale (highest possible)
 "algo A is two *times* better than algo B" is a meaningful statement
- assume a wide range of values
- meaningful (interpretable) with regard to the real world possible to transfer from benchmarking to real world

CPU timing not a good candidate

→depends on implementation/language/machine/...

time is spent on code optimization instead of science J.N. Hooker: Testing heuristics, we have it all wrong, 1995, J. of Heuristics

Measuring Performance Empirically

convergence graphs is all we have to start with...



How Do We Measure Performance?

Two objectives:

- Find solution with small(est possible) function/indicator value
- With the least possible search costs (number of function evaluations)

For measuring performance: fix one and measure the other

Measuring Performance Empirically

convergence graphs is all we have to start with...



Collect for a given target (several target), the number of function evaluations needed to reach a target

Repeat several times:

if algorithms are stochastic, never draw a conclusion from a single run

if deterministic algorithm, repeat by changing (randomly) the initial conditions

ECDF:

Empirical Cumulative Distribution Function of the Runtime [aka data profile]

Cumulative Distribution Function (CDF)

Given a random variable T, the cumulative distribution function (CDF) is defined as

 $CDF_T(t) = Pr(T \le t)$ for all $t \in \mathbb{R}$

It characterizes the probability distribution of *T*

If two random variables have the same CDF, they have the same probability distribution

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Empirical Cumulative Distribution Function

Given a collection of data $T_1, T_2, ..., T_k$ (e.g. an empirical sample of a random variable) the *empirical* cumulative distribution function (ECDF) is a step function that jumps by 1/k at each value in the data.



It is an estimate of the CDF that generated the points in the sample.

Empirical Cumulative Distribution Function

$$ECDF_{(T_1,...,T_k)}(t) = \frac{\text{number of } T_i \le t}{k} = \frac{1}{k} \sum_{i=1}^k \mathbb{1}_{\{T_i \le t\}}$$

For $\{T_i: i \ge 1\}$ i.i.d. realization of a random variable T, by the LLN



A Convergence Graph



First Hitting Time is Monotonous



15 Runs



15 Runs ≤ 15 Runtime Data Points



Empirical Cumulative Distribution



the ECDF of run lengths to reach the target

has for each data point a vertical step of constant size

displays for

 each x-value
 (budget) the
 count of
 observations to
 the left (first
 hitting times)

Empirical Cumulative Distribution



- interpretations possible:
- 80% of the runs reached the target
- e.g. 60% of the runs need
 between 2000
 and 4000
 evaluations

Reconstructing A Single Run



Reconstructing A Single Run



50 equally spaced targets






he empirical **CDF** makes a step for each star, is monotonous and displays for each budget the fraction of targets achieved within the budget







15 runs



15 runs50 targets



15 runs50 targets



15 runs 50 targets ECDF with 750 steps



50 targets from 15 runs ...integrated in a single graph

Interpretation



area over the **ECDF** curve average log runtime (or geometric avg. runtime) over all targets (difficult and easy) and all runs

Fixed-target: Measuring Runtime



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Fixed-target: Measuring Runtime

Idea: Simulated restarts by bootstrapping from measured runtimes until we see a success

Algo Restart A:

Algo Restart B:

 $\frac{RT_B^r}{p_s(Algo Restart A)} = 1$

 $p_s(Algo Restart A) = 1$

 $- RT_A^r$

Fixed-target: Measuring Runtime

• Expected running time of the restarted algorithm:

$$E[RT^{r}] = \frac{1 - p_{s}}{p_{s}} E[RT_{unsuccessful}] + E[RT_{successful}]$$

Estimator average running time (aRT/ERT/Enes/SP2*, w/o proof):

$$\widehat{p_s} = \frac{\# \text{successes}}{\# \text{runs}}$$

 $\widehat{RT_{unsucc}}$ = Average evals of unsuccessful runs

 $\widehat{RT_{succ}}$ = Average evals of successful runs

$$aRT = \frac{\text{total #evals}}{\text{#successes}}$$

* The concept is so essential that it has been discovered/proposed multiple times under different names in the past.

ECDFs with Simulated Restarts

What we typically plot are ECDFs of the simulated restarted algorithms:



Measuring Performance

On

- real world problems
 - expensive
 - comparison typically limited to certain domains
 - experts have limited interest to publish
- "artificial" benchmark functions
 - cheap
 - controlled
 - data acquisition is comparatively easy
 - problem of representativeness

Test Functions

define the "scientific question"

the relevance can hardly be overestimated

- should represent "reality"
- are often too simple?

remind separability

- a number of testbeds are around
- account for invariance properties

prediction of performance is based on "similarity", ideally equivalence classes of functions

What to Benchmark?

Furious activity is no substitute for understanding (H.H. Williams)

Taking all possible functions from a repository?

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What to Benchmark?

Furious activity is no substitute for understanding (H.H. Williams)

- Taking all possible functions from a repository?
- Bad idea if
 - function difficulties are unbalanced too many small dimensional problems, convex problems...
 - and performance are aggregated
- Leads to bias in the performance assessment

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What to Benchmark?

- test functions should be representative of difficulties we want to test therefore NFL has no relevance as assumption of being closed under permutation has no relevance wrt real world problems
- related to real-word difficulties

for performance to be generalizable to RW

scalable

dimension plays a big role in performance curse of dimensionality

comprehensible but not too easy

BB optimization does not mean BB benchmarking

 we should still hide properties from the solver (hide optimum, ...) solvers should not be able to exploit the benchmark intentionally or not

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automated benchmarking: COCO

Comparing Continuous Optimizers Platform https://github.com/numbbo/coco

COCO implements a reasonable, well-founded, and well-documented pre-chosen methodology





```
import cocoex
import scipy.optimize
### input
suite name = "bbob" # or "bbob-biobj" or ...
output folder = "scipy-optimize-fmin"
### prepare
suite = cocoex.Suite(suite name, "", "")
observer = cocoex.Observer(suite name,
                           "result folder: " + output folder)
### ao
for problem in suite: # this loop will take several minutes
   problem.observe with (observer) # generates the data for
                                    # cocopp post-processing
    scipy.optimize.fmin(problem, problem.initial solution)
```





https://github.com/numbbo/coco



How to benchmark algorithms with COCO?

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E README.md

numbbo/coco: Comparing Continuous Optimizers

This code reimplements the original Comparing Continous Optimizer platform, now rewritten fully in ANSI c with other languages calling the c code. As the name suggests, the code provides a platform to benchmark and compare continuous optimizers, AKA non-linear solvers for numerical optimization. Languages currently available are

- C/C++
- Java
- MATLAB/Octave

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numbbo/coco: Comparing Continuous Optimizers

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- C/C++
- Java
- MATLAB/Octave
- Python

Contributions to link further languages (including a better example in C++) are more than welcome.

For more information,

- read our benchmarking guidelines introduction
- read the COCO experimental setup description


installation I: experiments

As easy (in python) as: pip install cocoex

installation II: postprocessing

pip install cocopp

for other languages, you can use the development branch

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| python do.py install-postprocessing | | | | | | | | |
| to (user-locally) install the post-processing. From here on, do builds to a new release. | b.py has done its job and is only needed | again | for u | pdati | ing th | ie | | |
| 4. Copy the folder code-experiments/build/YOUR-FAVORIT sufficient to copy the file example_experiment.py . Run vary, see the respective read-me's and/or example experi- | TE-LANGUAGE and its content to another the example experiment (it already is con iment files: | ocatio npiled | n. In I I). As t | Pytho the d | on it is etails | ; | | |
| C read me and example experiment Java read me and example experiment Matlab/Octave read me and example experiment Python read me and example experiment | coupling alg | 0 + | - C | 0 | С | D | | |
| If the example experiment runs, connect your favorite algorithe the example experiment file by a call to your algorithm (see a and algorithm_info of the observer options in the example | hm to Coco: replace the call to the rando above). Update the output result_folde e experiment file. | om sea er , the | rch o e alg | ptimi oritł | zerin m_na | me | | |
| Another entry point for your own experiments can be the co | de-experiments/examples folder. | | | | | | | |
| 5. Now you can run your favorite algorithm on the bbob s bbob-biobj-ext suites (for multi-objective algorithms). | uite (for single-objective algorithms) or o Output is automatically generated in the | on the speci | bbob fied d | -bioł ata | bj an | ıd | | |

result_folder . By now, more suites might be available, see below.

Simplified Example Experiment in Python

```
import cocoex
import scipy.optimize
### input
suite name = "bbob"
output folder = "scipy-optimize-fmin"
fmin = scipy.optimize.fmin
### prepare
suite = cocoex.Suite(suite name, "", "")
observer = cocoex.Observer(suite name,
                           "result folder: " + output folder)
### go
for problem in suite: # this loop will take several minutes
   problem.observe with (observer) # generates the data for
                                    # cocopp post-processing
    fmin(problem, problem.initial solution)
```

Note: the actual example_experiment.py contains more advanced things like restarts, batch experiments, other algorithms (e.g. CMA-ES), etc.



automatically). Results of each batch must be kept under their separate folder as is. These folders then must be



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Derivative-free Optimization, M2 Optimization, U. Paris-Saclay, Dec. 15, 2023 82



| Post processing results × + | | | | x |
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Available Test Suites in COCO

- bbob
- bbob-noisy
- bbob-biobj
- bbob-largescale 24 noiseless fcts
- bbob-mixint
 24 mixed-int. fcts
- bbob-constrained 54 fcts w/ varying constr. 9 algo data sets

24 noiseless fcts

55 bi-objective fcts

30 noisy fcts

240+ algo data sets 40+ algo data sets 30+ algo data sets 16 algo data sets 5 algo data sets

Worth to Note: ECDFs in COCO

In COCO, ECDF graphs

- never aggregate over dimension
 - but often over targets and functions
- can show data of more than 1 algorithm at a time



The single-objective BBOB functions

https://numbbo.github.io/gforge/downloads/download16.00/bbobdocfunctions.pdf

The bbob Testbed

24 functions in 5 groups:

| 1 Separable Functions | | 4 Multi-modal functions with adequate global structure | | | | | |
|---|--|--|--|--|--|--|--|
| f1 | Sphere Function | f15 | Rastrigin Function | | | | |
| f2 | Ellipsoidal Function | f16 | Weierstrass Function | | | | |
| f3 | Rastrigin Function | f17 | Schaffers F7 Function | | | | |
| f4 | Büche-Rastrigin Function | f18 | Schaffers F7 Functions, moderately ill-conditioned | | | | |
| f5 | ♥Linear Slope | f19 | Composite Griewank-Rosenbrock Function F8F2 | | | | |
| 2 Functions with low or moderate conditioning | | | 5 Multi-modal functions with weak global structure | | | | |
| f6 | Attractive Sector Function | f20 | Schwefel Function | | | | |
| f7 | Step Ellipsoidal Function | f21 | Gallagher's Gaussian 101-me Peaks Function | | | | |
| f8 | Rosenbrock Function, original | f22 | Gallagher's Gaussian 21-hi Peaks Function | | | | |
| f9 | Rosenbrock Function, rotated | f23 | GKatsuura Function | | | | |
| 3 F | unctions with high conditioning and unimodal | f24 | Cunacek bi-Rastrigin Function | | | | |
| f10 | Ellipsoidal Function | | | | | | |
| f11 | ODiscus Function | | | | | | |
| f12 | Bent Cigar Function | | | | | | |
| f13 | Sharp Ridge Function | | | | | | |

6 dimensions: 2, 3, 5, 10, 20, (40 optional)

f14 ODifferent Powers Function

Notion of Instances

- All COCO problems come in form of instances
 - e.g. as translated/rotated versions of the same function
- Prescribed instances typically change from year to year
 - avoid overfitting
 - 5 instances are always kept the same

Plus:

 the bbob functions are locally perturbed by nonlinear transformations

Notion of Instances

- All COCO problems come in form of instances
 - e.a. as translated/rotated versions of the same



Exercise

Objectives:

- investigate the performance of these 6 algorithms:
 - CMA-ES ("IPOP-CMA-ES" version)
 - CMA-ES ("BIPOP-CMA-ES" version)
 - Nelder-Mead simplex (use "NelderDoerr" version here)
 - BFGS quasi-Newton
 - Genetic Algorithm: discretization of cont. variables ("GA")
 - ONEFIFTH: (1+1)-ES with 1/5 rule
- postprocessed available here: http://www.cmap.polytechnique.fr/~dimo.brock hoff/advancedOptSaclay/2019/exercises/cocoresults/
- so now: investigate the data!

Exercise

Objective:

investigate the data:

- a) which algorithms are the best ones?
- b) does this depend on the dimension? Or on other things?
- c) look at single graphs: can we say something about the algorithms' invariances, e.g. wrt. rotations of the search space?
- d) what's the impact of covariance-matrix-adaptation?
- e) what do you think: are the displayed algorithms well-suited for problems with larger dimension?