Advanced Optimization
Lecture 8: Benchmarking and Branch&Bound

December 1, 2021

CentraleSupélec / ESSEC Business School

dimo.brockhoff@inria.fr

Dimo Brockhoff

Inria Saclay – Ile-de-France

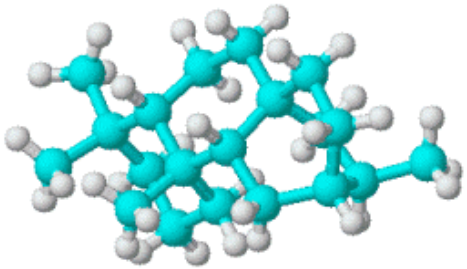
INSTITUT POLYTECHNIQUE DE PARIS

Course Overview

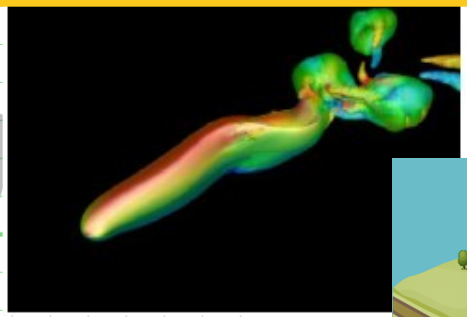
		Topic
Wed, 13.10.2021	PM	Introduction, examples of problems, problem types
Wed, 20.10.2021	PM	Continuous (unconstrained) optimization: convexity, gradients, Hessian, … [technical test Evalmee]
Wed, 27.10.2021	PM	Continous optimization II: [1st mini-exam] Constrained optimization: Lagrangian, optimality conditions
Wed, 03.11.2021	PM	gradient descent, Newton direction, quasi-Newton (BFGS) Linear programming: duality, maxflow/mincut, simplex algo
Wed, 10.11.2021	PM	derivative-free algorithms: Nelder-Mead and CMA-ES
Wed, 17.11.2021	PM	CMA-ES, Part II, Stochastic Gradient Descent, Bayesian optimization
Wed, 24.11.2021	PM	Benchmarking solvers: runtime distributions, the COCO platform, recommendations **[2nd mini-exam]**
Wed, 01.12.2021	PM	Benchmarking (cont.), discrete optimization: branch and bound
Fri, 3.12.2021	23:59	Deadline open source project (PDF sent by email)
Wed, 15.12.2021	PM	Exam

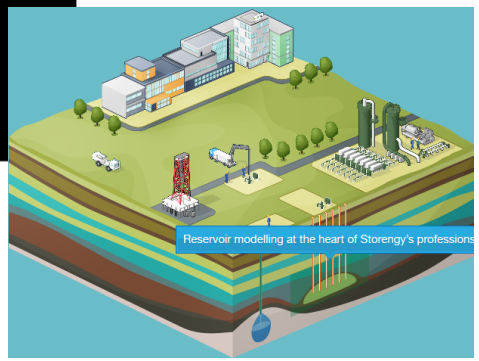
Benchmarking Optimization Algorithms

or: critical performance assessment



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





Practical (Numerical) Blackbox Optimization

Given:

derivatives not available or not useful

Not clear:

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

Need: Benchmarking

- understanding of algorithms
- algorithm selection
- putting algorithms to a standardized test
  - simplify judgement
  - simplify comparison
  - regression test under algorithm changes

Kind of everybody has to do it (and it is tedious):

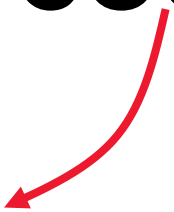
- choosing (and implementing) problems, performance measures, visualization, stat. tests, ...
- running a set of algorithms

wouldn’t

automatized benchmarking

be cool?

for this, we developed COCO



Comparing Continuous Optimizers Platform

`https://github.com/numbbo/coco`

benchmarking is non-trivial

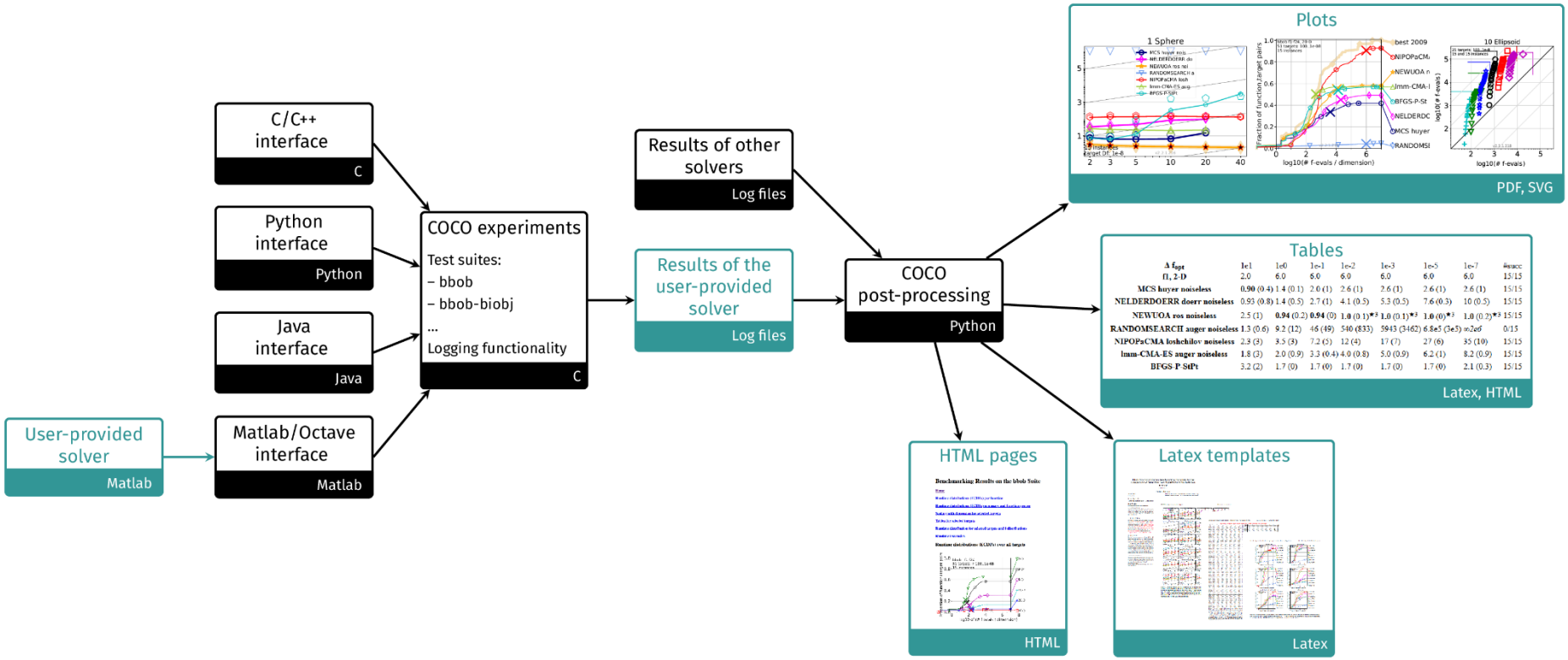
hence, COCO implements a

reasonable, well-founded, and well-documented

pre-chosen methodology

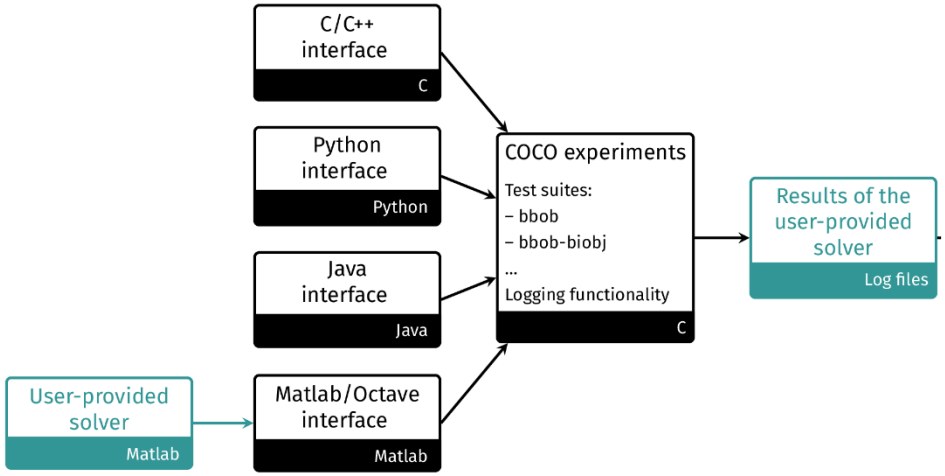
The Comparing Continuous Optimizers Platform

https://github.com/numbbo/coco



The Comparing Continuous Optimizers Platform

https://github.com/numbbo/coco

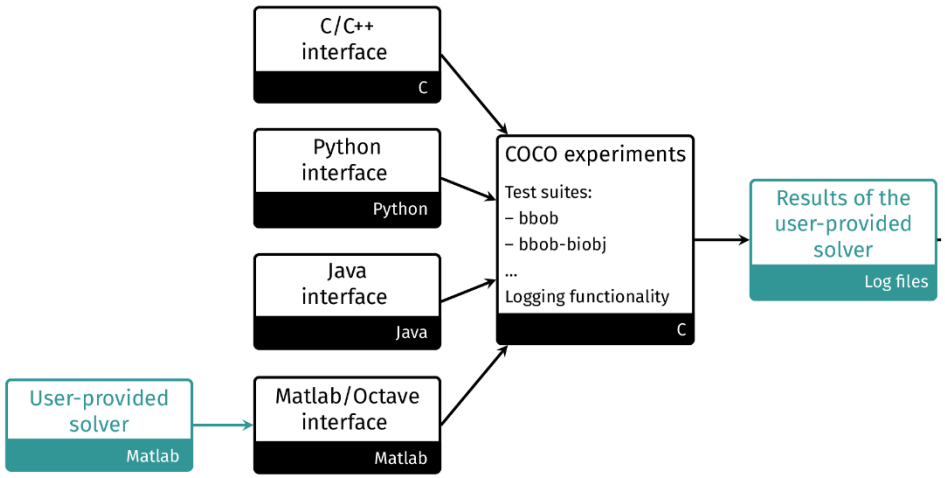


Experiments are as simple as (after installation)…

```
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)

### go
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)
```

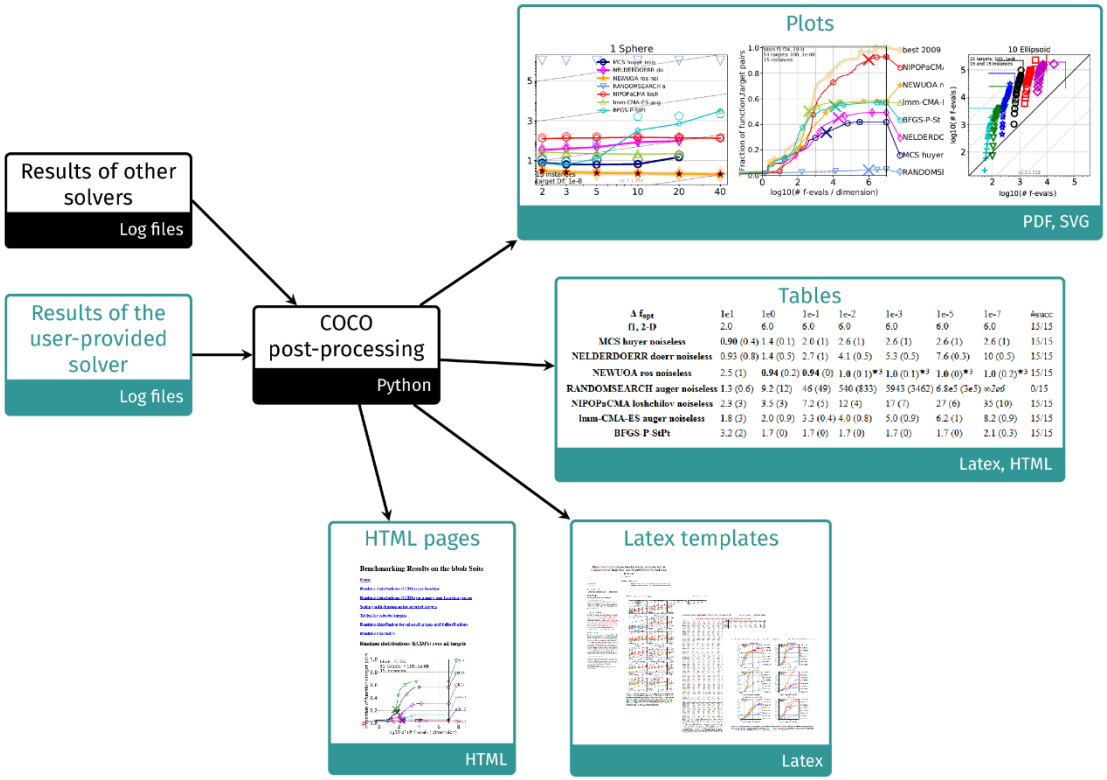
The Comparing Continuous Optimizers Platform

https://github.com/numbbo/coco



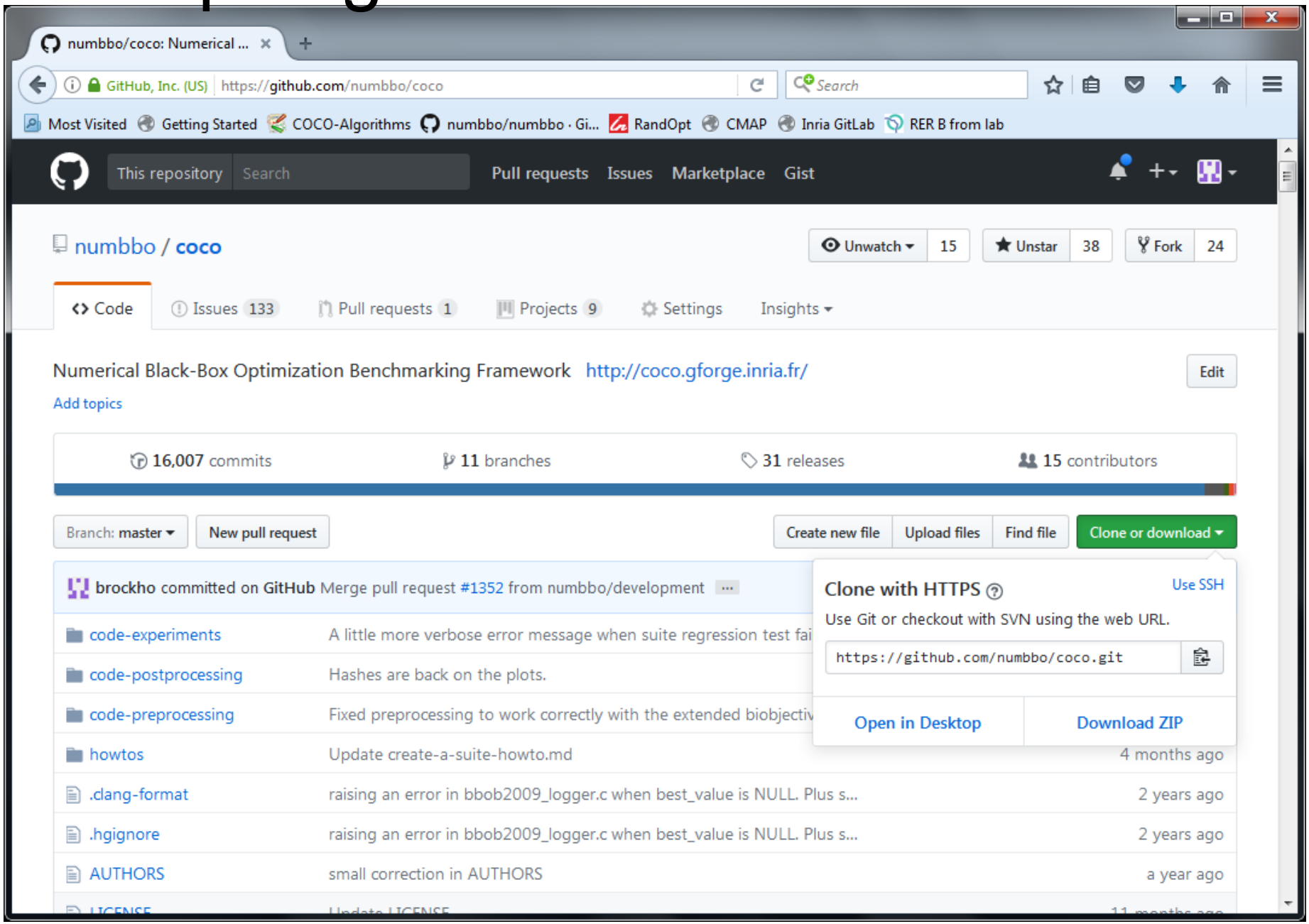
The Comparing Continuous Optimizers Platform

https://github.com/numbbo/coco

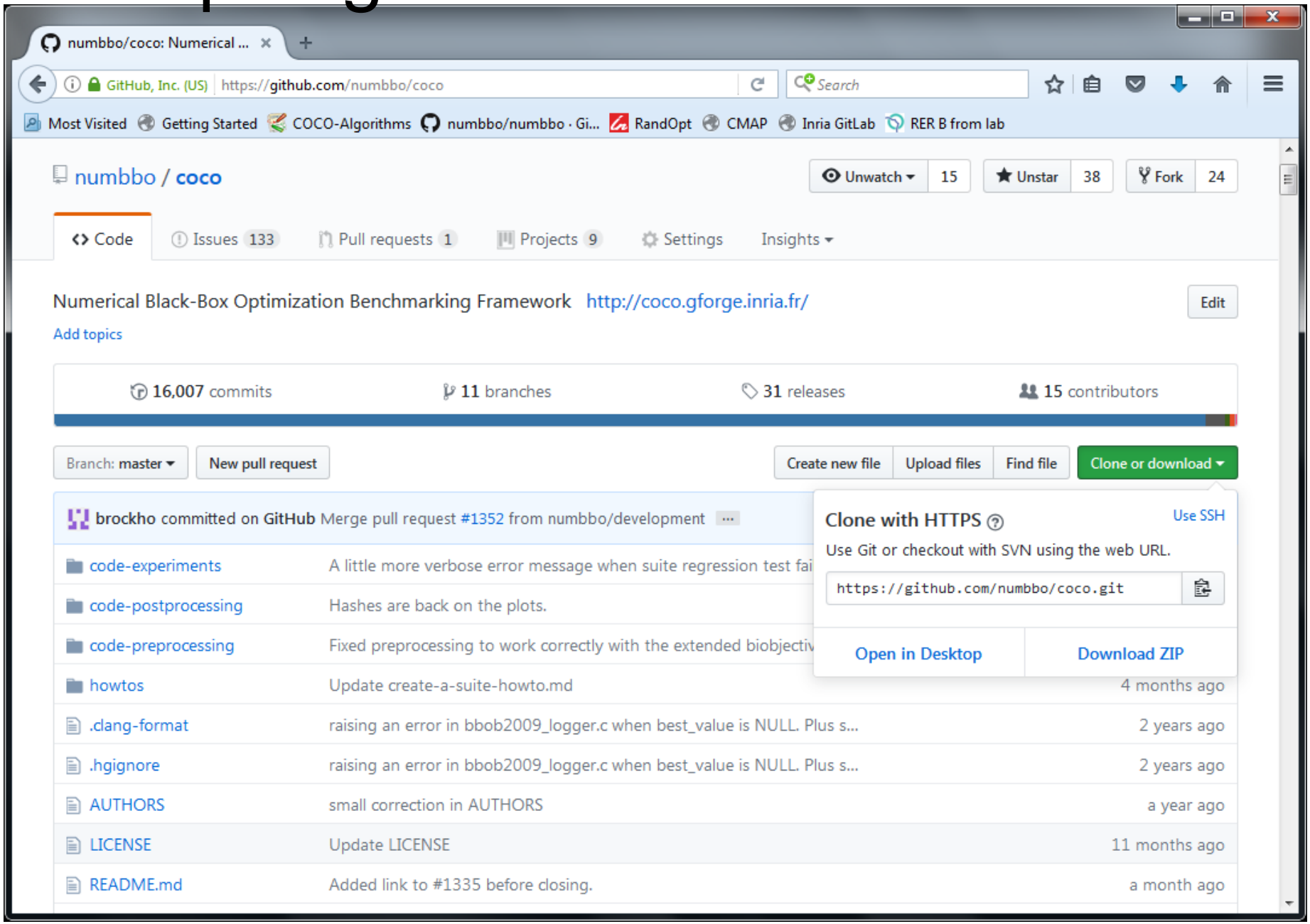


How to benchmark algorithms with COCO?

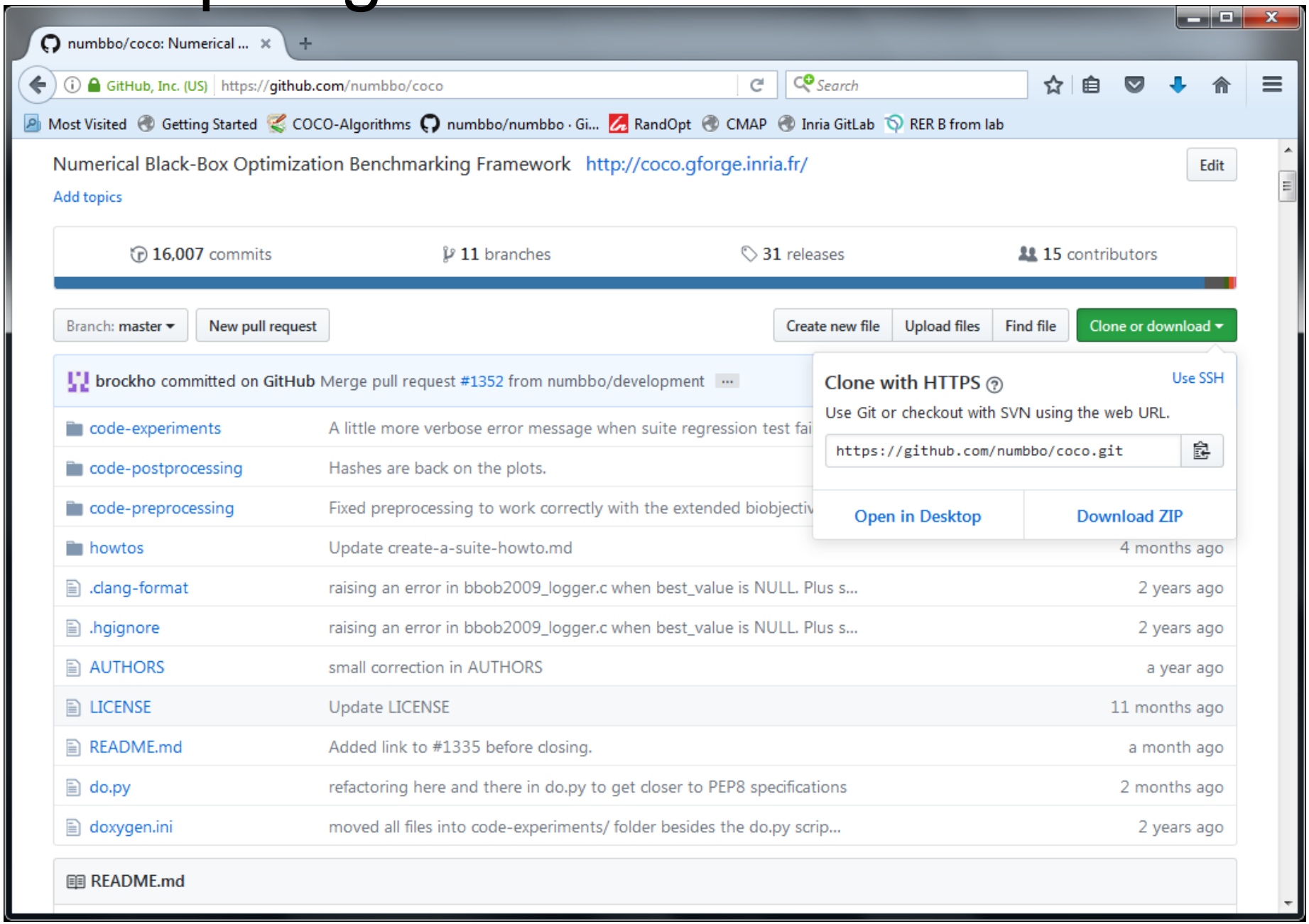
https://github.com/numbbo/coco



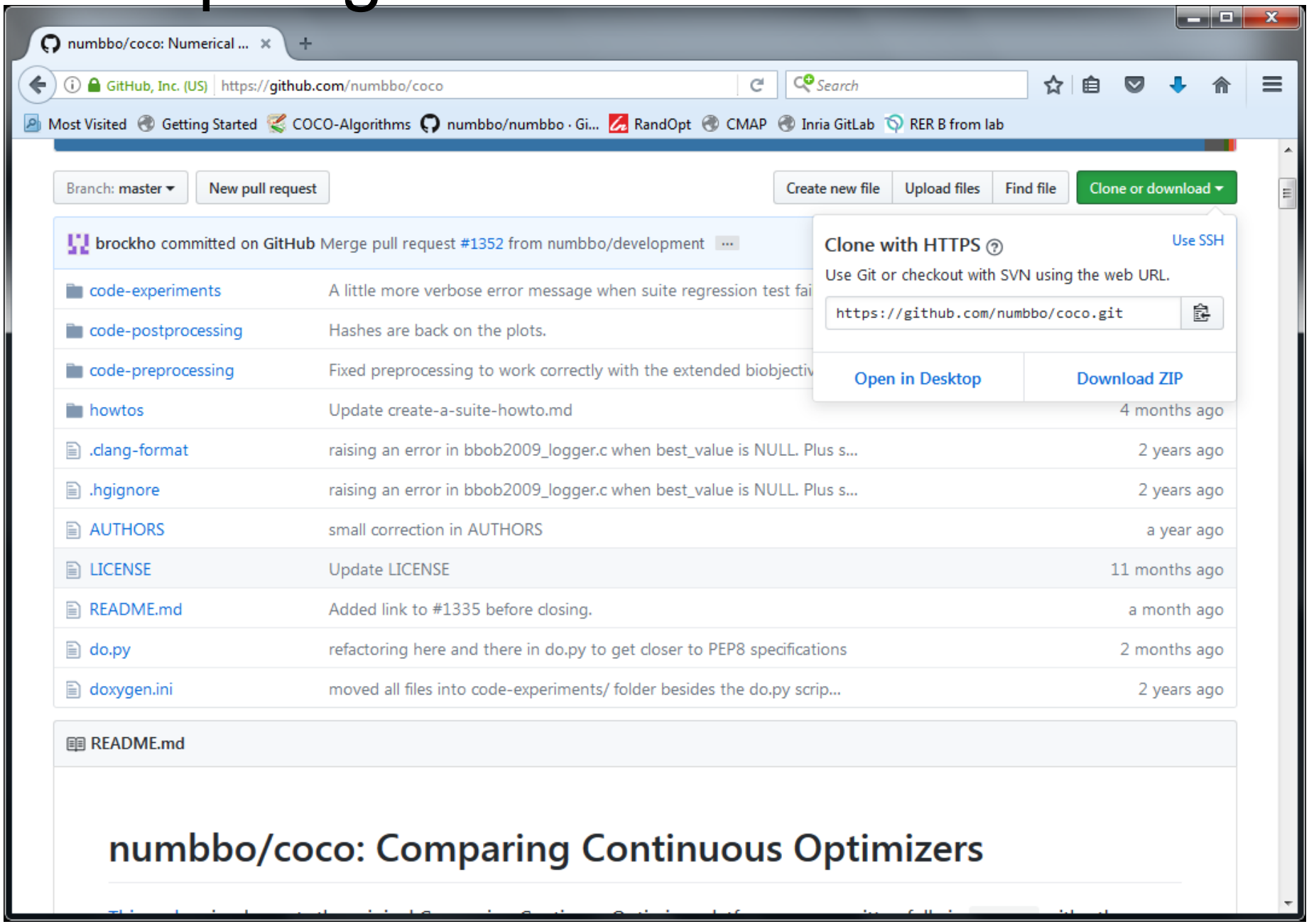
https://github.com/numbbo/coco



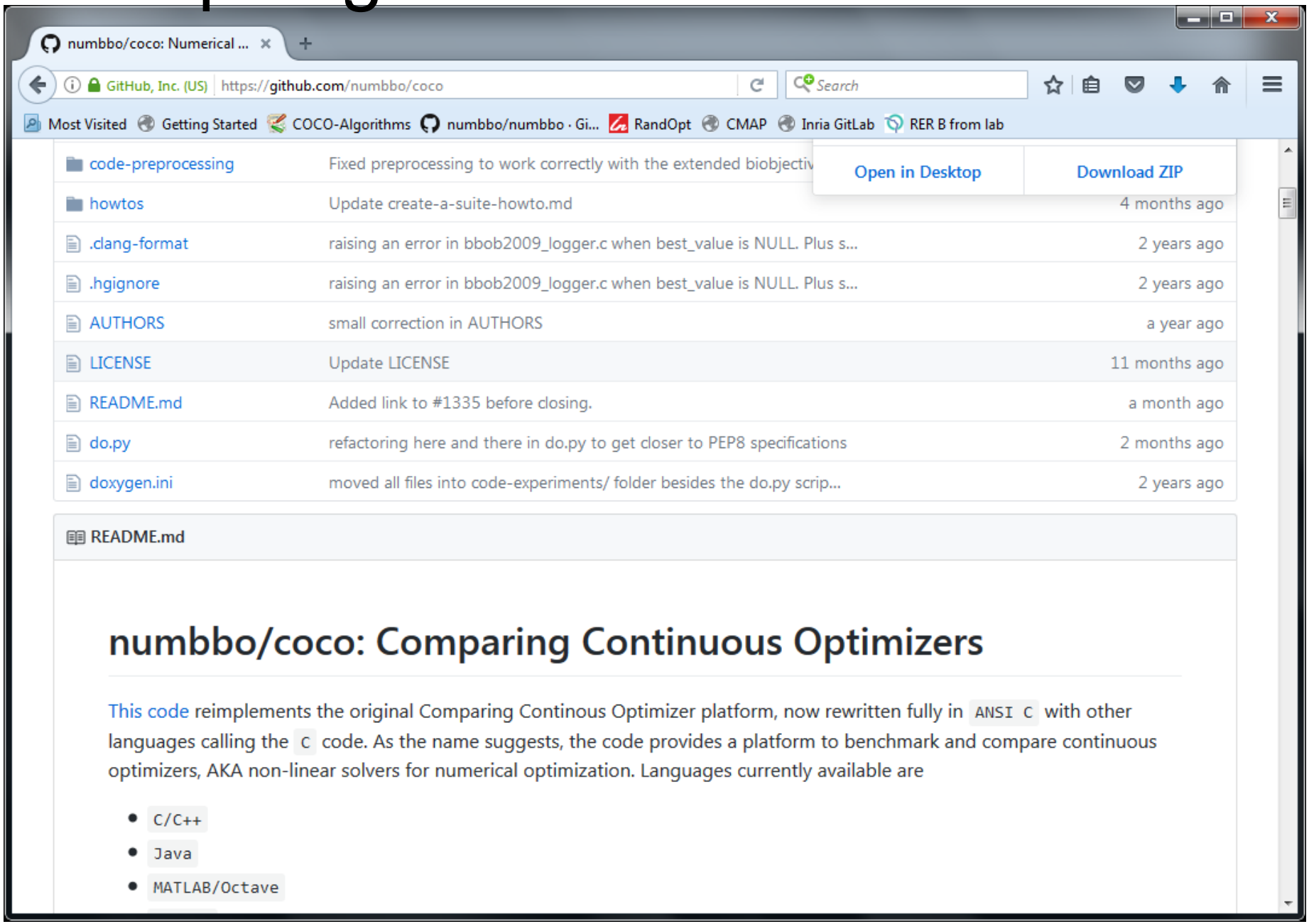
https://github.com/numbbo/coco



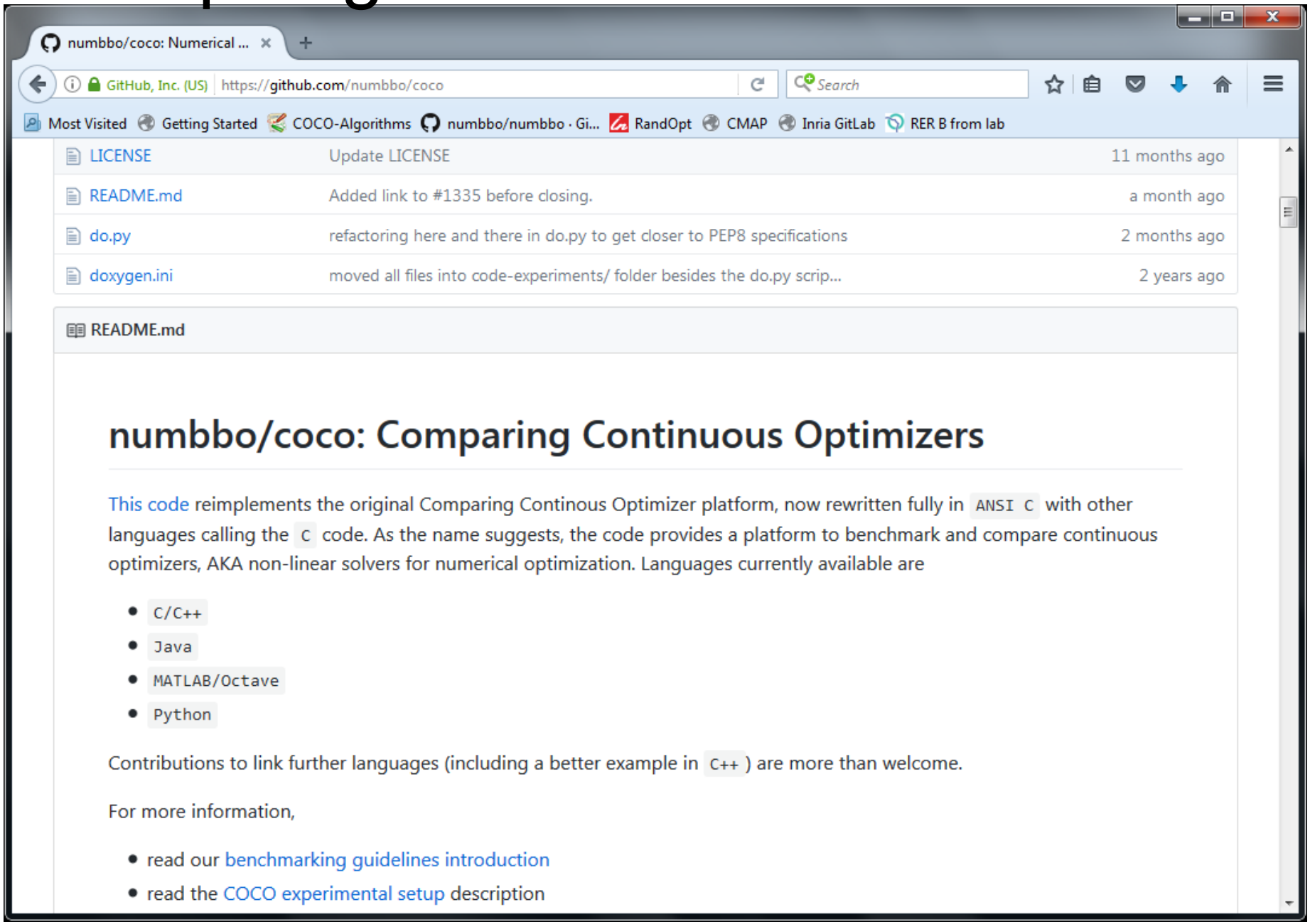
https://github.com/numbbo/coco



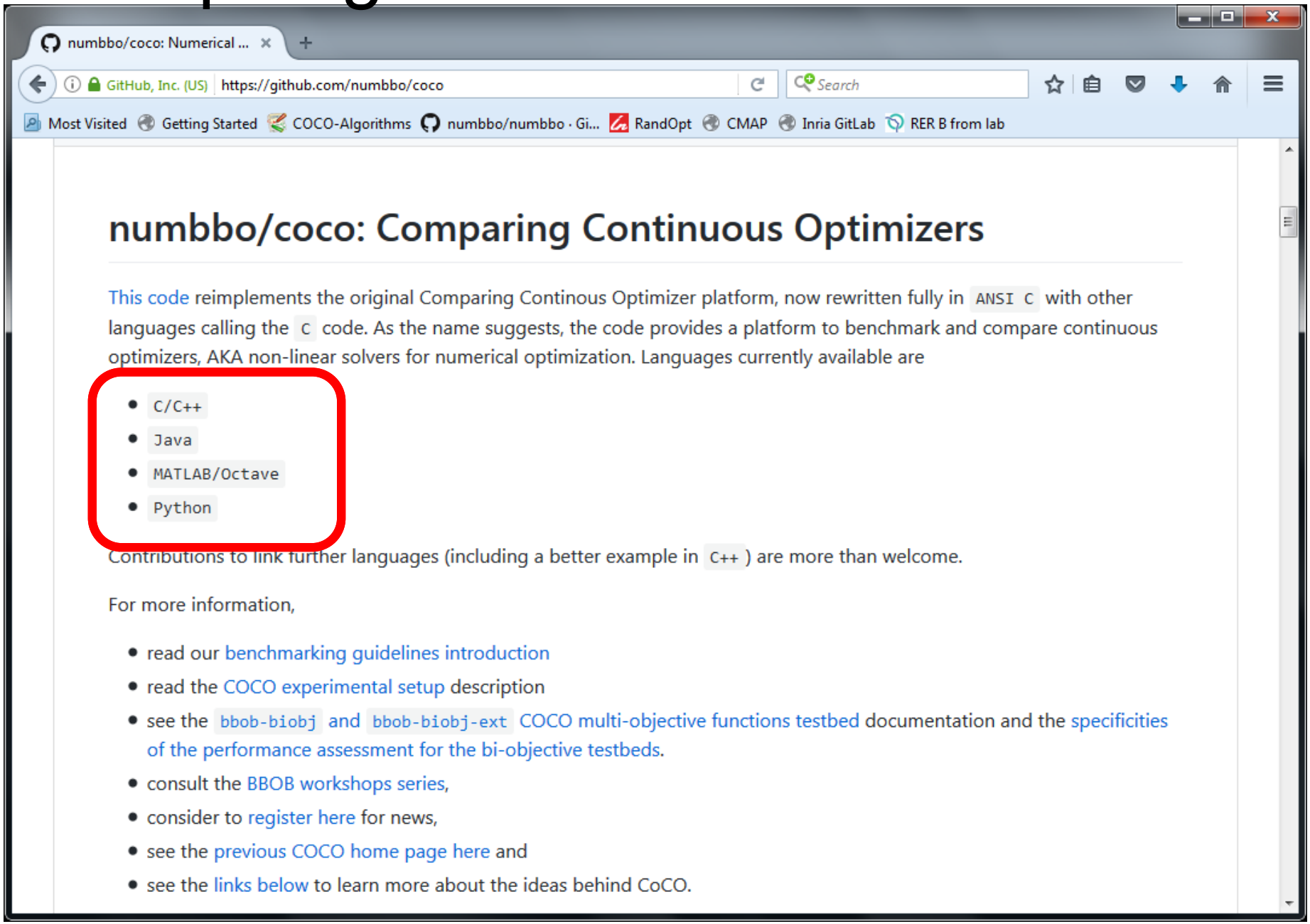
https://github.com/numbbo/coco



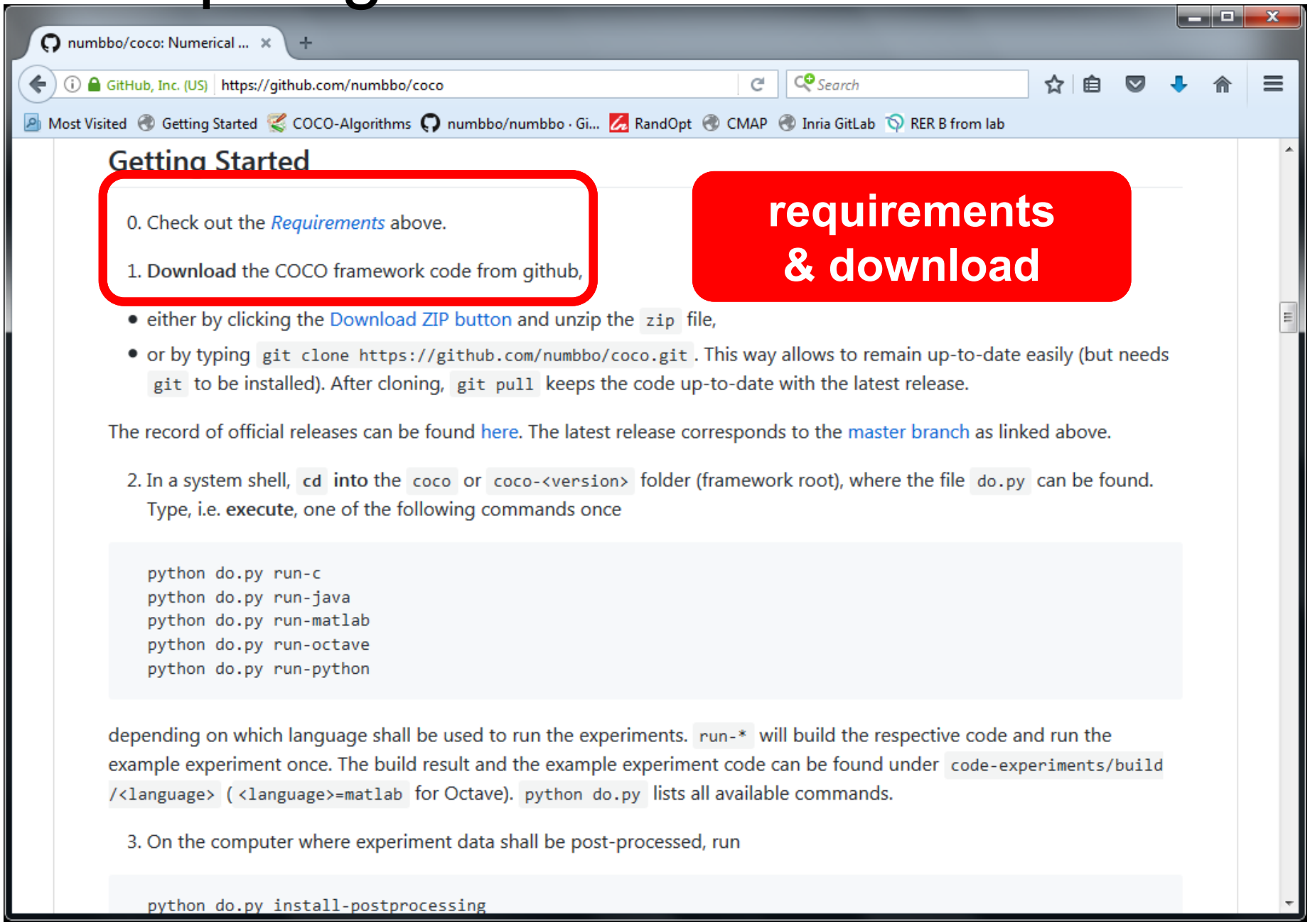
https://github.com/numbbo/coco



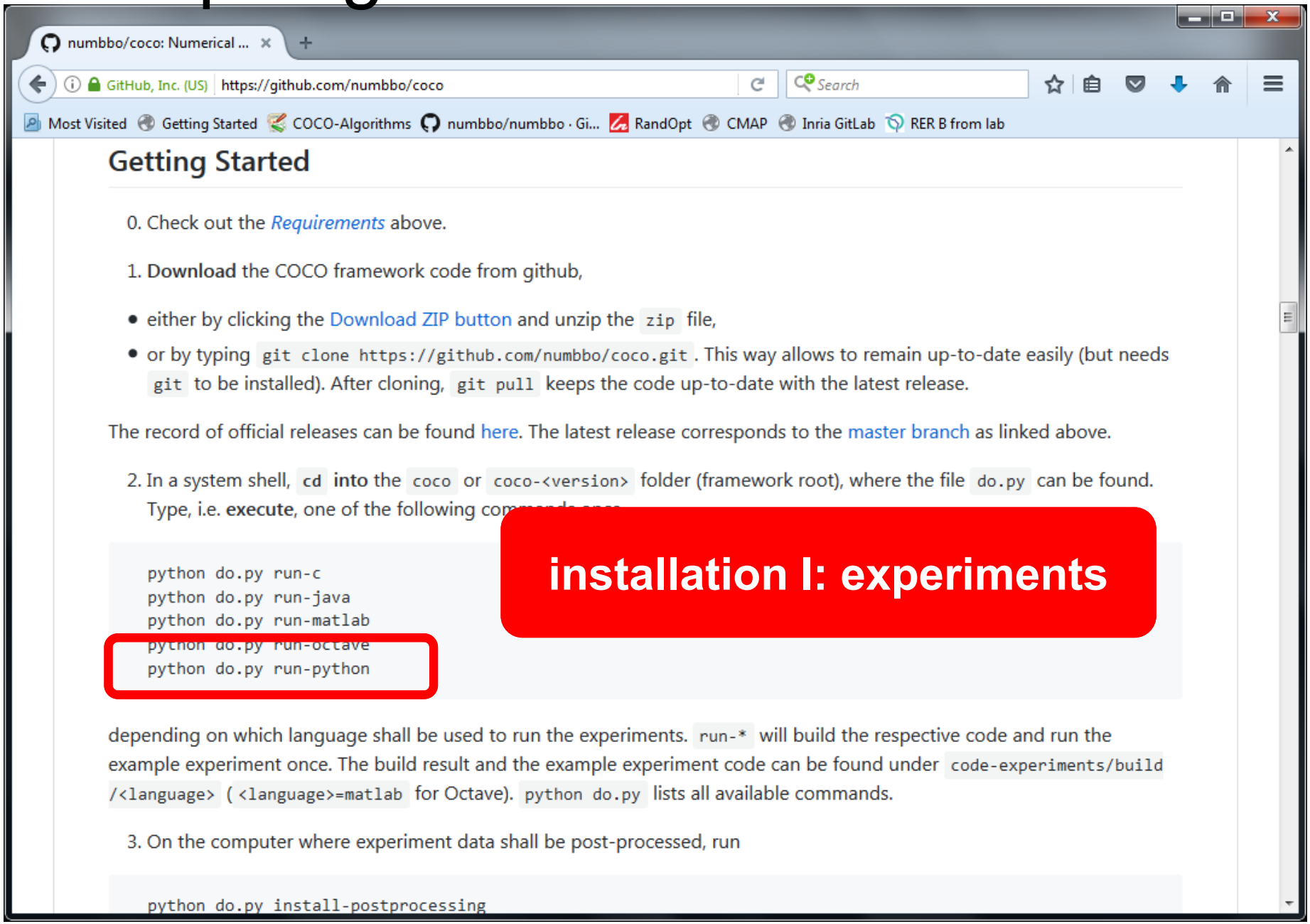
https://github.com/numbbo/coco



https://github.com/numbbo/coco



https://github.com/numbbo/coco



Getting Started

0. Check out the *Requirements* above.

1. **Download** the COCO framework code from github,

- either by clicking the Download ZIP button and unzip the `zip` file,
- or by typing `git clone https://github.com/numbbo/coco.git`. This way allows to remain up-to-date easily (but needs `git` to be installed). After cloning, `git pull` keeps the code up-to-date with the latest release.

The record of official releases can be found here. The latest release corresponds to the master branch as linked above.

2. In a system shell, `cd` **into** the `coco` or `coco-<version>` folder (framework root), where the file `do.py` can be found. Type, i.e. **execute**, one of the following commands once

```
python do.py run-c
python do.py run-java
python do.py run-matlab
python do.py run-octave
python do.py run-python
```

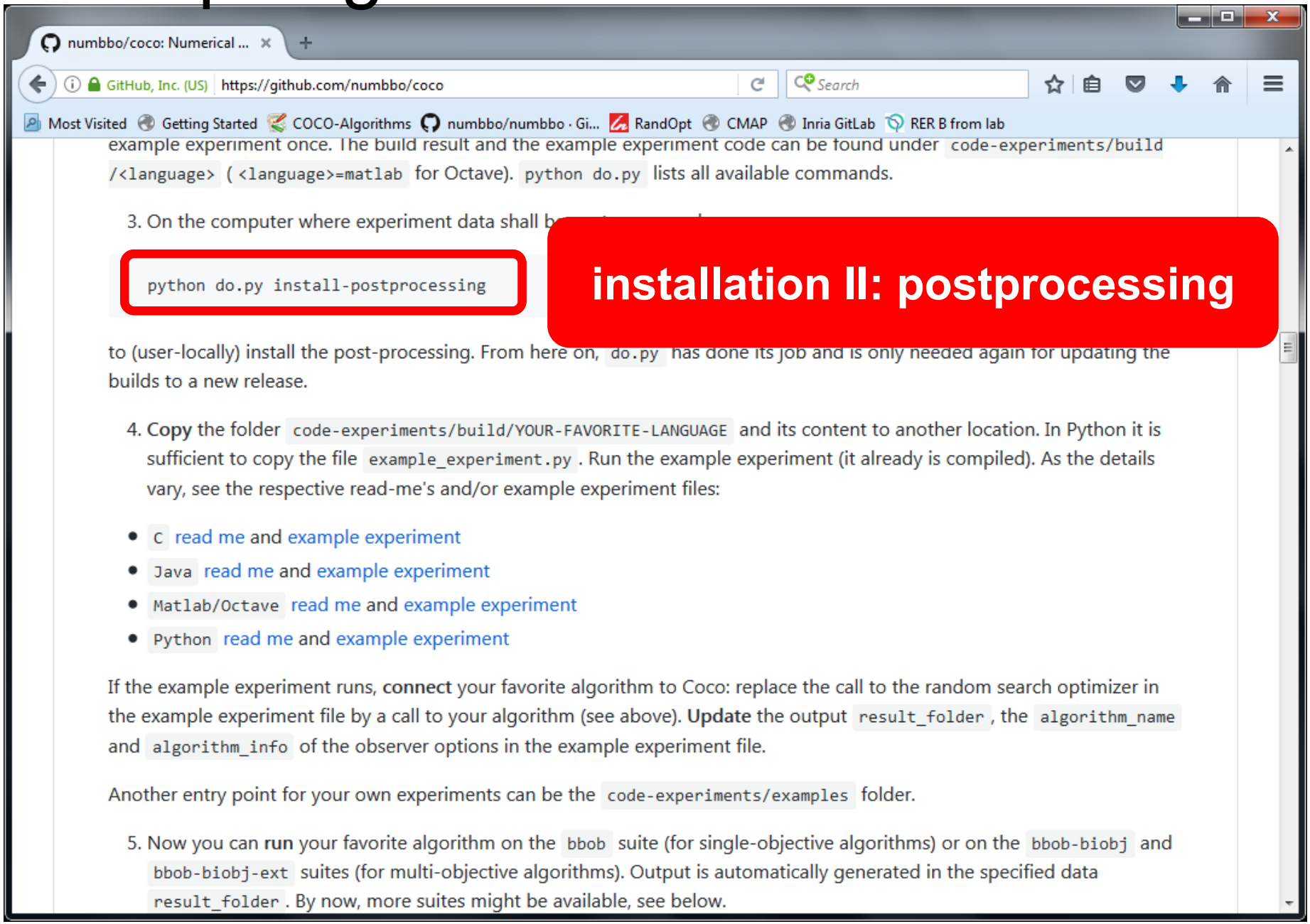
installation I: experiments

depending on which language shall be used to run the experiments. `run-*` will build the respective code and run the example experiment once. The build result and the example experiment code can be found under `code-experiments/build/<language>` (`<language>=matlab` for Octave). `python do.py` lists all available commands.

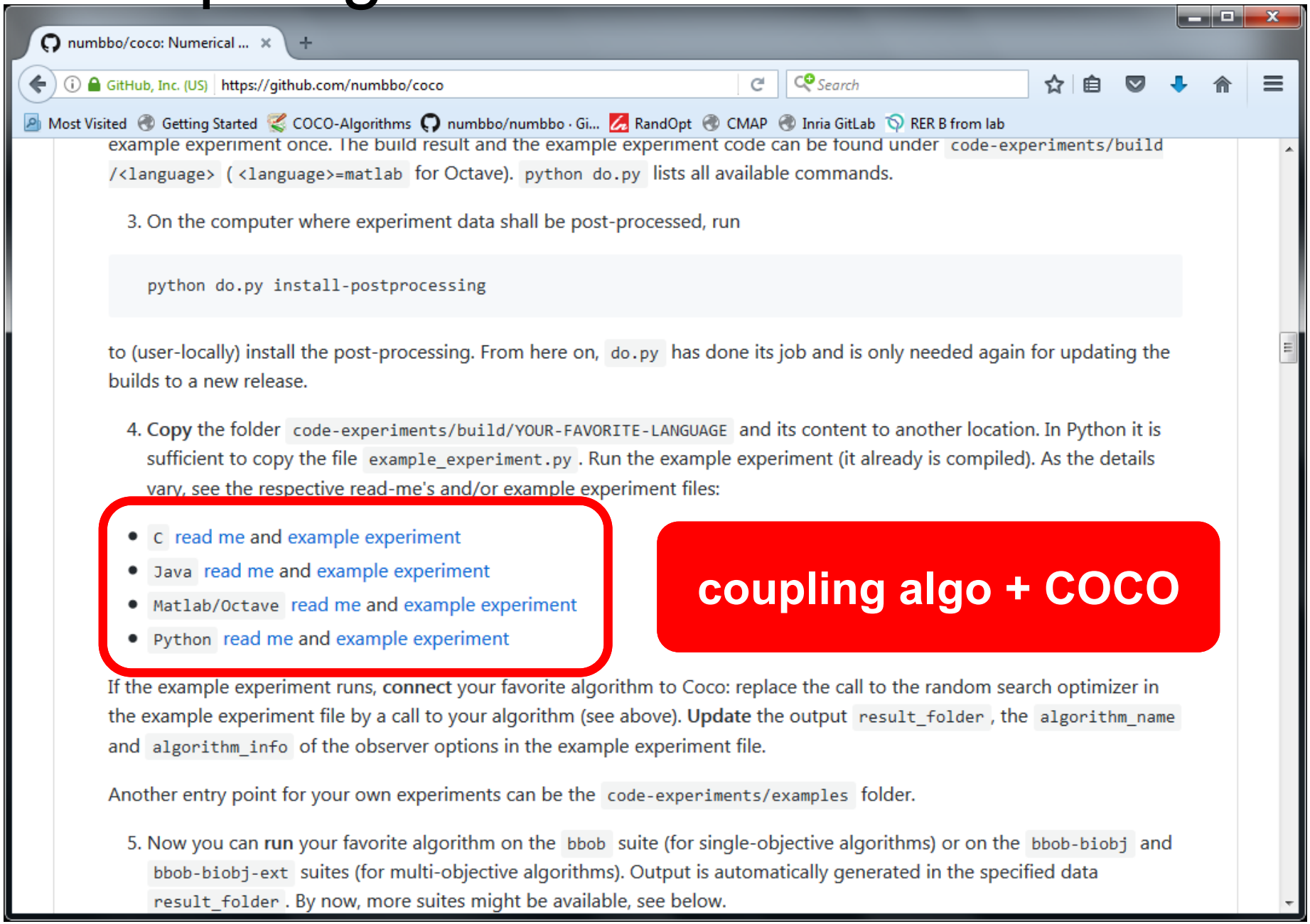
3. On the computer where experiment data shall be post-processed, run

```
python do.py install-postprocessing
```

https://github.com/numbbo/coco



https://github.com/numbbo/coco

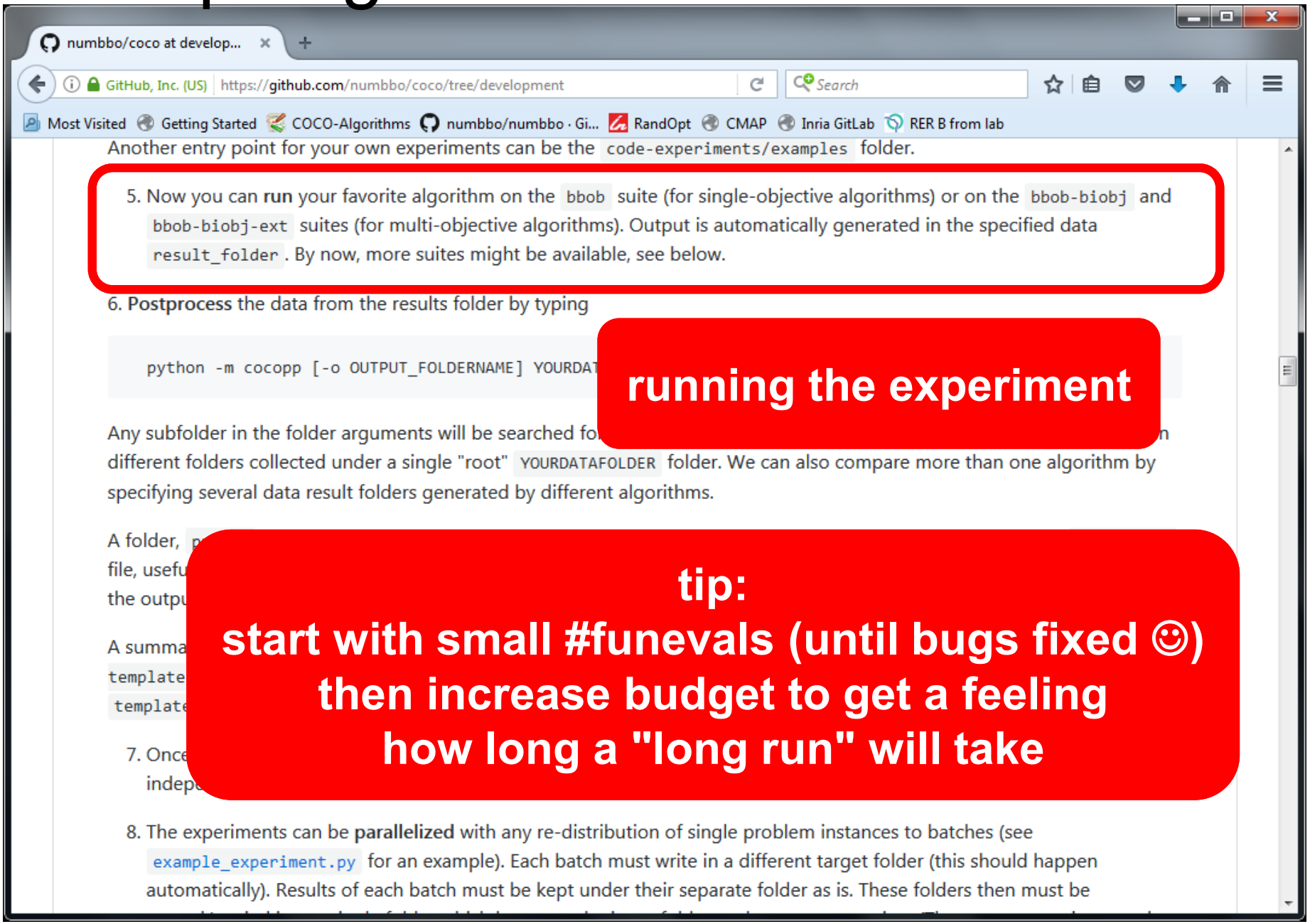


Simplified Example Experiment in Python

```
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.

https://github.com/numbbo/coco

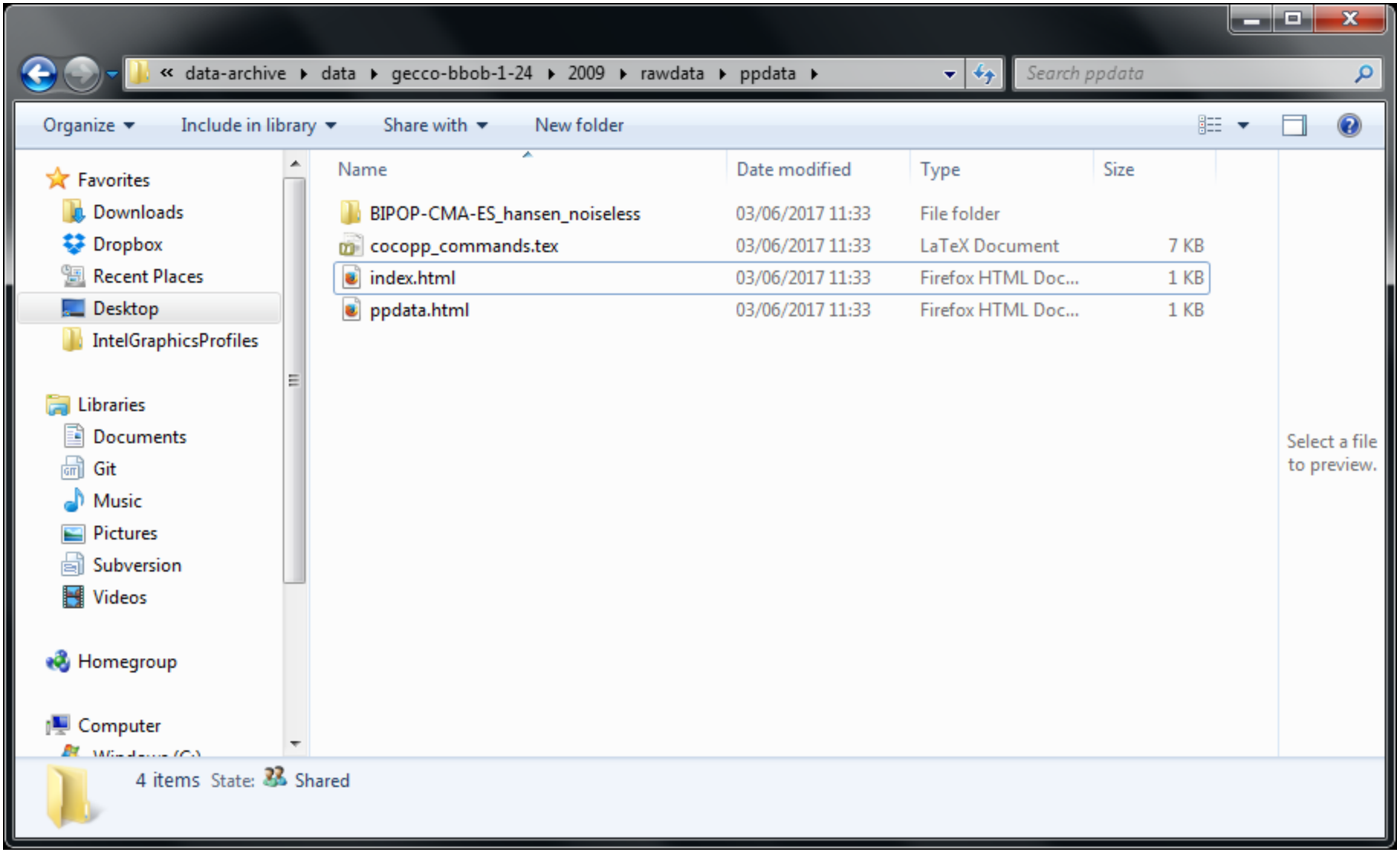


https://github.com/numbbo/coco

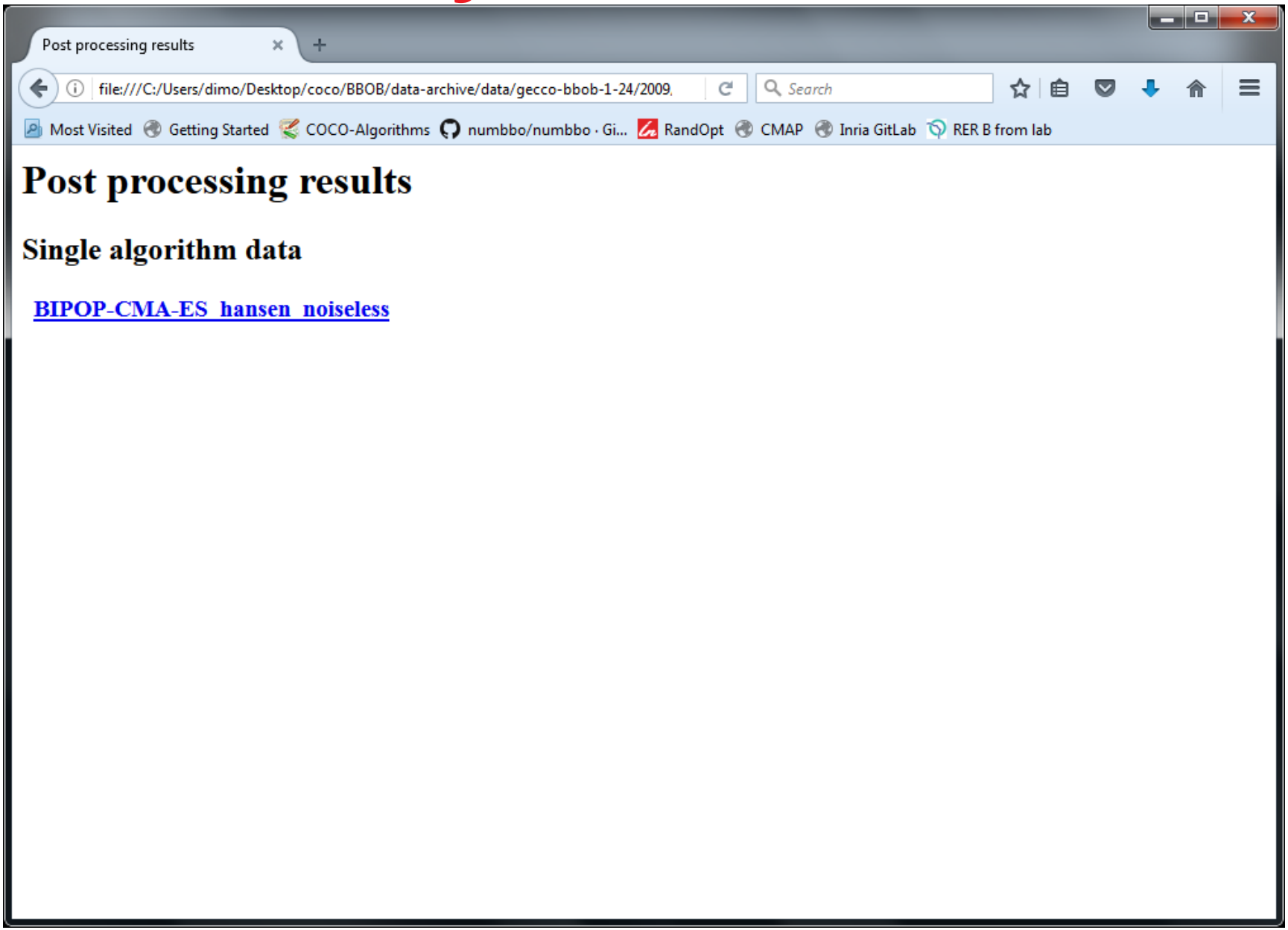
data from 200+ algorithms can be accessed directly through its name

(see `https://numbbo.github.io/data-archive/`)

Result Folder



Automatically Generated Results



Automatically Generated Results

BIPOP-CMA-ES, templateBBOB...

file:///C:/Users/dimo/Desktop/coco/BBOB/data-archive/data/gecco-bbob-1-24/2009

Search

Most Visited | Getting Started | COCO-Algorithms | numbbo/numbbo · Gi... | RandOpt | CMAP | Inria GitLab | RER B from lab

BIPOP-CMA-ES

Home

Runtime distributions (ECDFs) per function

Runtime distributions (ECDFs) summary and function groups

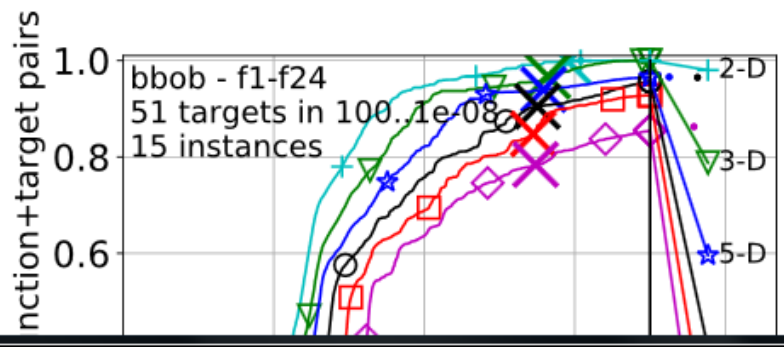
Scaling with dimension for selected targets

Tables for selected targets

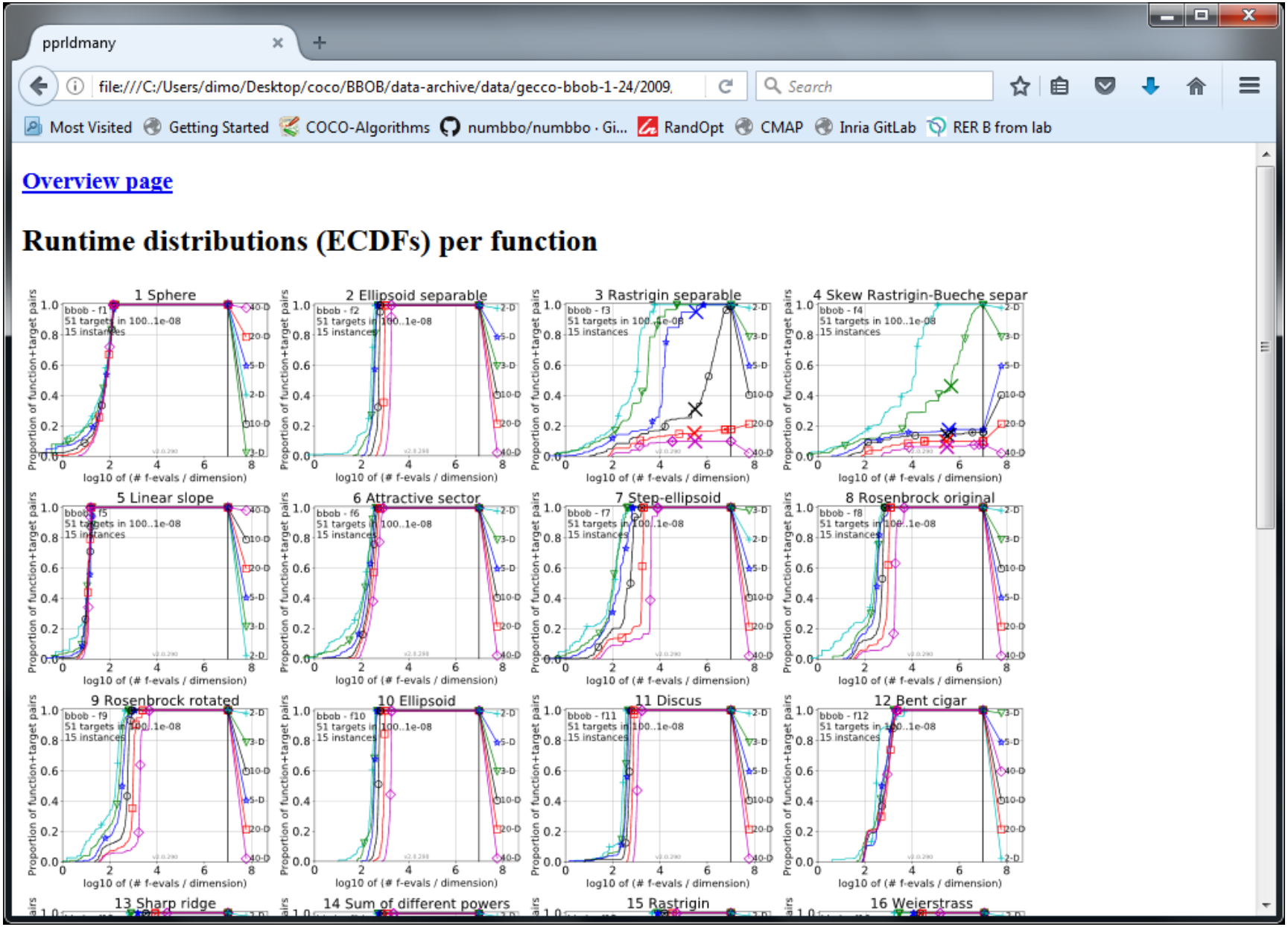
Runtime distribution for selected targets and f-distributions

Runtime loss ratios

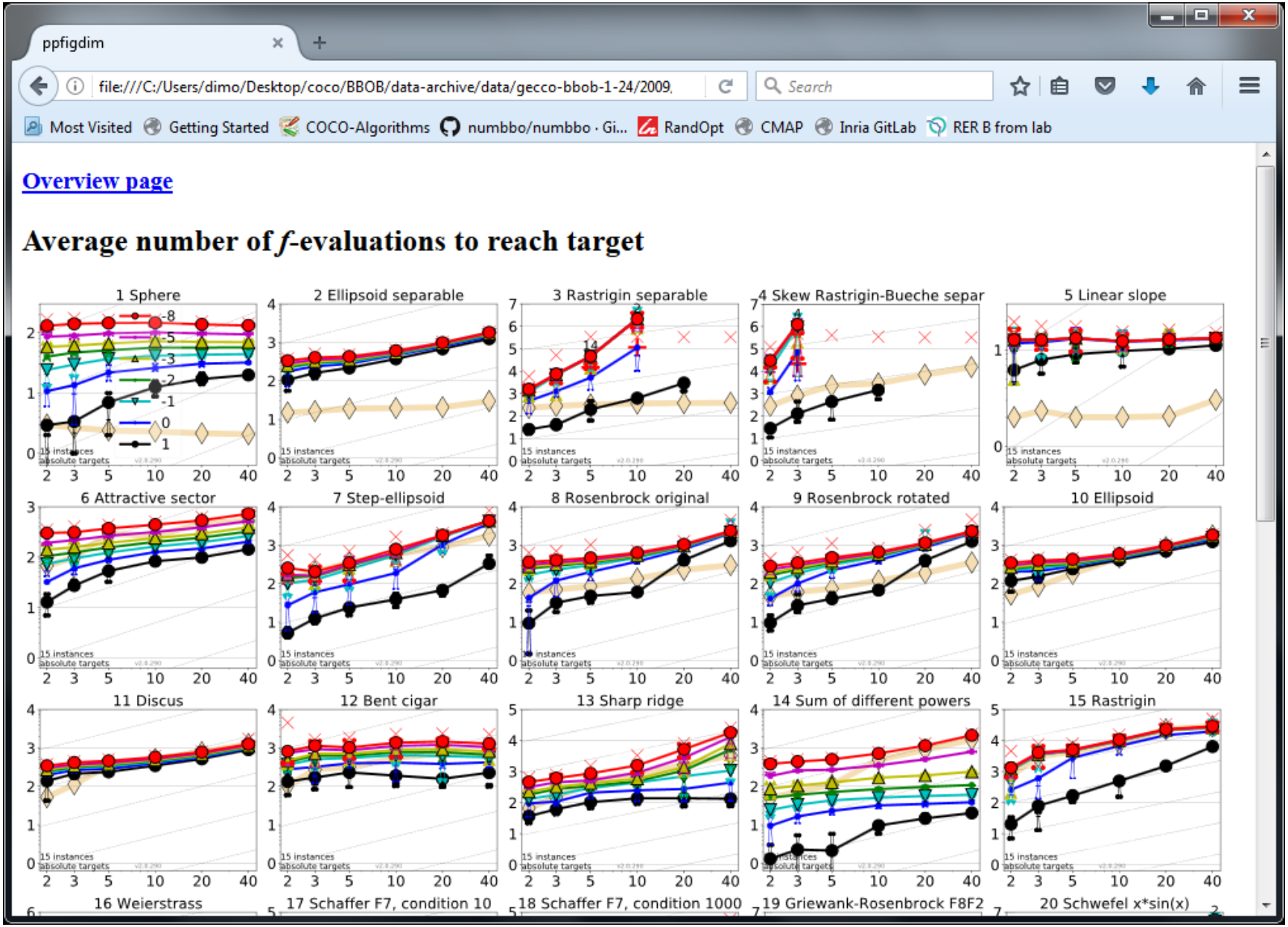
Runtime distributions (ECDFs) over all targets



Automatically Generated Results



Automatically Generated Results



so far:

data for 300+ algorithm variants

(some of which on noisy/multiobjective/mixed-integer test functions)

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

Available Test Suites in COCO

▪ bbob	24 noiseless fcts	220+ algo data sets
▪ bbob-noisy	30 noisy fcts	40+ algo data sets
▪ bbob-biobj	55 bi-objective fcts	30+ algo data sets
▪ bbob-largescale	24 noiseless fcts	11 algo data sets
▪ bbob-mixint	24 mixed integer fcts	
▪ bbob-biobj-mixint	92 mixed integer fcts	

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

runtime or first hitting time is the prime candidate
(we don't have many choices anyway)

How Do We Measure Performance?

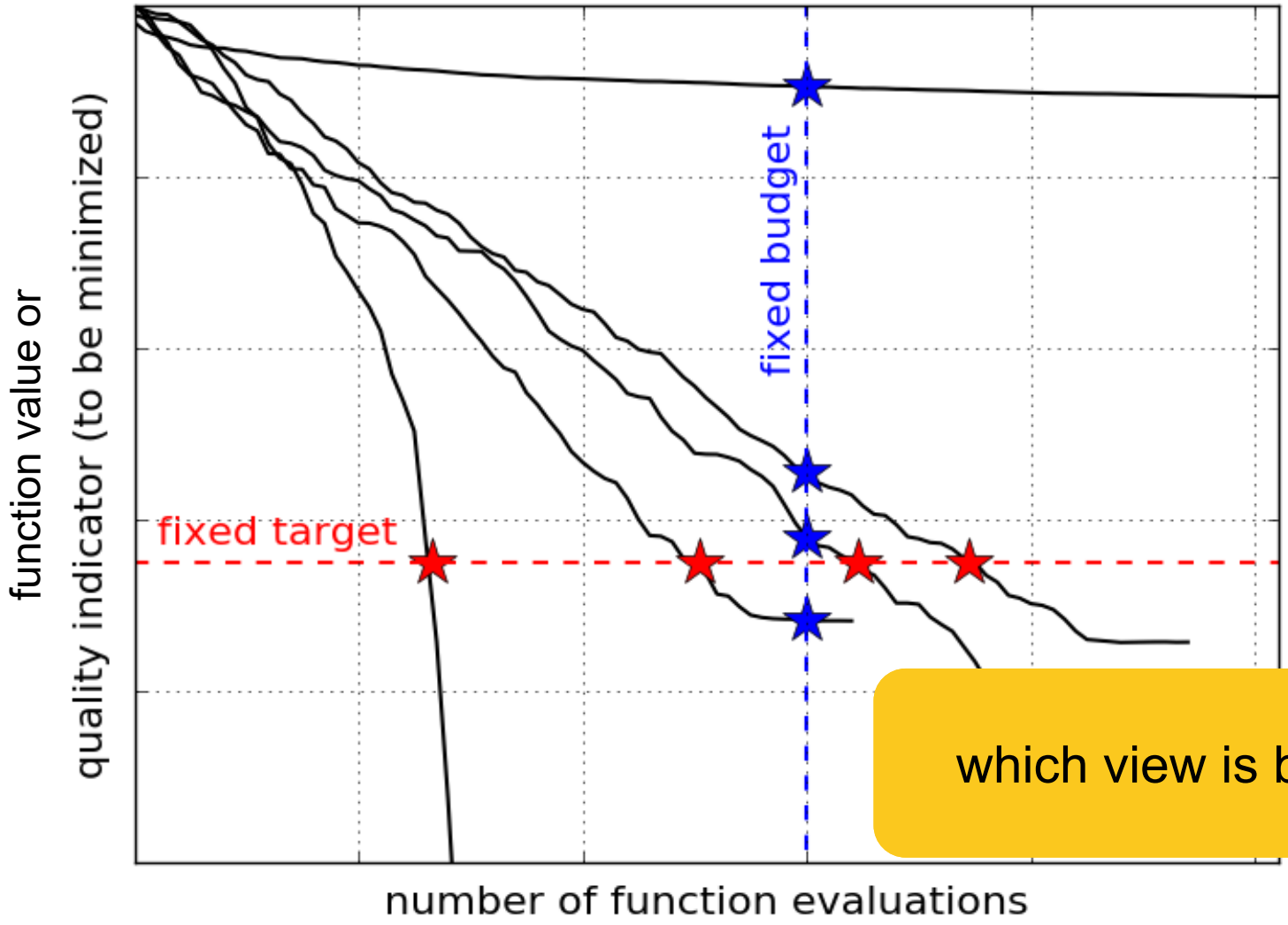
Two objectives:

- 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...



which view is better?

Runtime is the prime candidate

Why?

- runtimes are easier to interpret than f-values
- runtimes are interpretable in a meaningful way
- runtimes have a natural zero (hence: ratio scale)

Another reason:

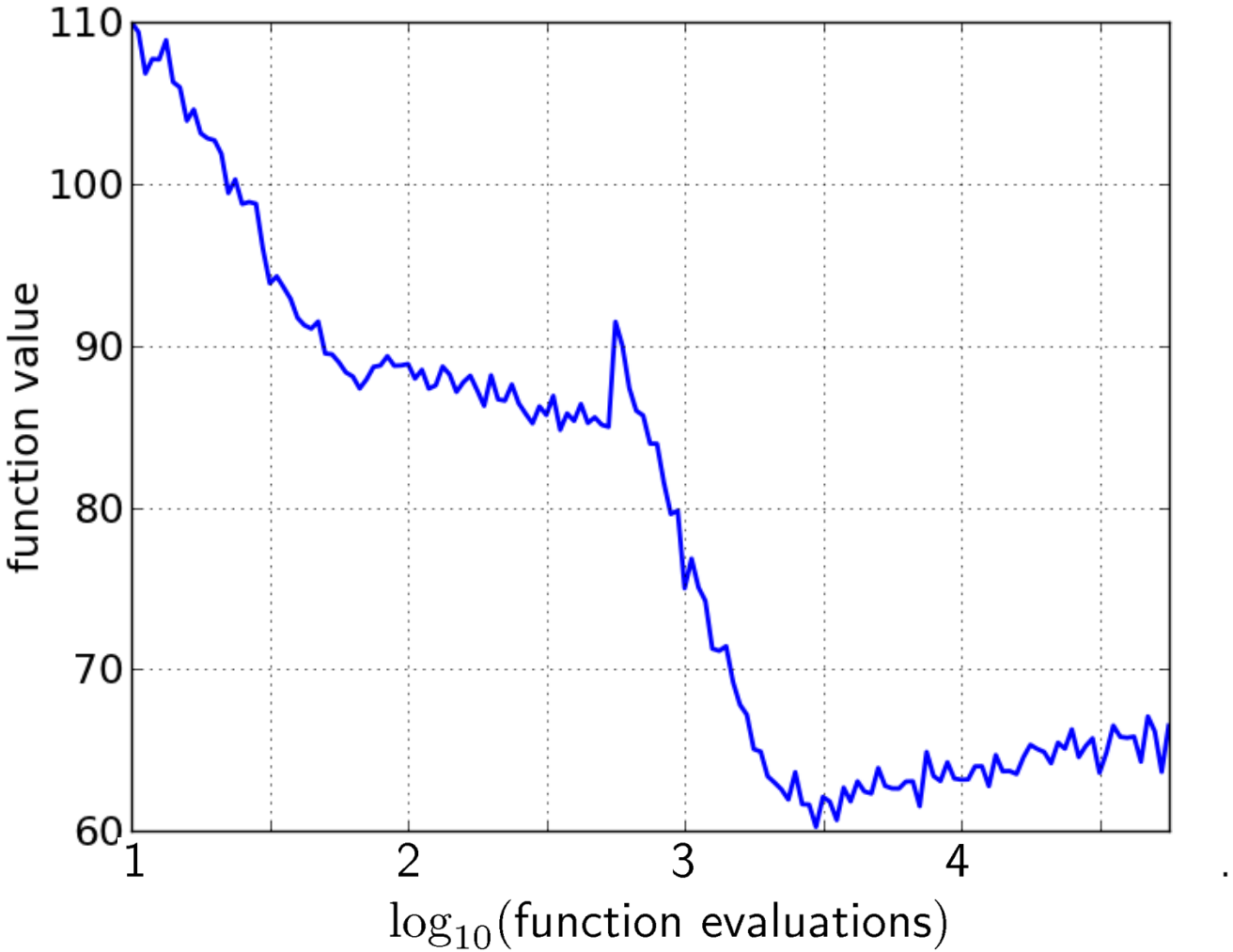
- in both cases, we have missing values
- in the fixed budget view, we miss values of "too good" algorithms
- in the fixed target view, we miss values of "bad/slow" algorithms

ECDF:

Empirical Cumulative Distribution Function of the Runtime

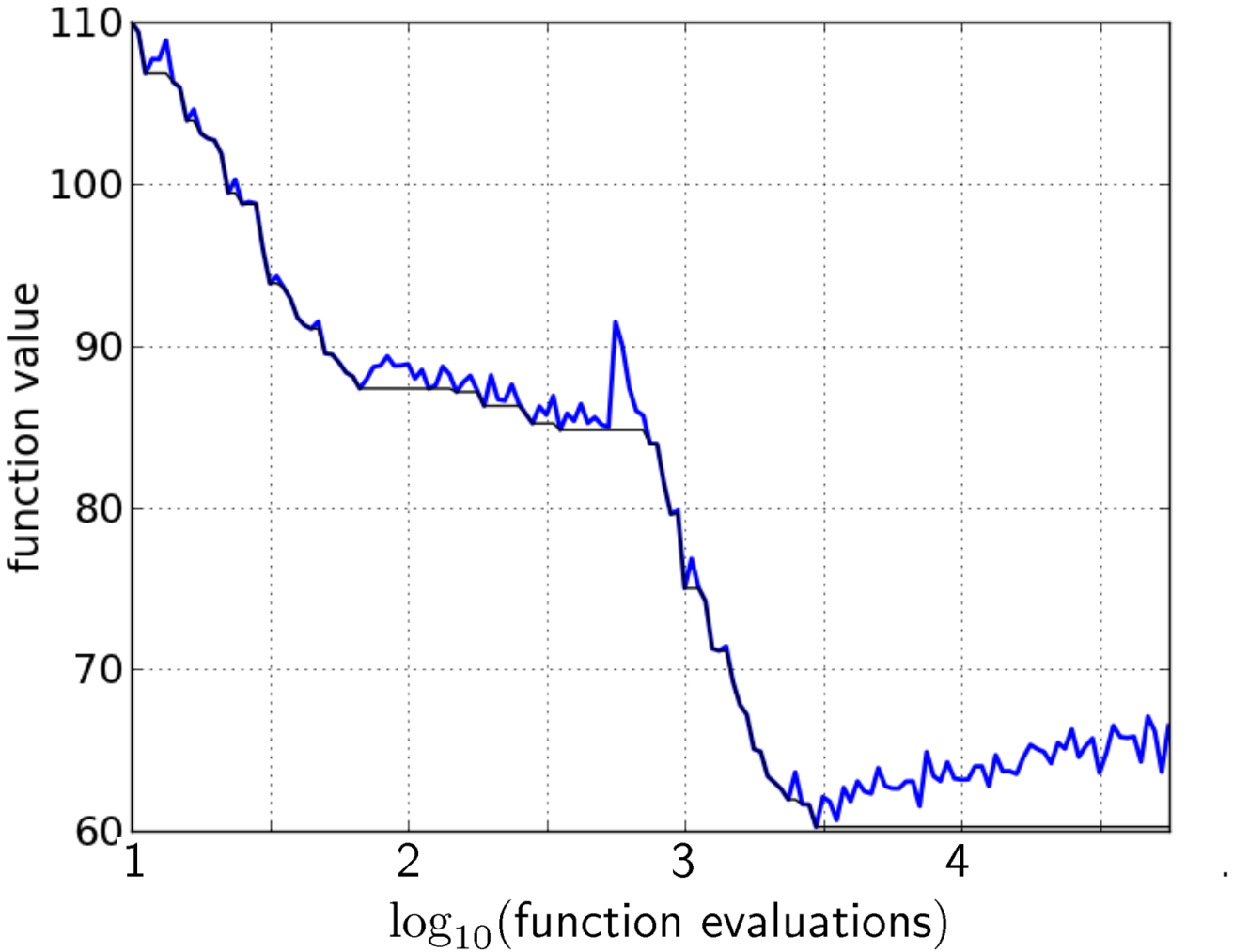
[aka data profile]

A Convergence Graph



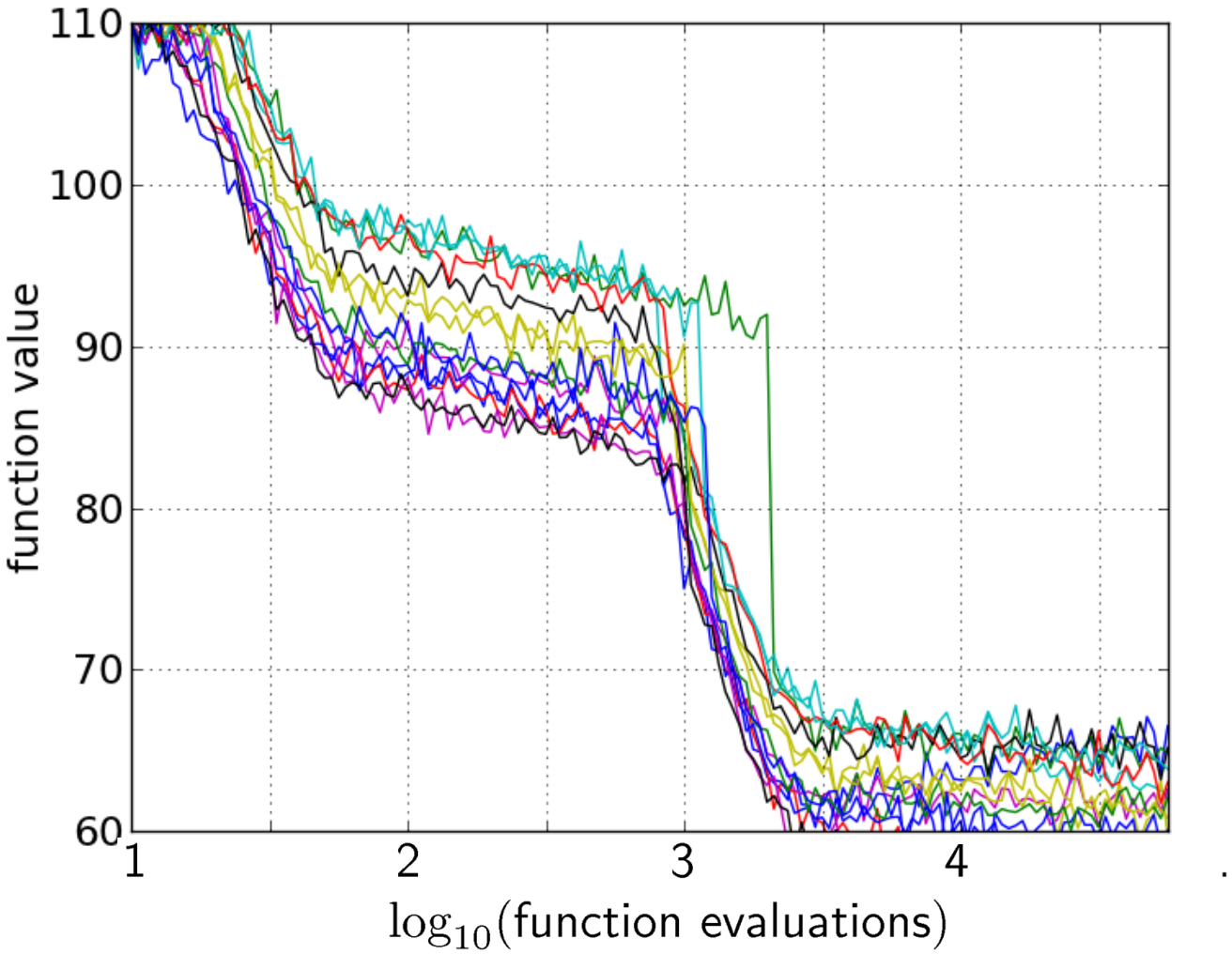
.

First Hitting Time is Monotonous



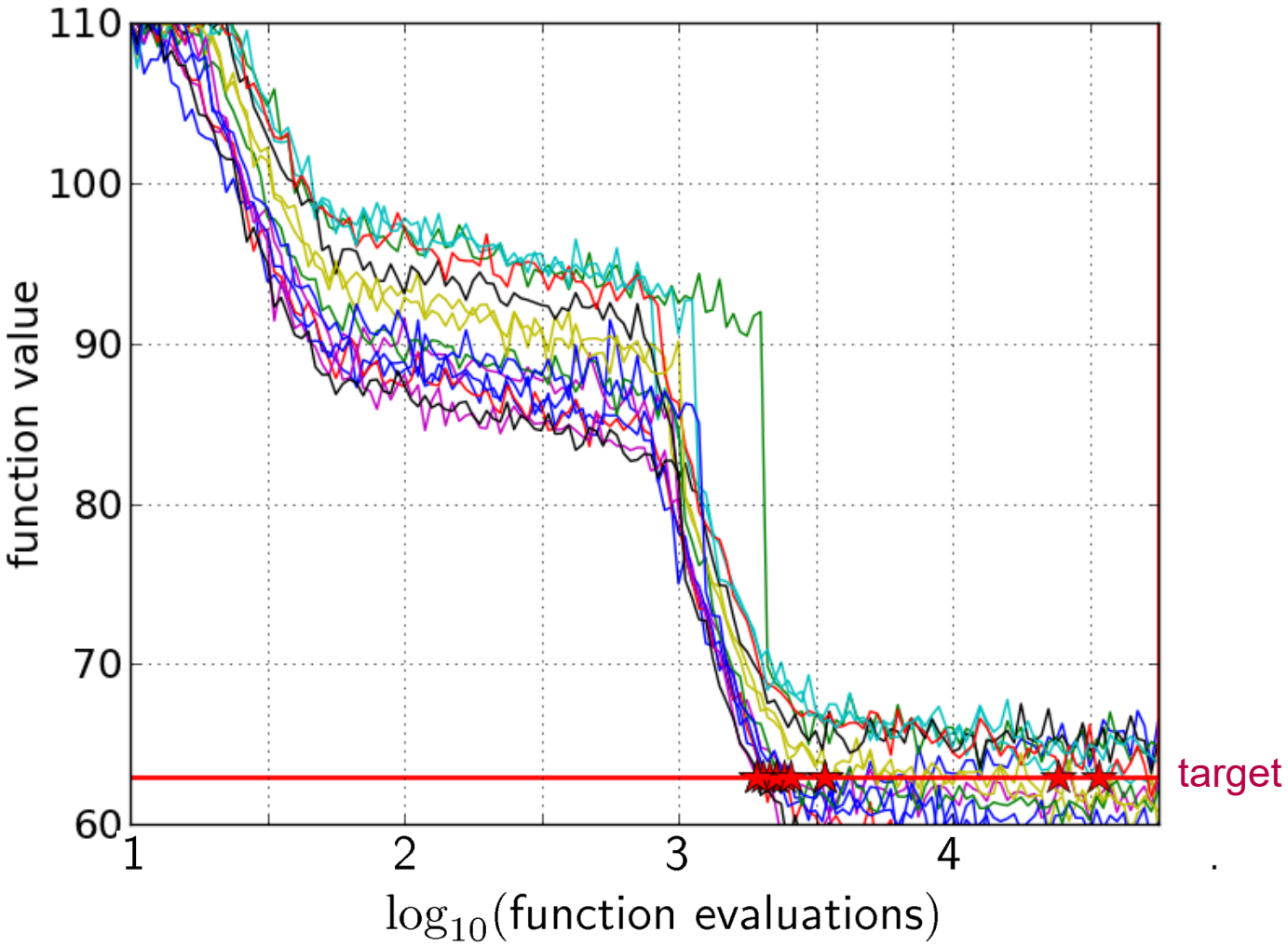
.

15 Runs


110
100
90
80
70
60
function value
1
2
3
4
$\log_{10}$(function evaluations)

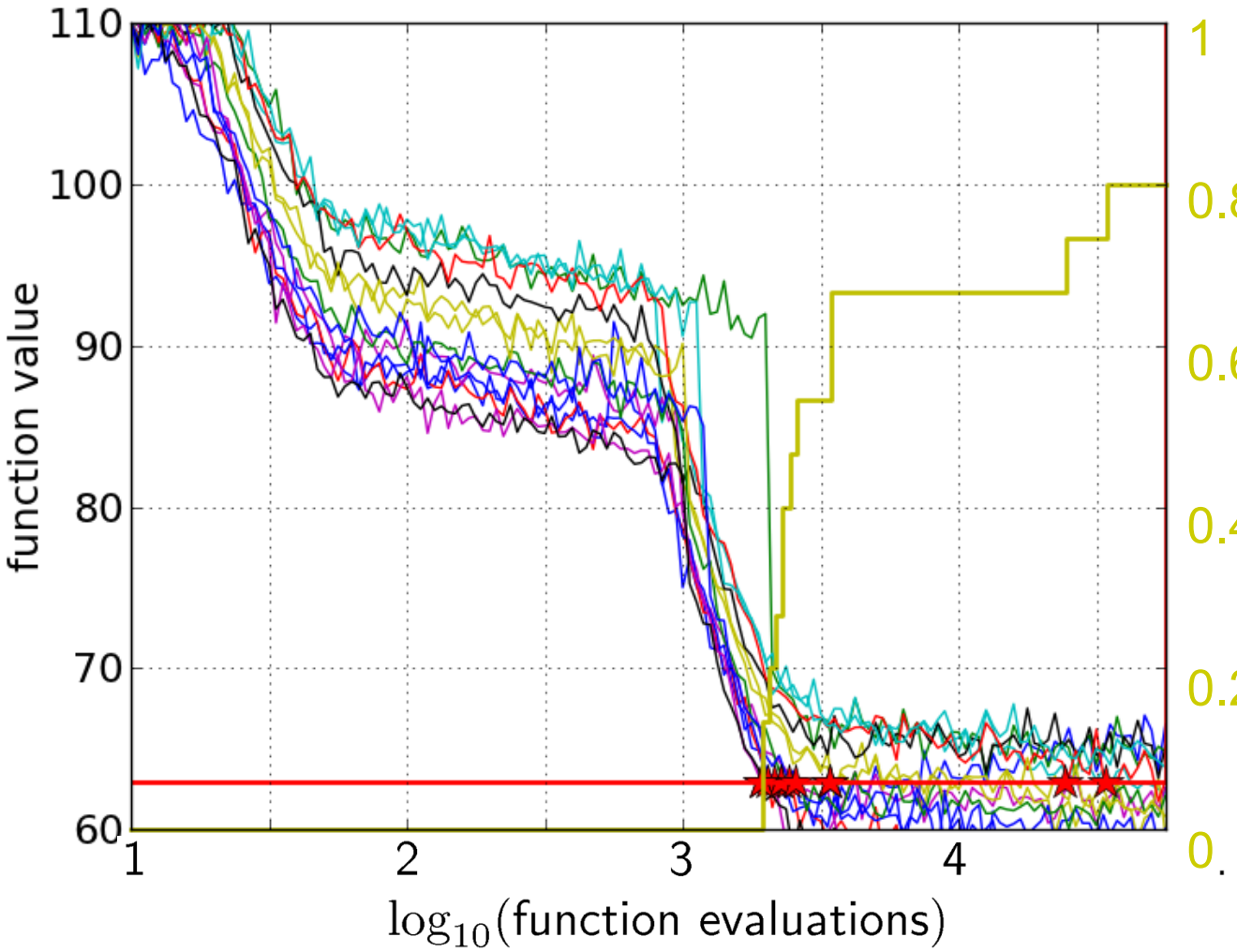
.

15 Runs ≤ 15 Runtime Data Points



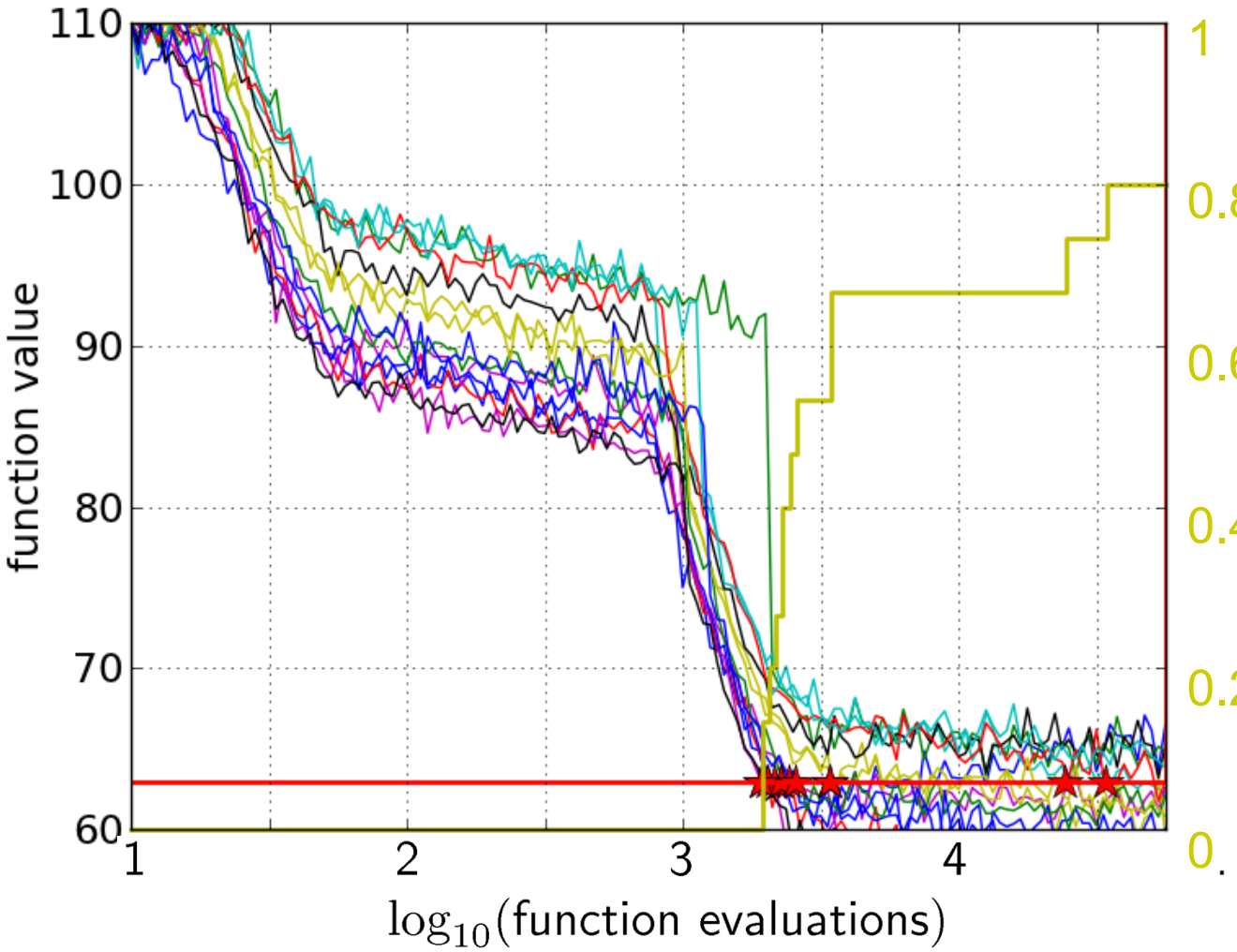
.

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)

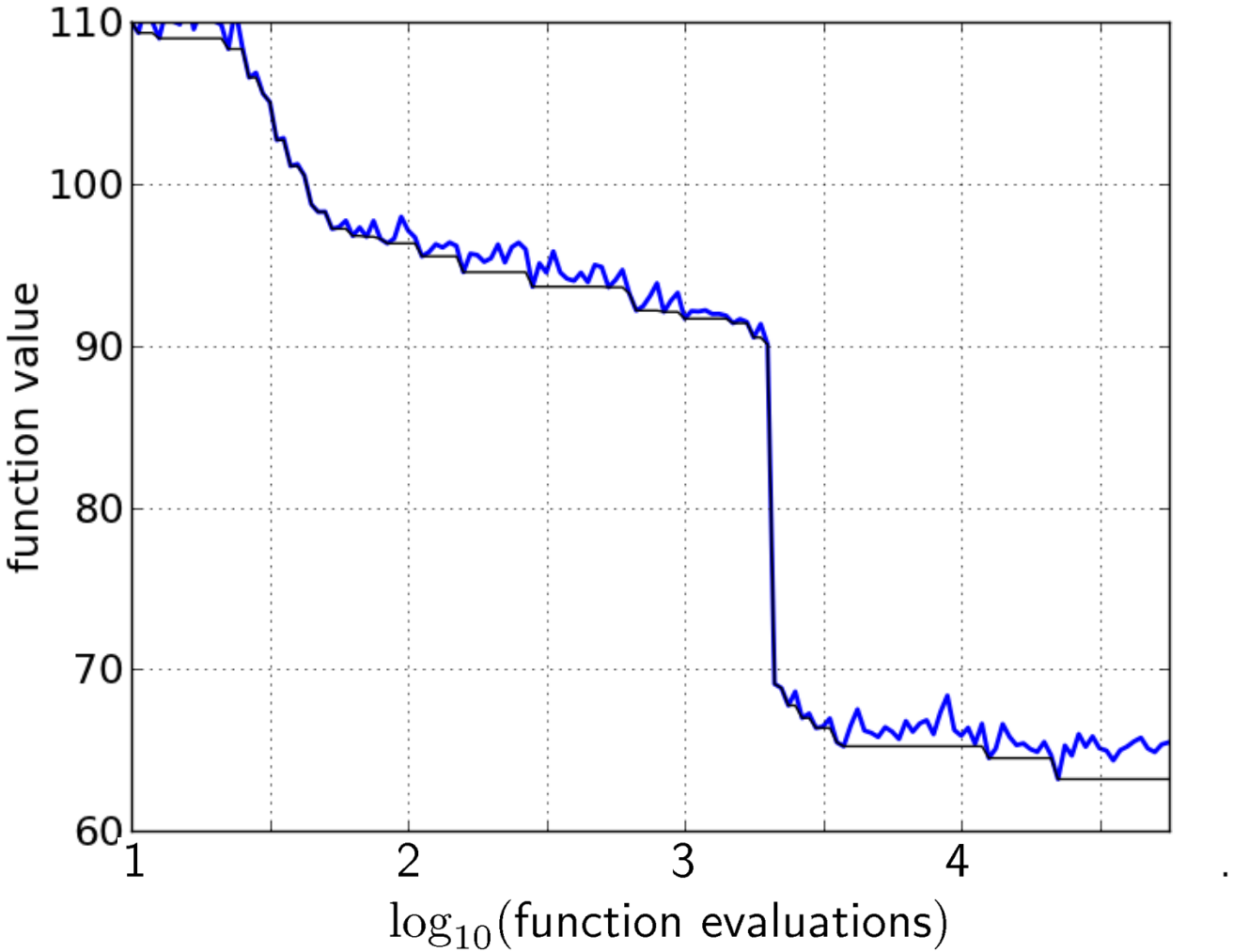
Empirical Cumulative Distribution



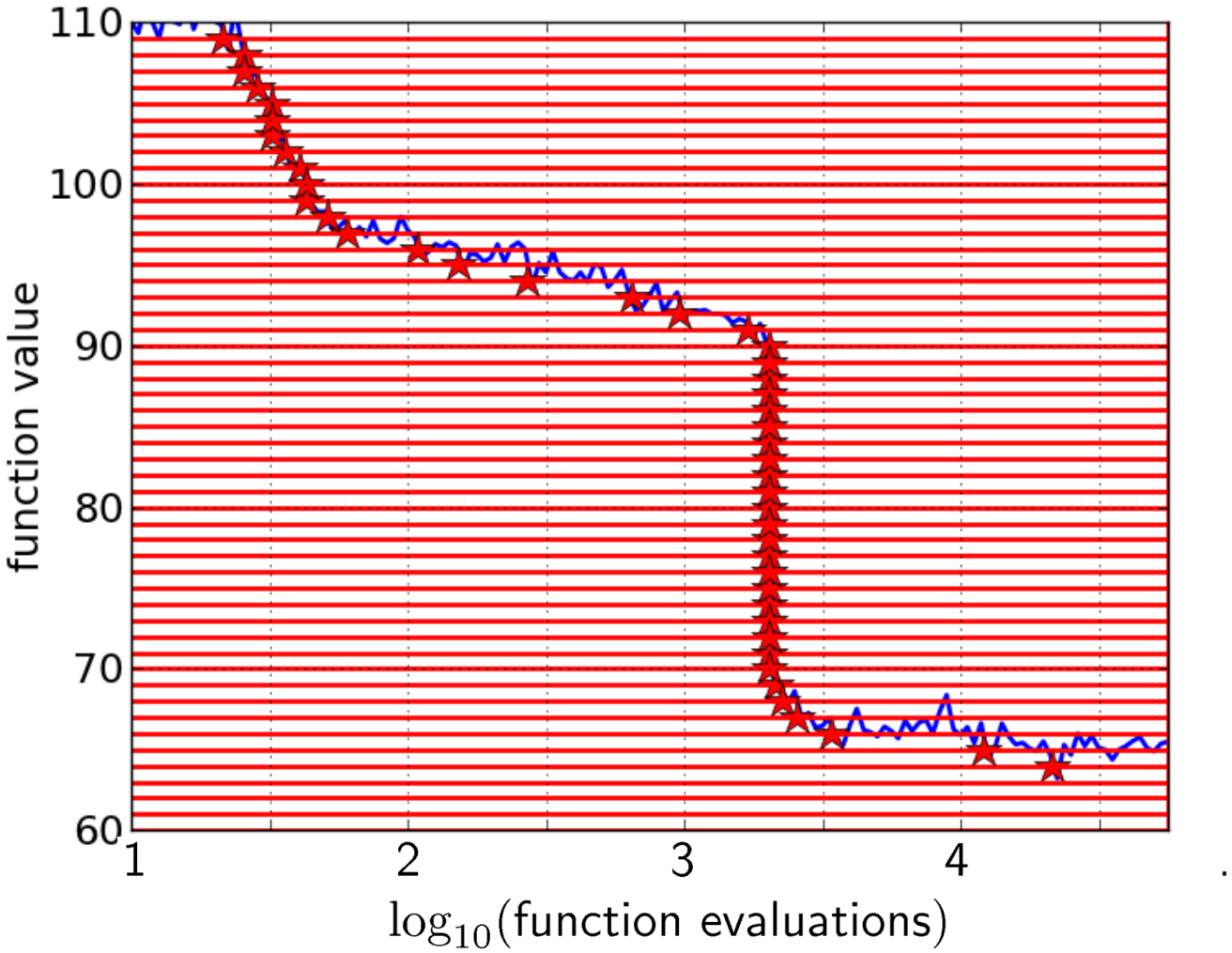
interpretations possible:

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

Reconstructing A Single Run

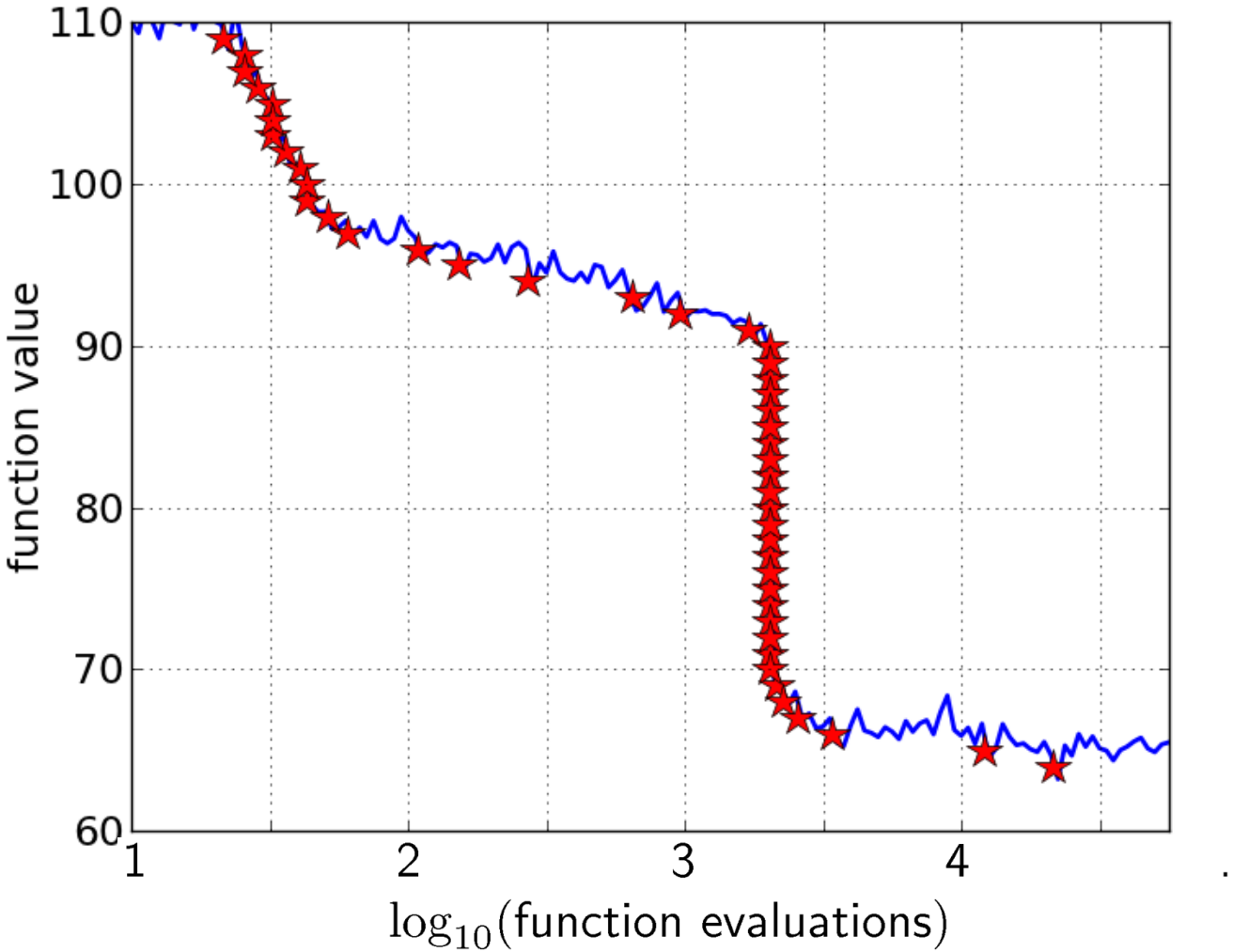


Reconstructing A Single Run

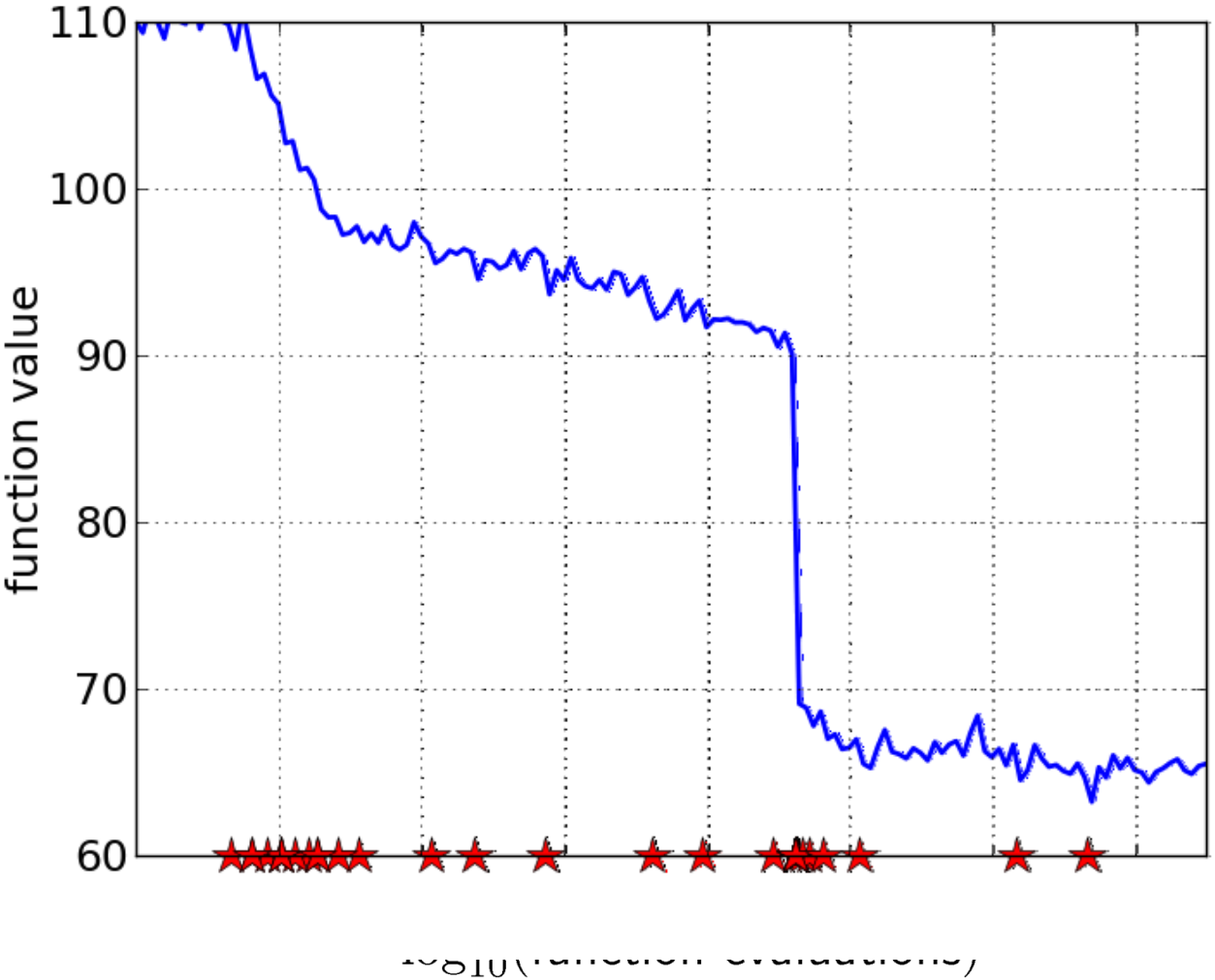


50 equally spaced targets

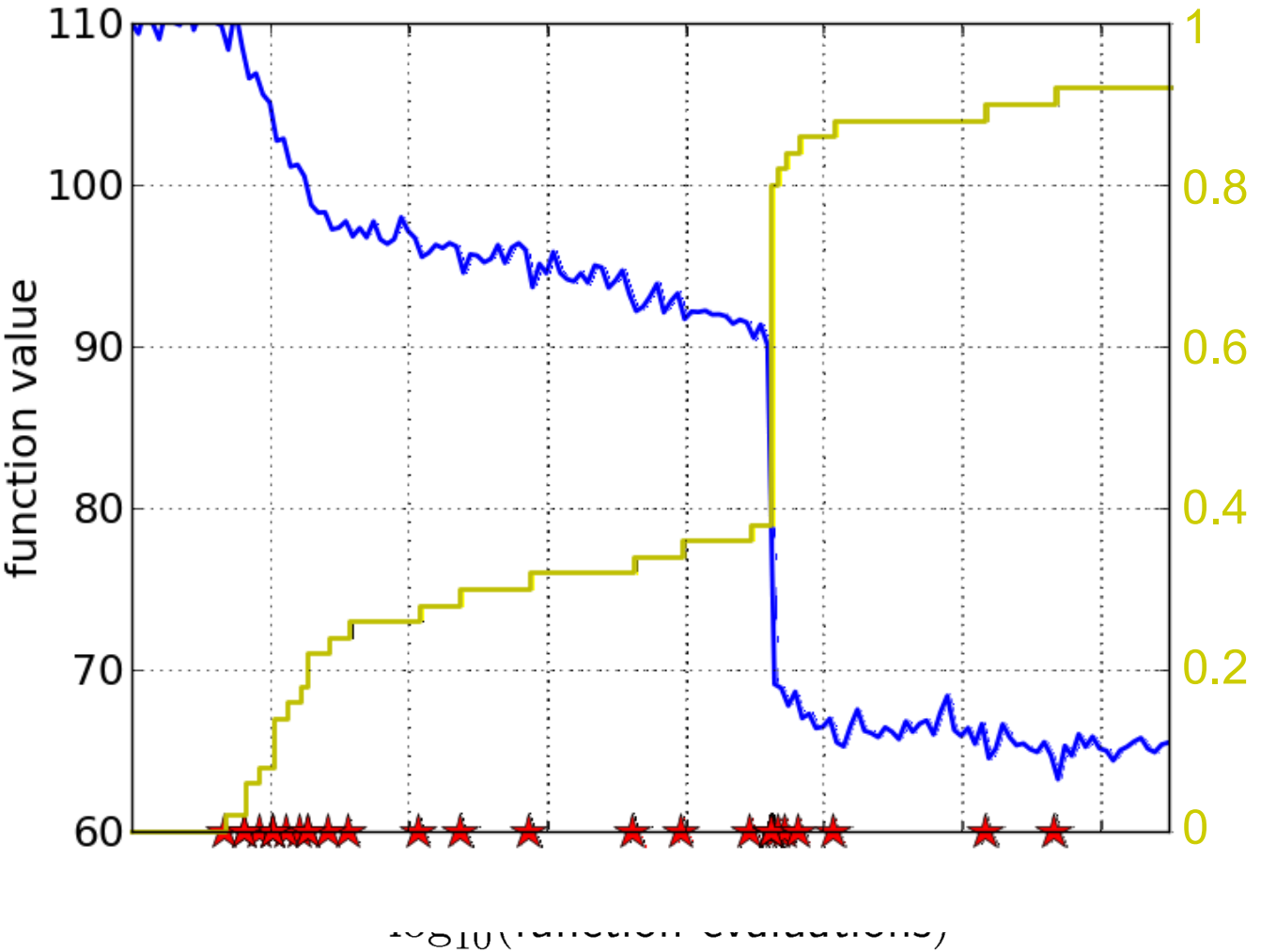
Reconstructing A Single Run



Reconstructing A Single Run

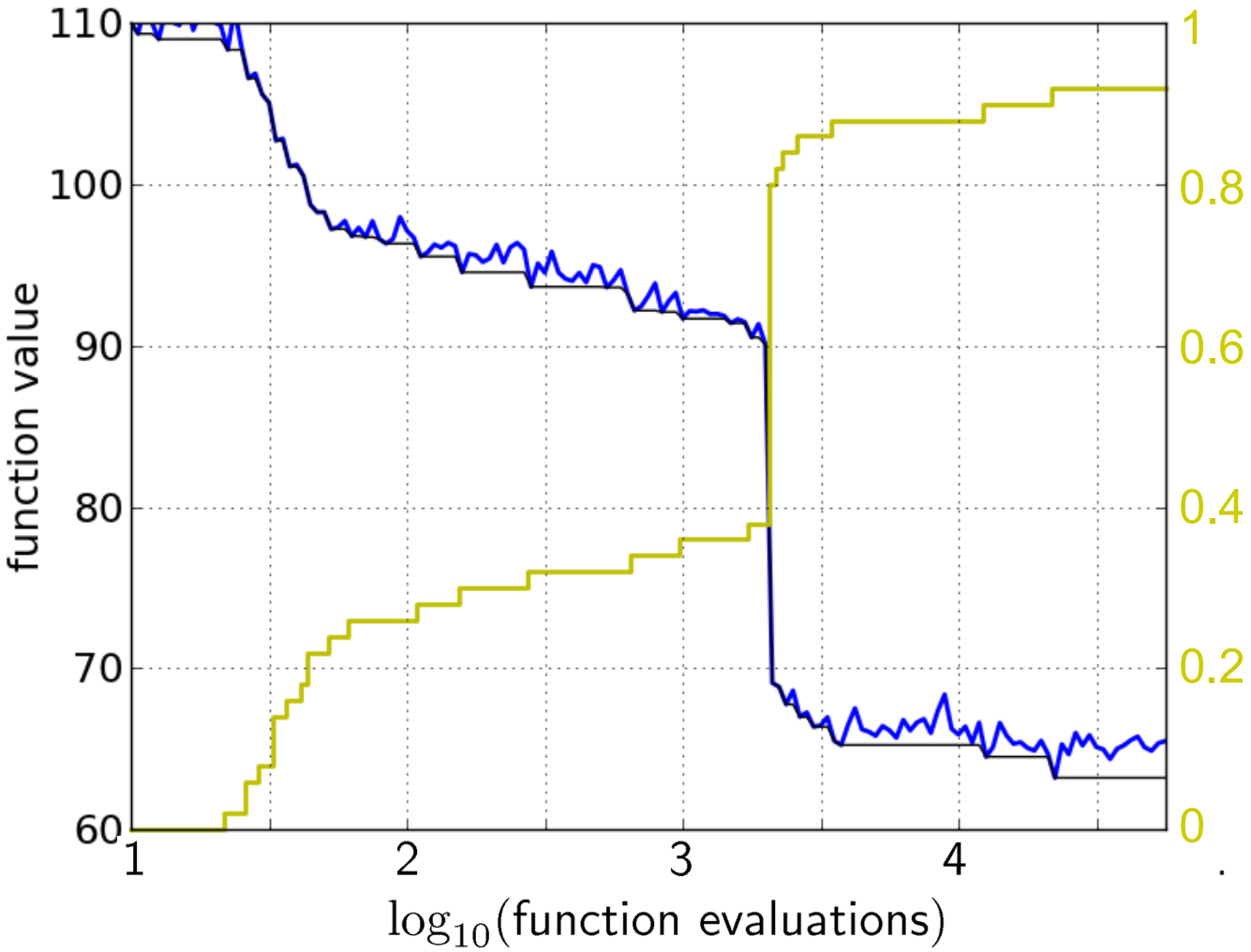


Reconstructing A Single Run



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

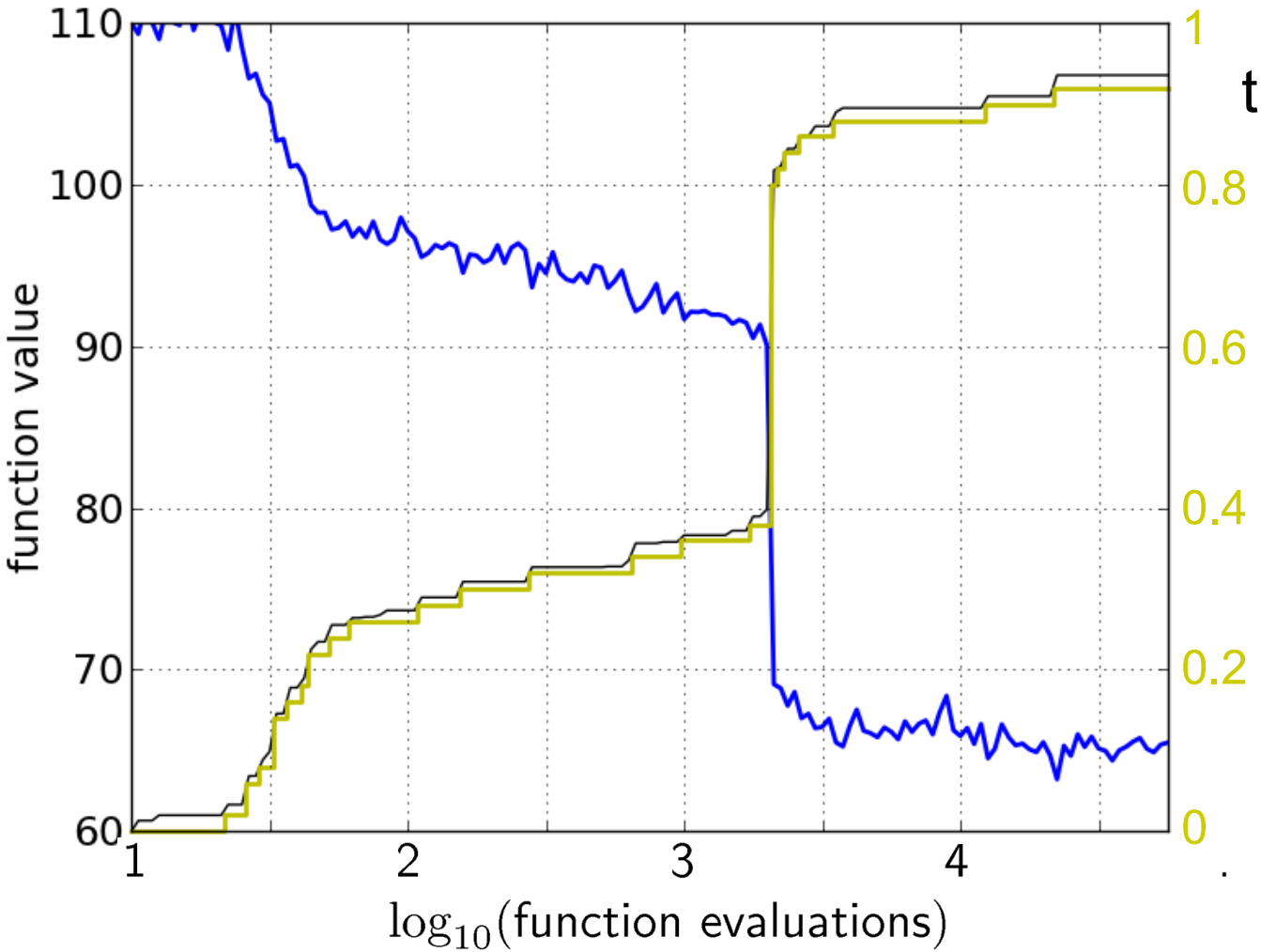
Reconstructing A Single Run



the ECDF recovers the monotonous graph, discretized and flipped

.

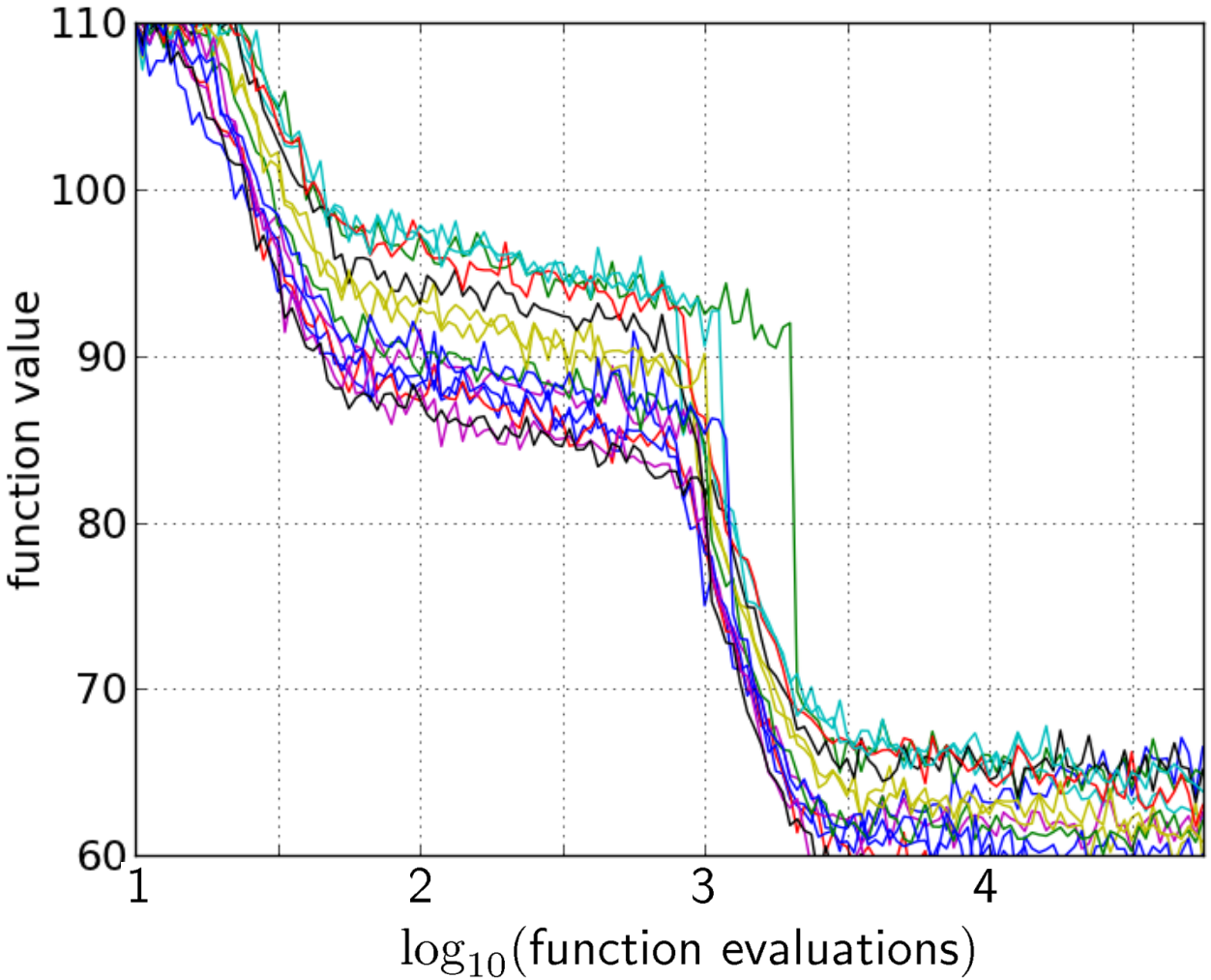
Reconstructing A Single Run



the ECDF recovers the monotonous graph, discretized and flipped

.

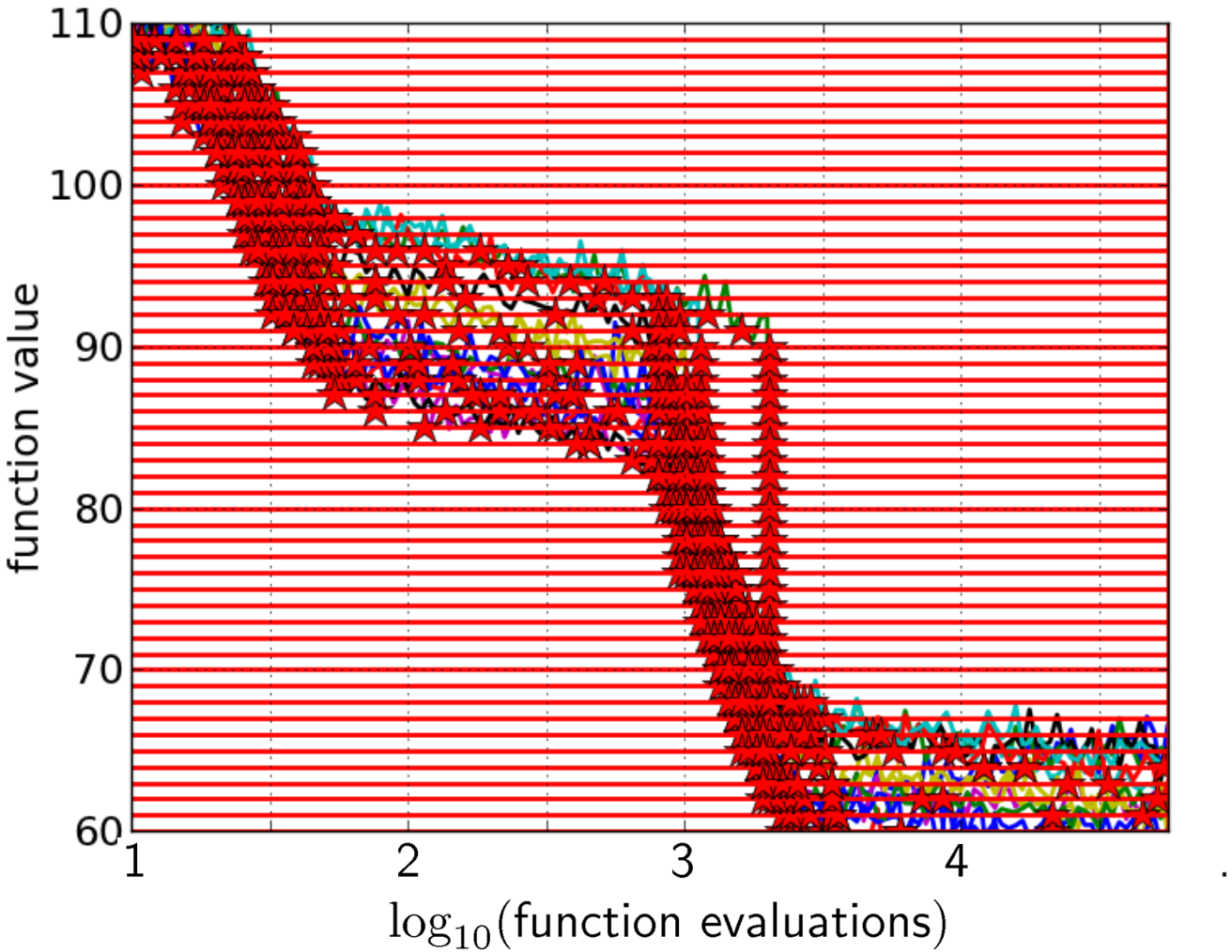
Aggregation



15 runs

.

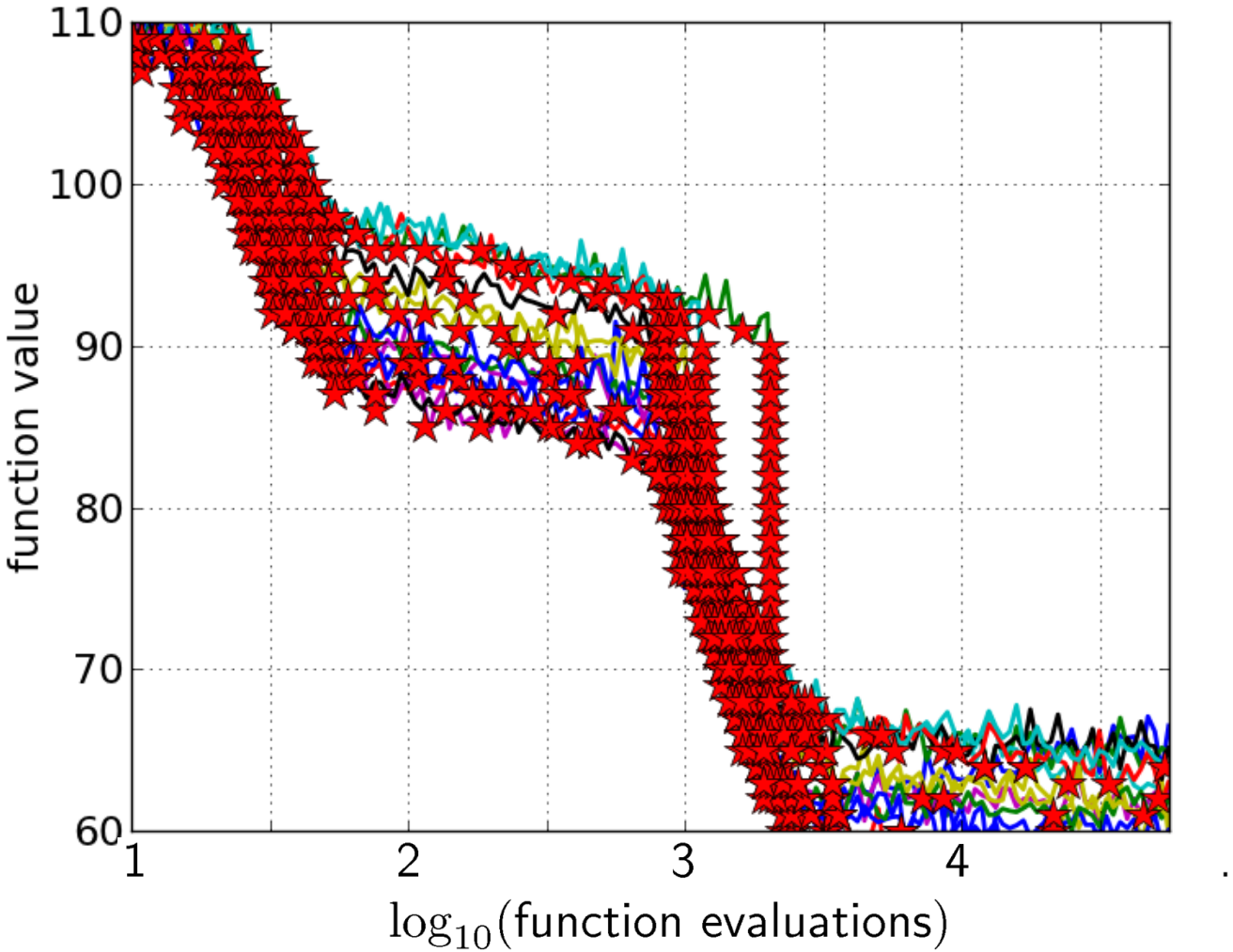
Aggregation



15 runs

50 targets

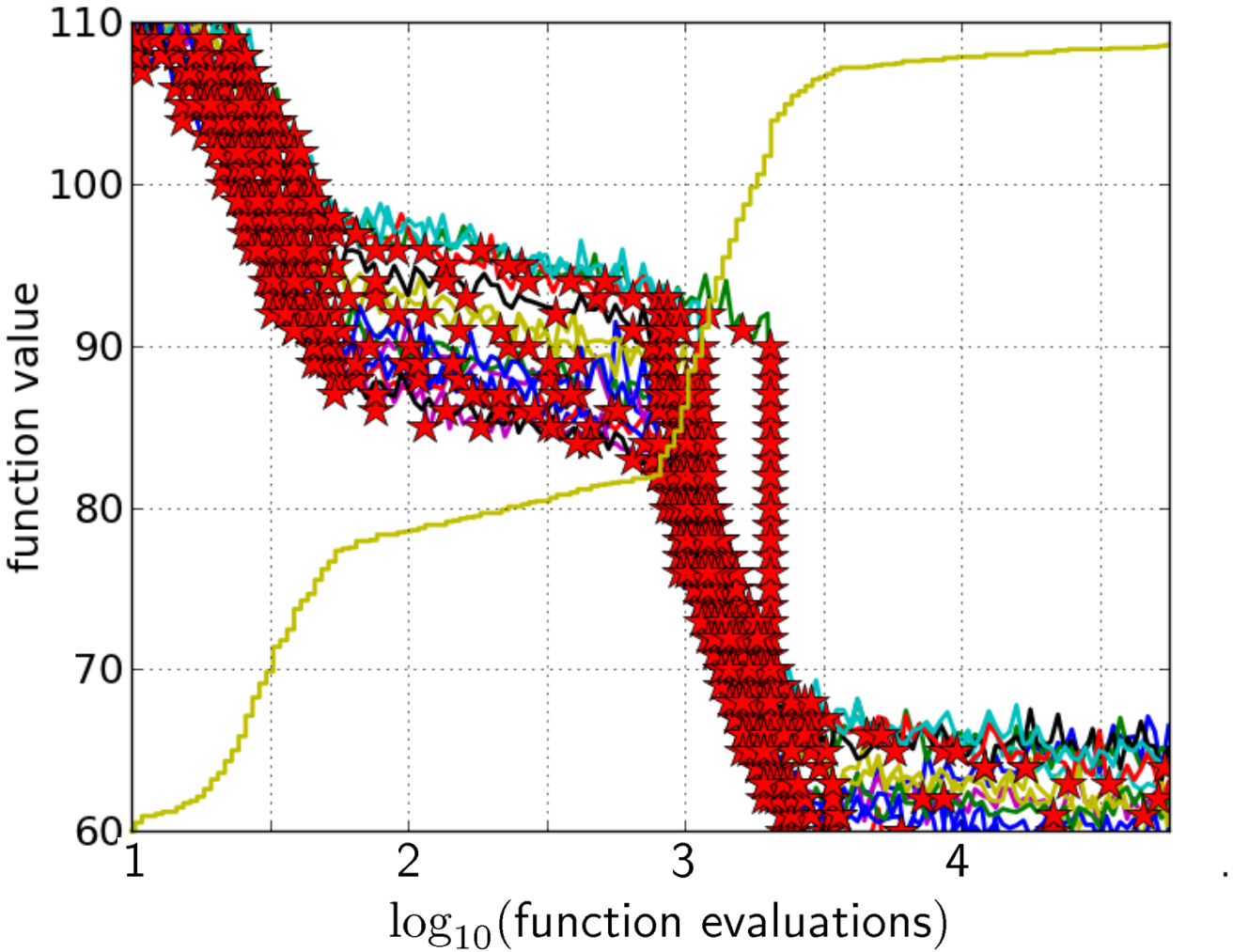
Aggregation



15 runs

50 targets

Aggregation

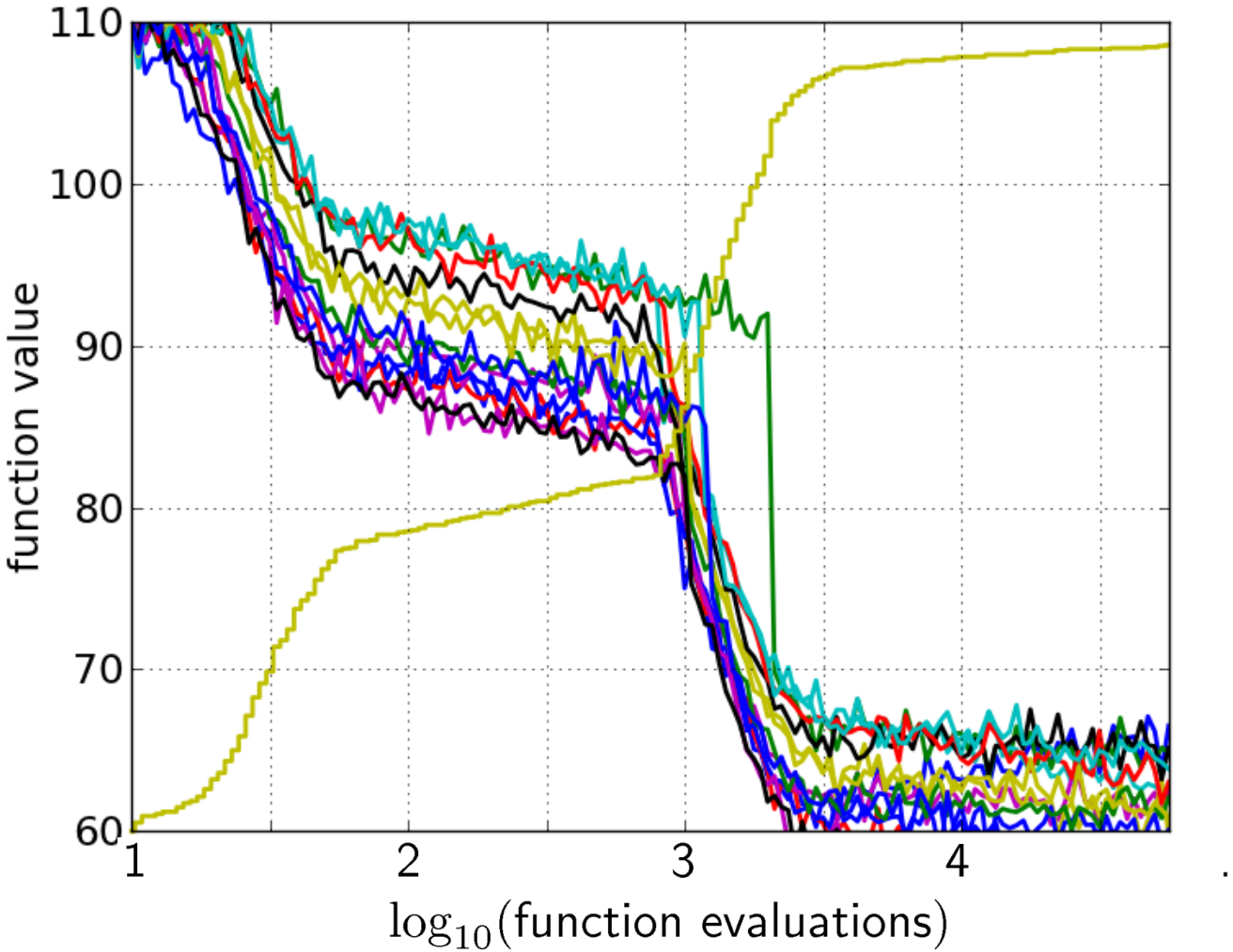


15 runs

50 targets

ECDF with 750 steps

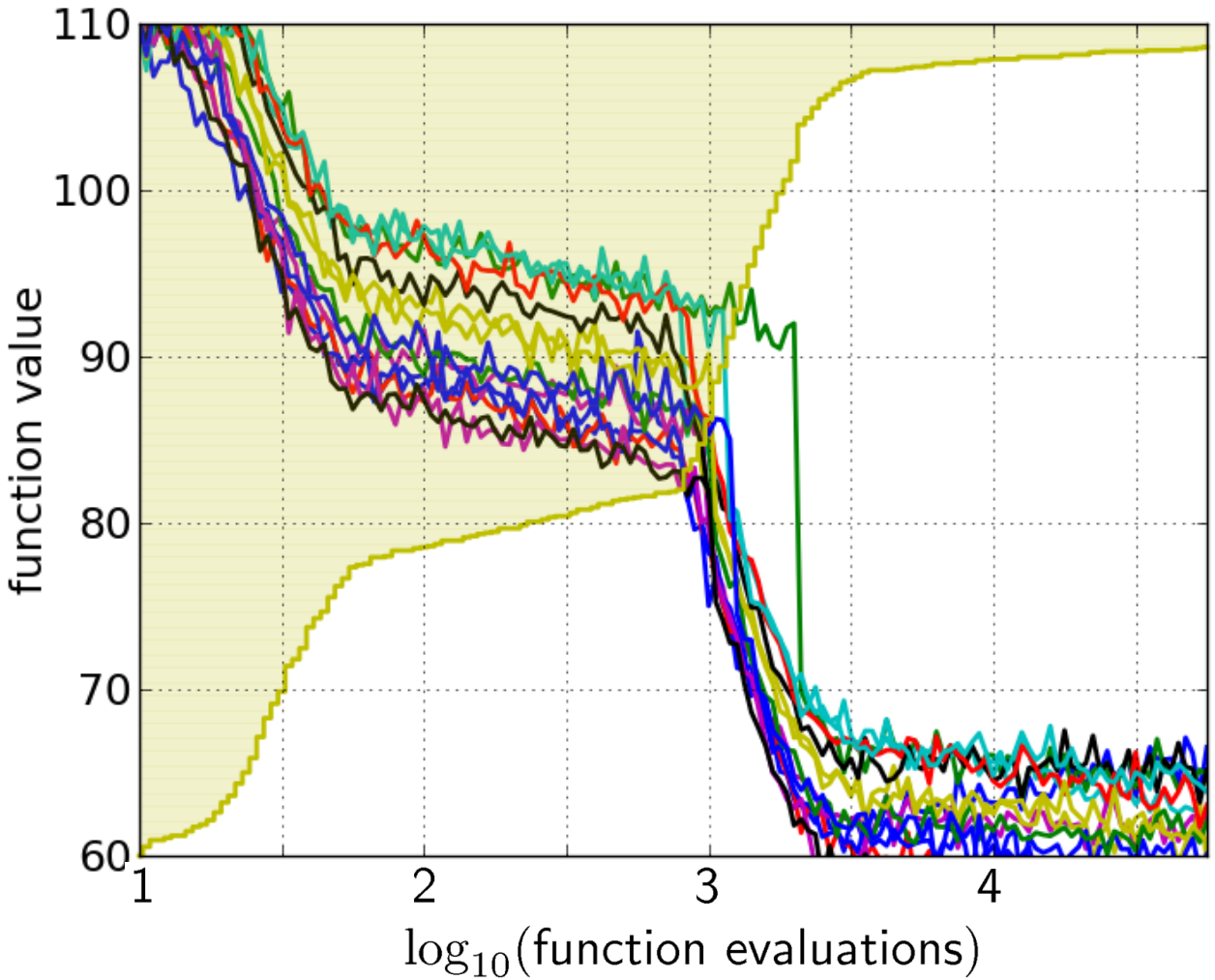
Aggregation



50 targets from 15 runs

...integrated in a single graph

Interpretation



50 targets from 15 runs integrated in a single graph

area over the ECDF curve

=

average log runtime

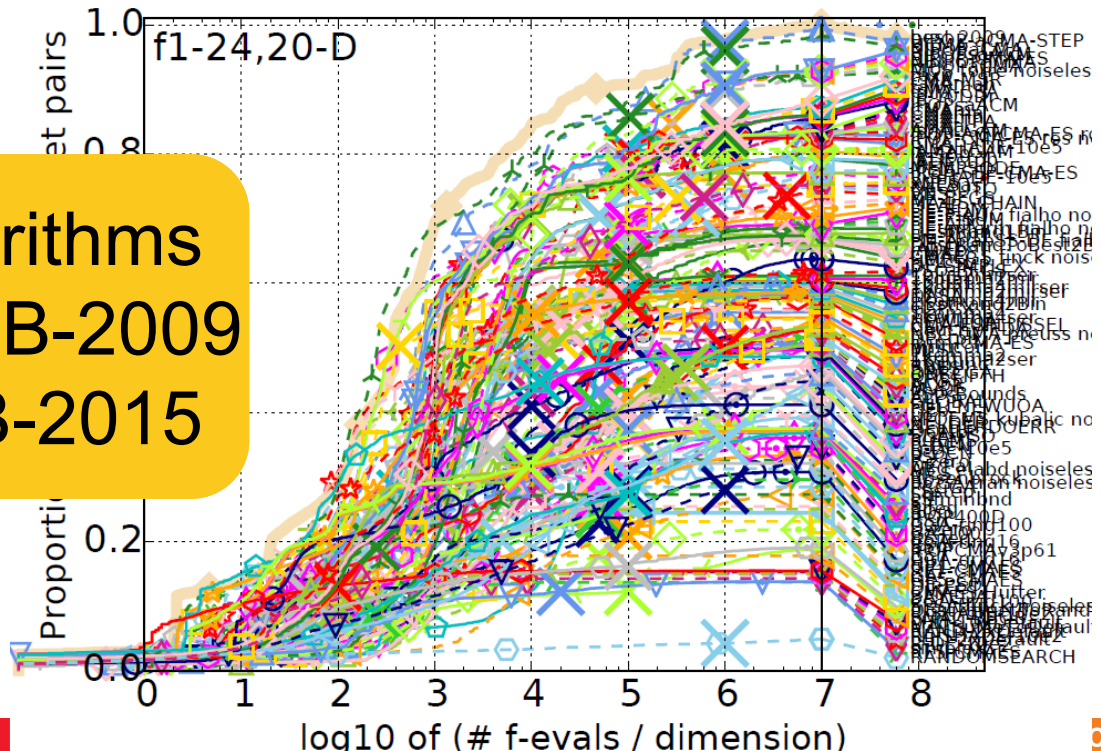
(or geometric avg. runtime) over all targets (difficult and easy) and all runs

Worth to Note: ECDFs in COCO

In COCO, ECDF graphs

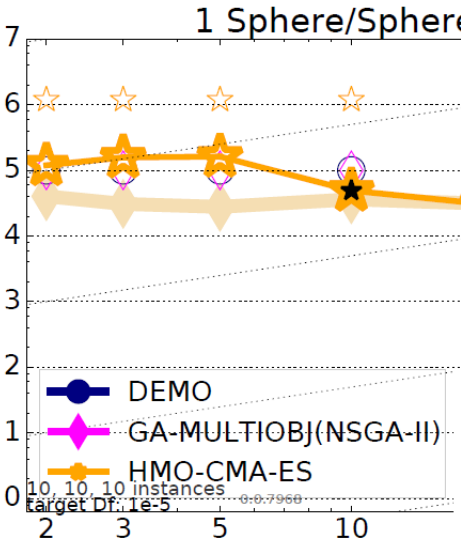
- never aggregate over dimension
  - but often over targets and functions
- can show data of more than 1 algorithm at a time

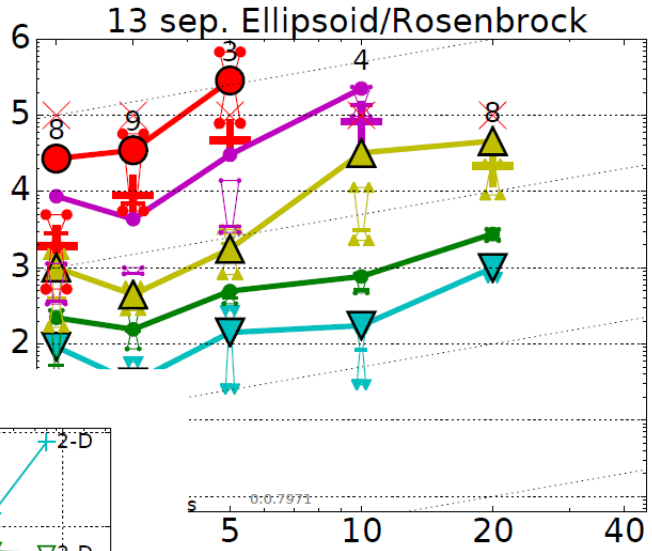
150 algorithms from BBOB-2009 till BBOB-2015

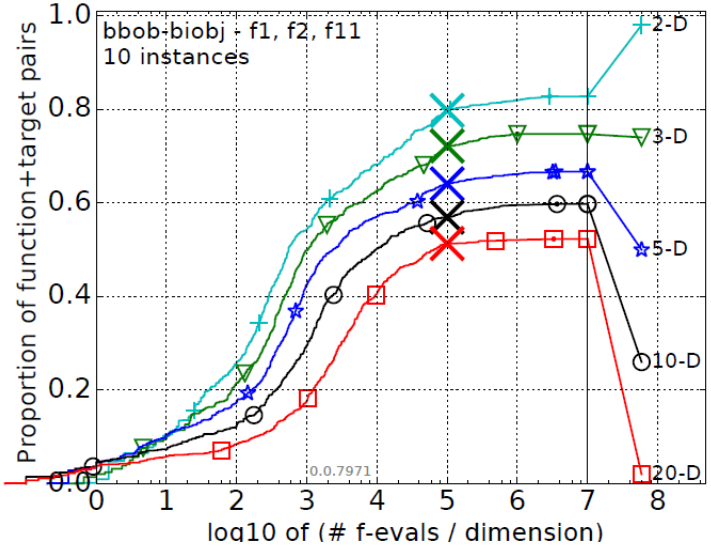


More Automated Plots with COCO

...but no time to explain them here ☹

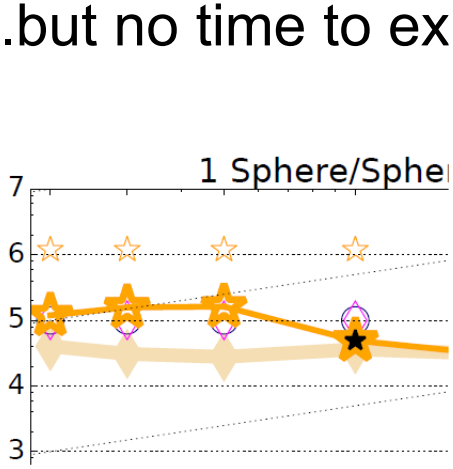


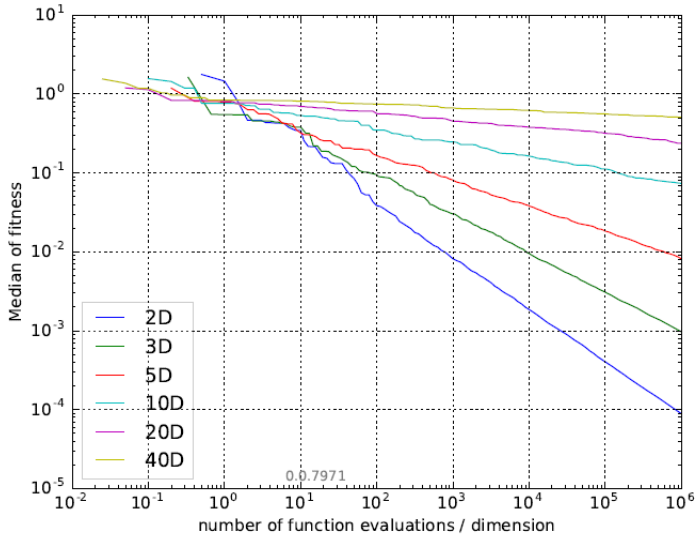


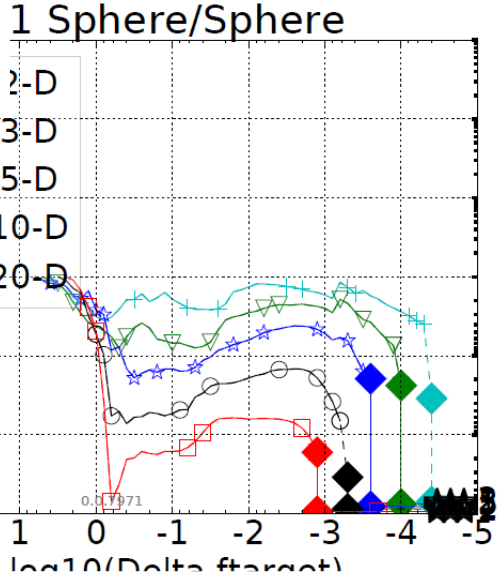


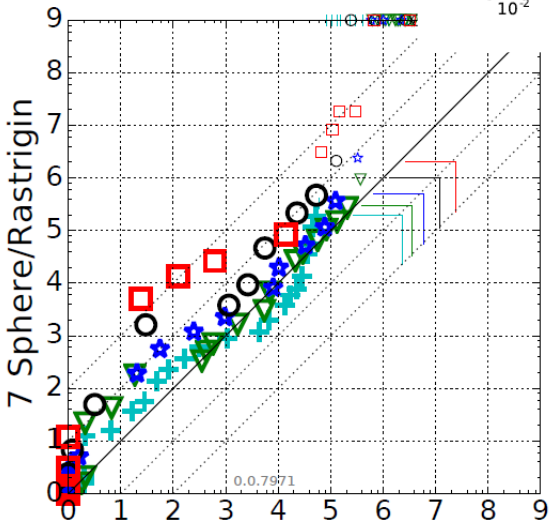
More Automated Plots with COCO

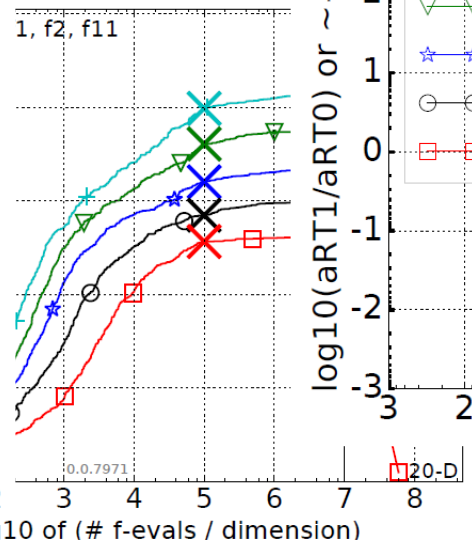
...but no time to ex











Take Home Messages Benchmarking

I hope it became clear...

...that benchmarking is a non-trivial task

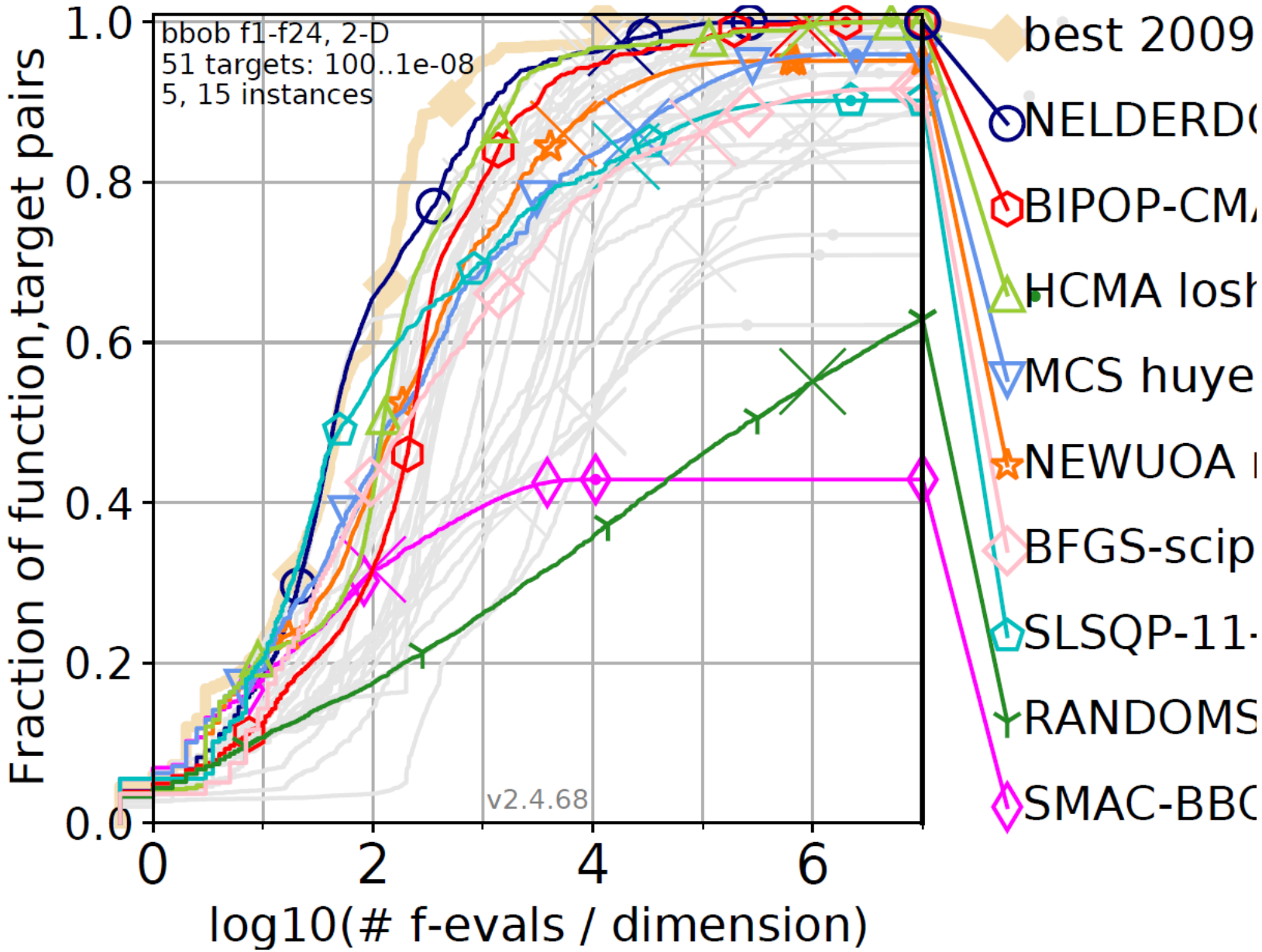
...details matter when comparing algorithms

...and that the COCO platform allows for an automated benchmarking and provides data from hundreds of benchmarking experiments

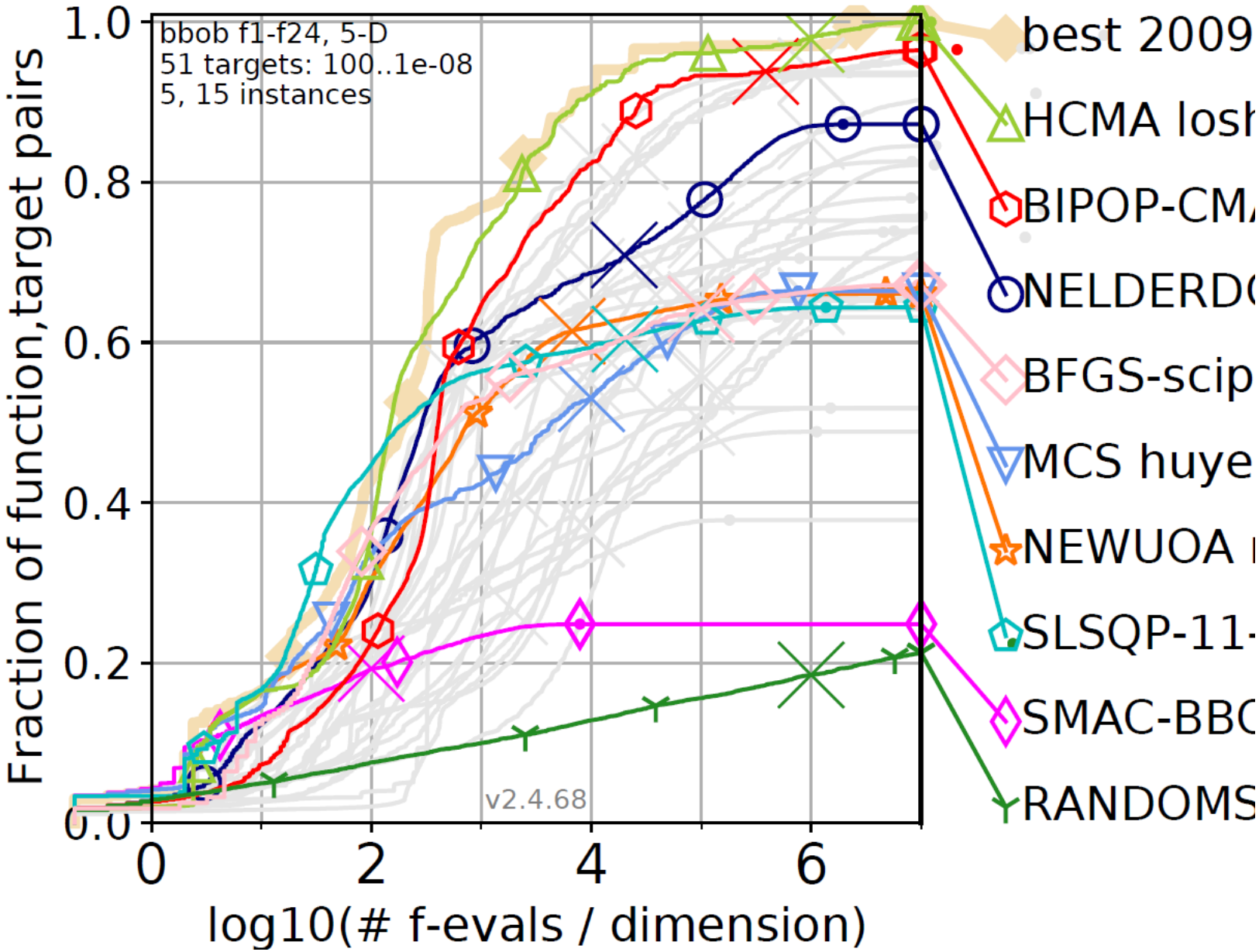
Final Observations

bringing it all together

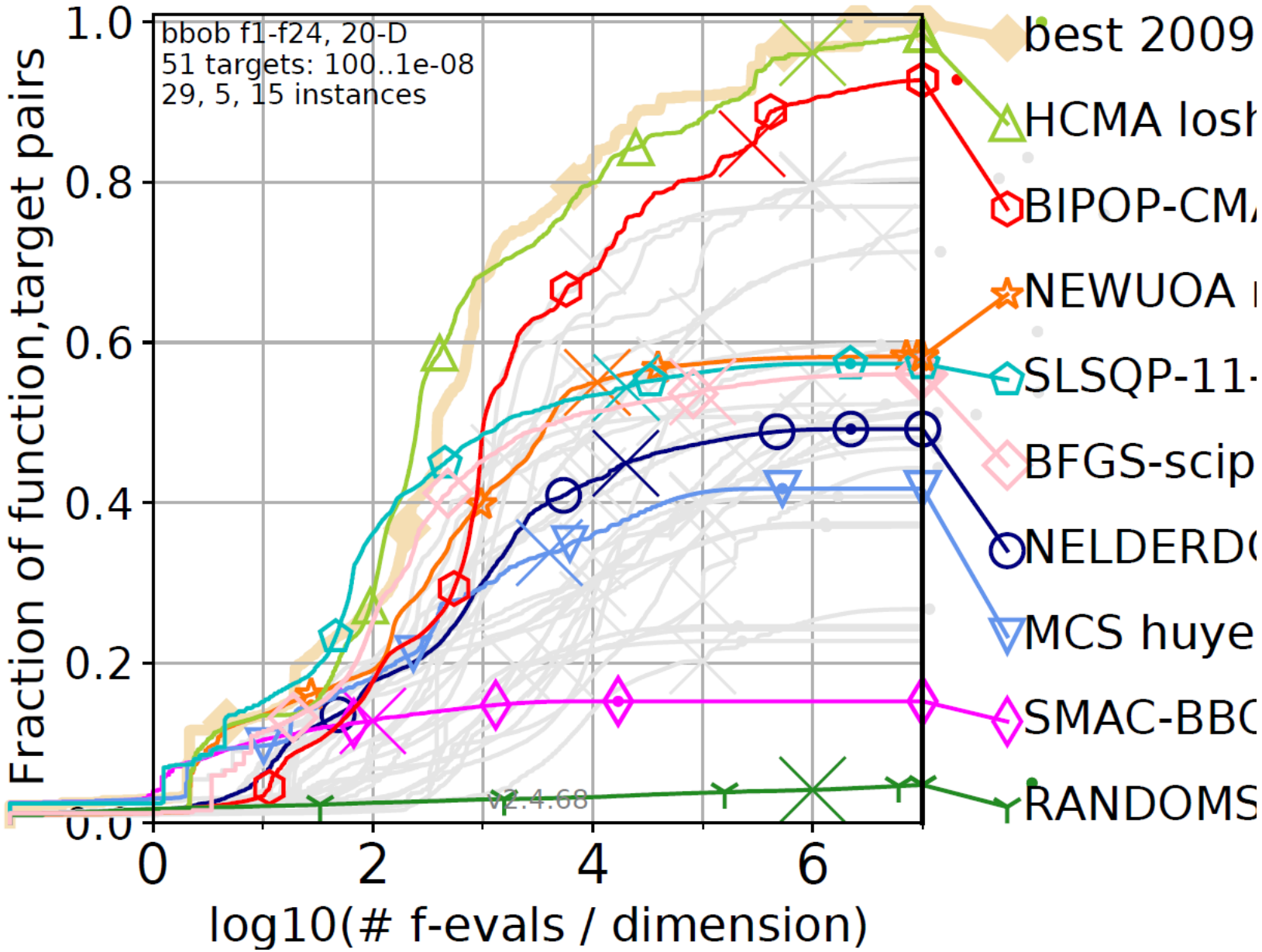
Some Algorithms in 2-D



Some Algorithms in 5-D



Some Algorithms in 20-D



Recommendations

Results of 240+ algorithms (noiseless test suite)

- low dimension (2-D, 3-D), small budget: Nelder Mead (implementation by B. Doerr et al.)
- very small budget (<50D funevals): BBOB-SMAC (an EGO variant) or SLSQP
- larger dimension, small budget (<500D funevals): NEWUOA, SLSQP, BFGS
- larger dimension, large budget (>500D funevals): CMA-ES variants
- portfolio algorithms can combine the best of all worlds, e.g. HCMA
- restarts of quick (local) algorithms for multimodality

Further Observations

Invariance

- many algorithms are not invariant under affine transformations of the search space (for example PSO), others like CMA-ES variants are
- as a consequence, other types of algorithms are good for separable and non-separable problems

Robustness of Algorithms

- CMA-ES was tested in several variants, in several programming languages and with several, slightly changing settings
- nevertheless, it showed throughout its variants consistently good behavior and can be considered as a robust algorithm if the budget is not too low

final topic…

Branch and Bound

Branch and Bound: Scenario and Idea

- A general optimization heuristic for discrete optimization
- Split the finite search space iteratively and solve each sub-problem separately ("branch")
- Why is this better than exhaustive search?
  - If we can get upper and lower bounds on the optimal function value of a subproblem ("bound")…

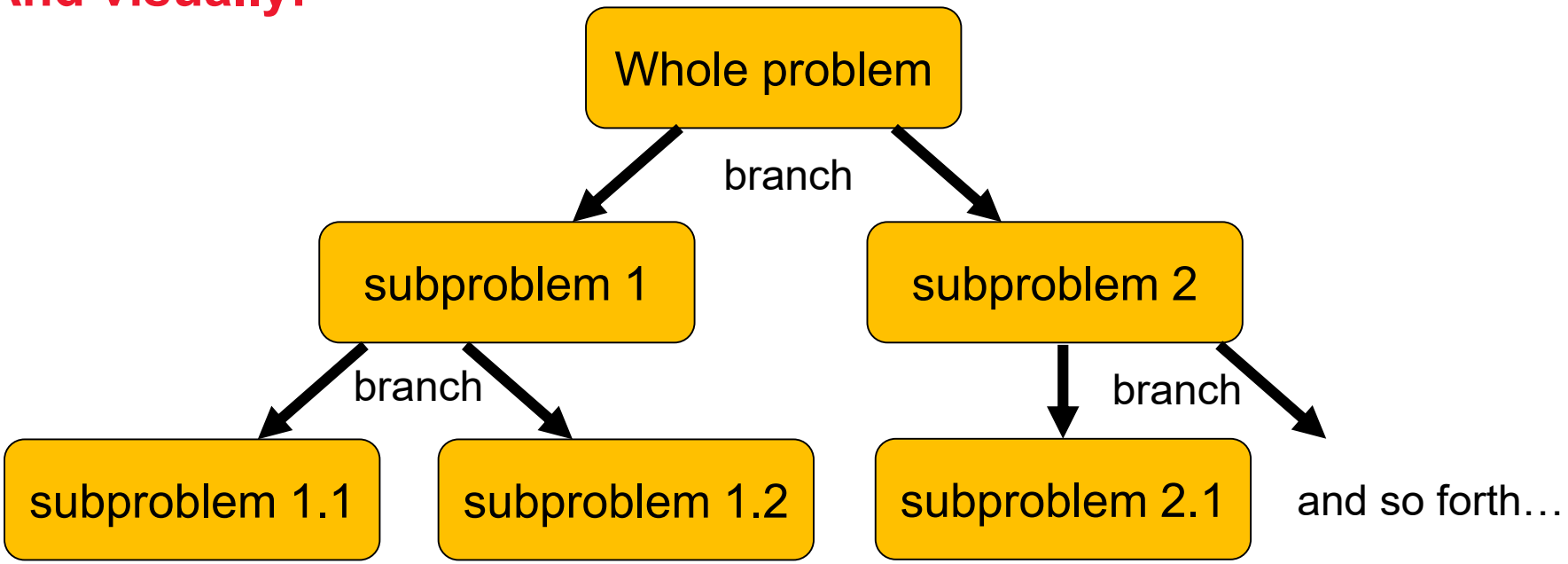
    should be quick, i.e. without computing the actual optimal value
  - …we can avoid solving subproblems if, for example the upper bound for problem P1 < lower bound for problem P2

Visualization of Branch and Bound

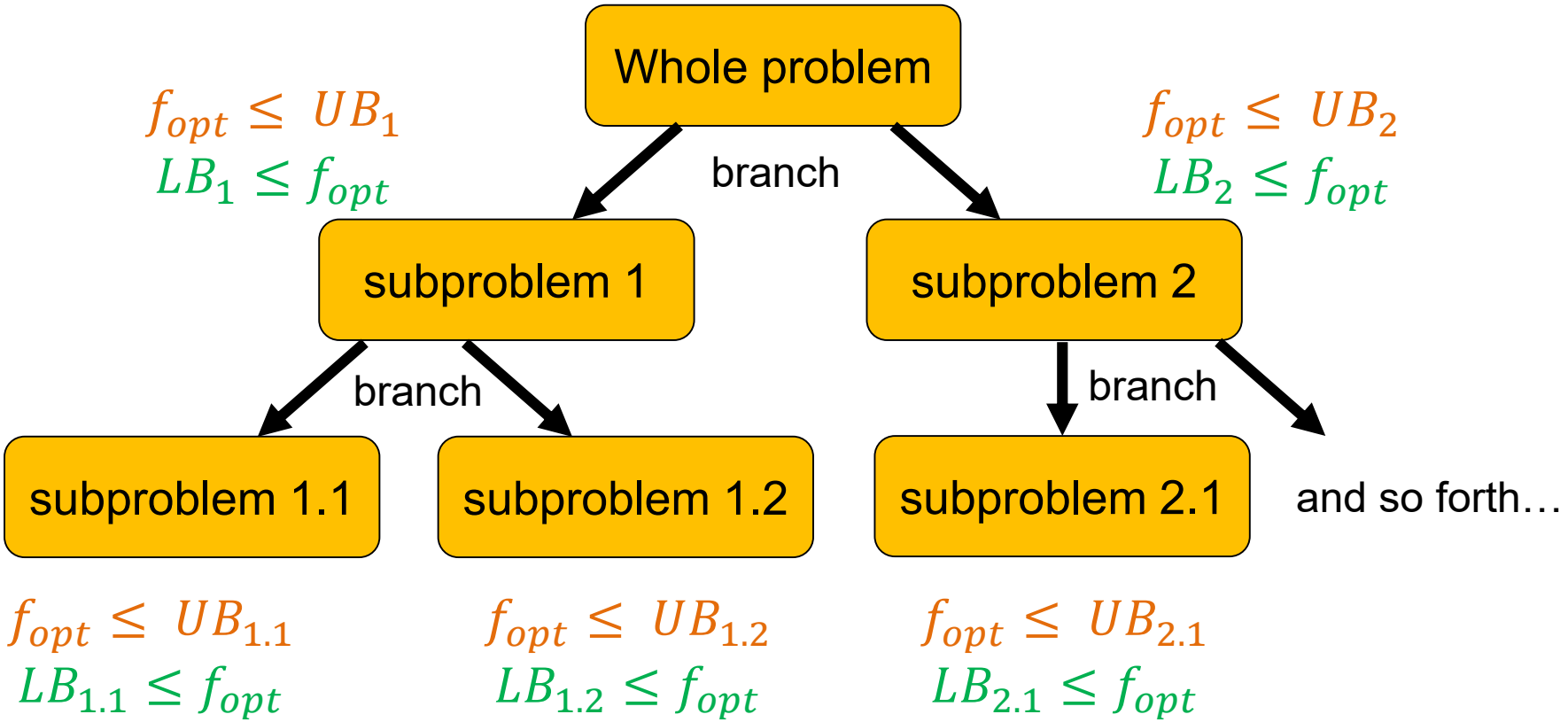
In other words:

- Basically enumerates the entire search space
- But uses clever strategies to avoid enumerations in bad areas

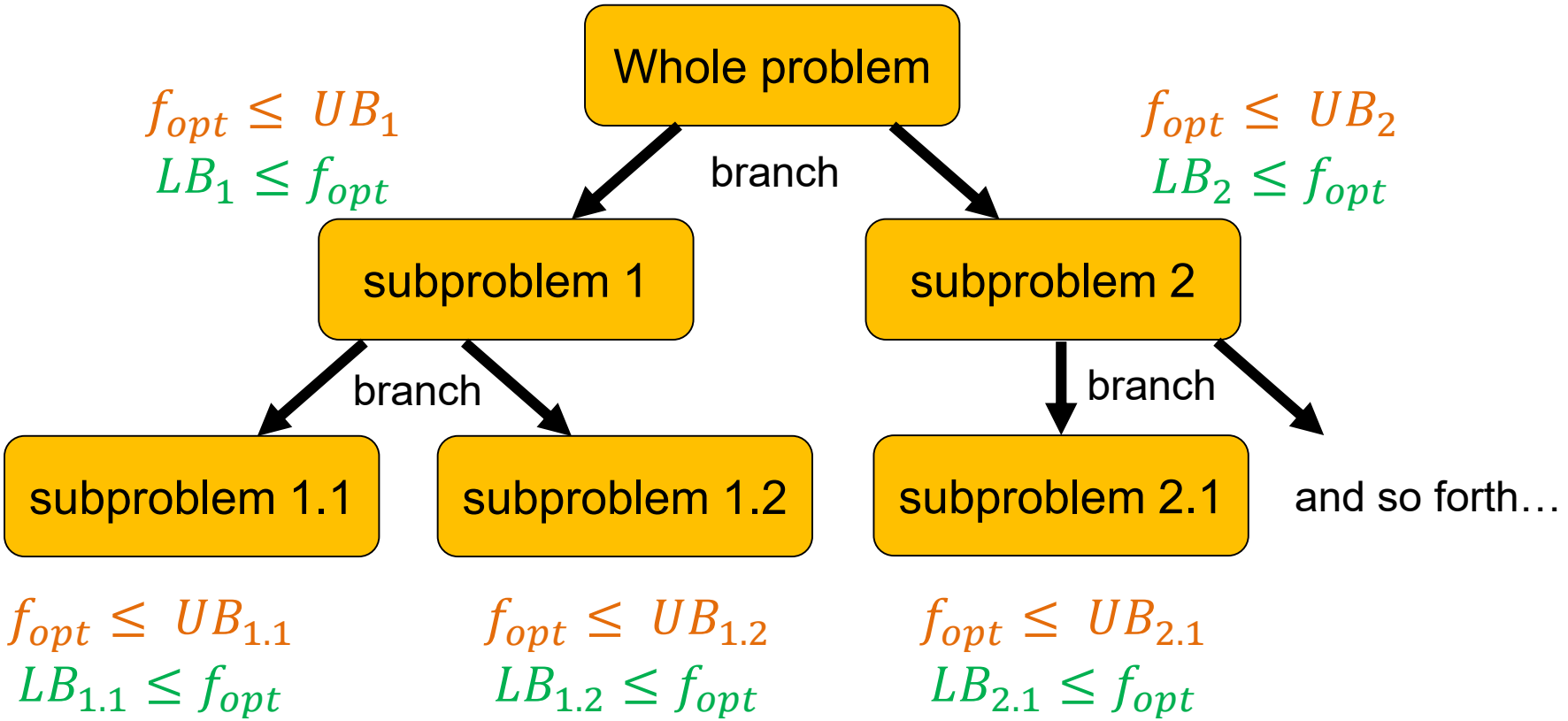
And visually:



Idea Behind Branch and Bound

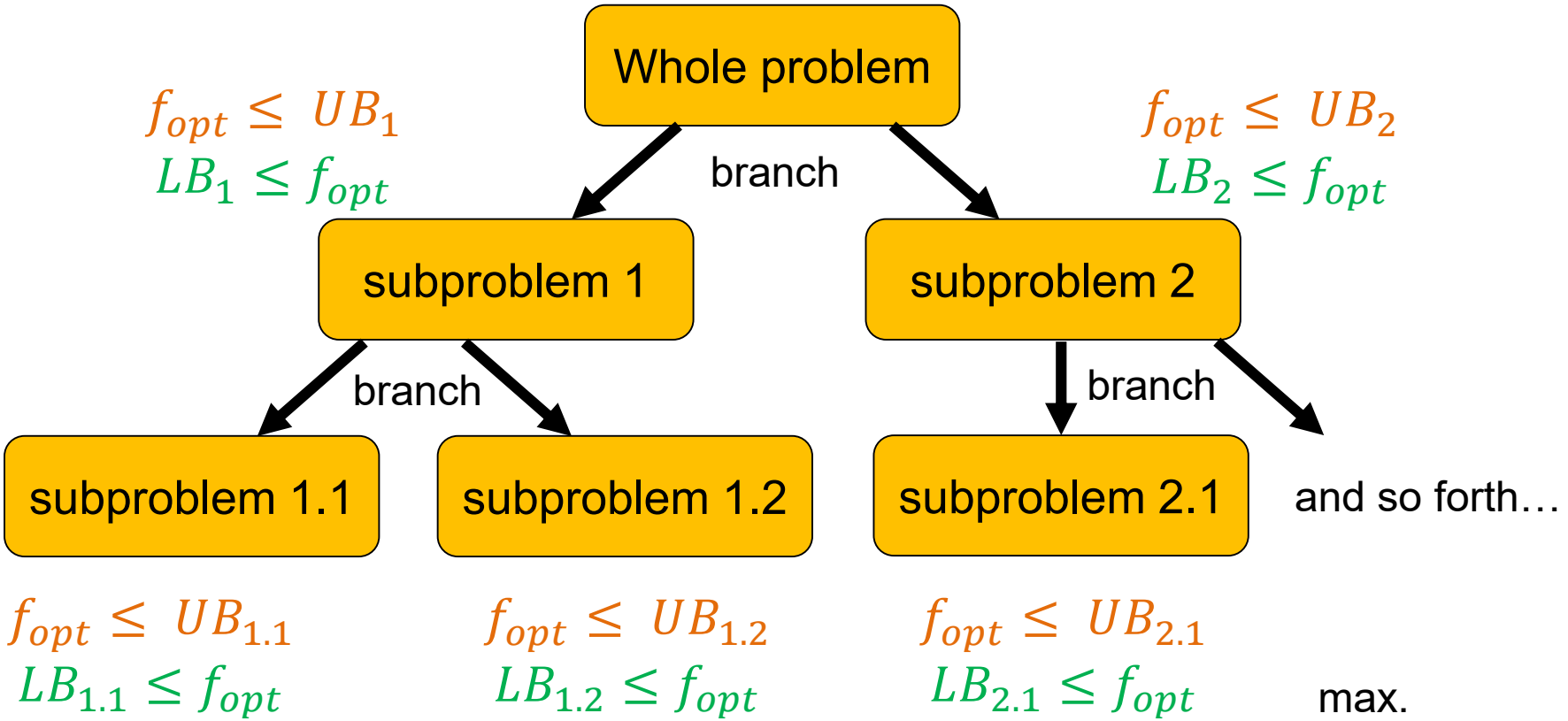


Idea Behind Branch and Bound



when can we actually avoid evaluating all solutions?

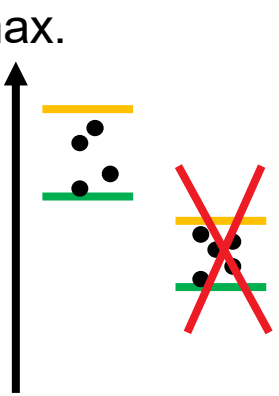
Idea Behind Branch and Bound



We can stop exploring/branching if

- UB=LB
- UB for new subproblem lower than LB for another

[when maximizing]



How do we get Upper and Lower Bounds?

We assume again maximization here…

- A feasible solution gives us a lower bound

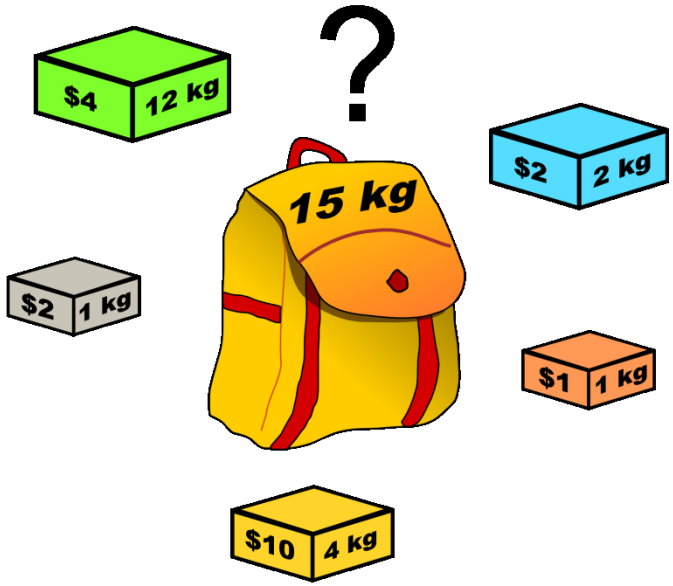
  the optimum will be at least as good as a solution, we know
- Hence, fast (non-exact) algorithms such as greedy can give us lower bounds
- For upper bounds, we can relax the problem

  for example, by removing constraints

An Example: Branch&Bound for the KP

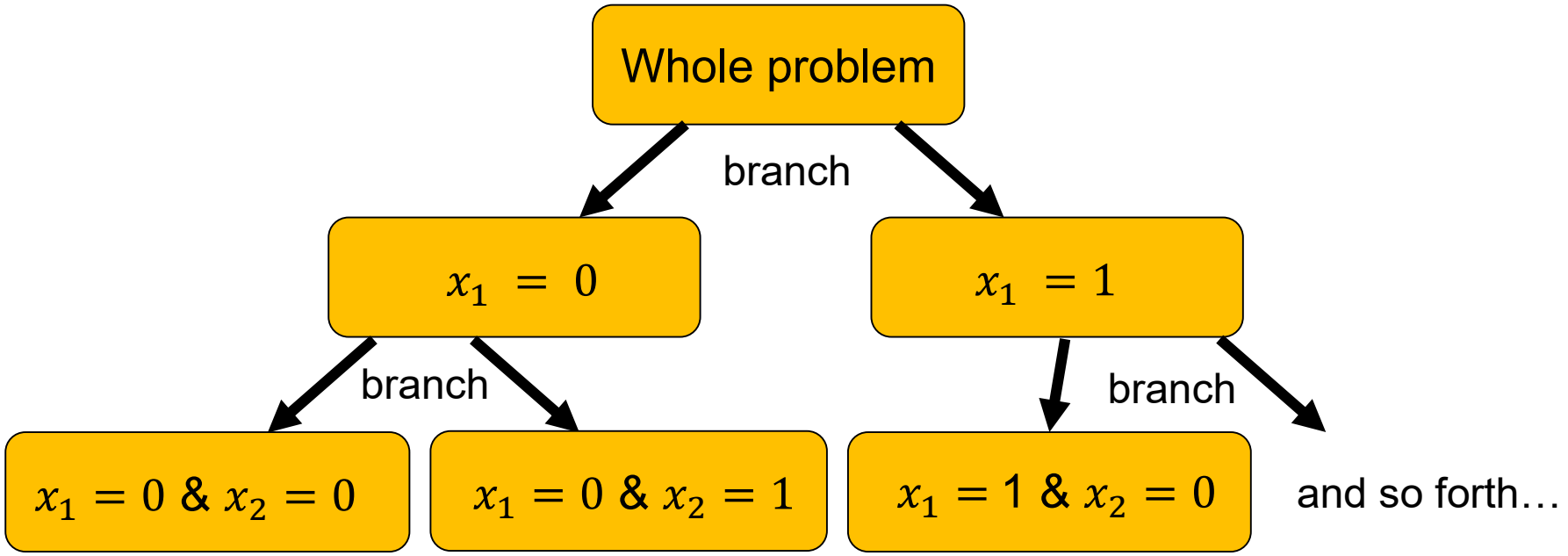
$$\max \sum_{j=1}^{n} p_j x_j \text{ with } x_j \in \{0,1\}$$

$$\text{s.t.} \sum_{j=1}^{n} w_j x_j \leq W$$



Dake

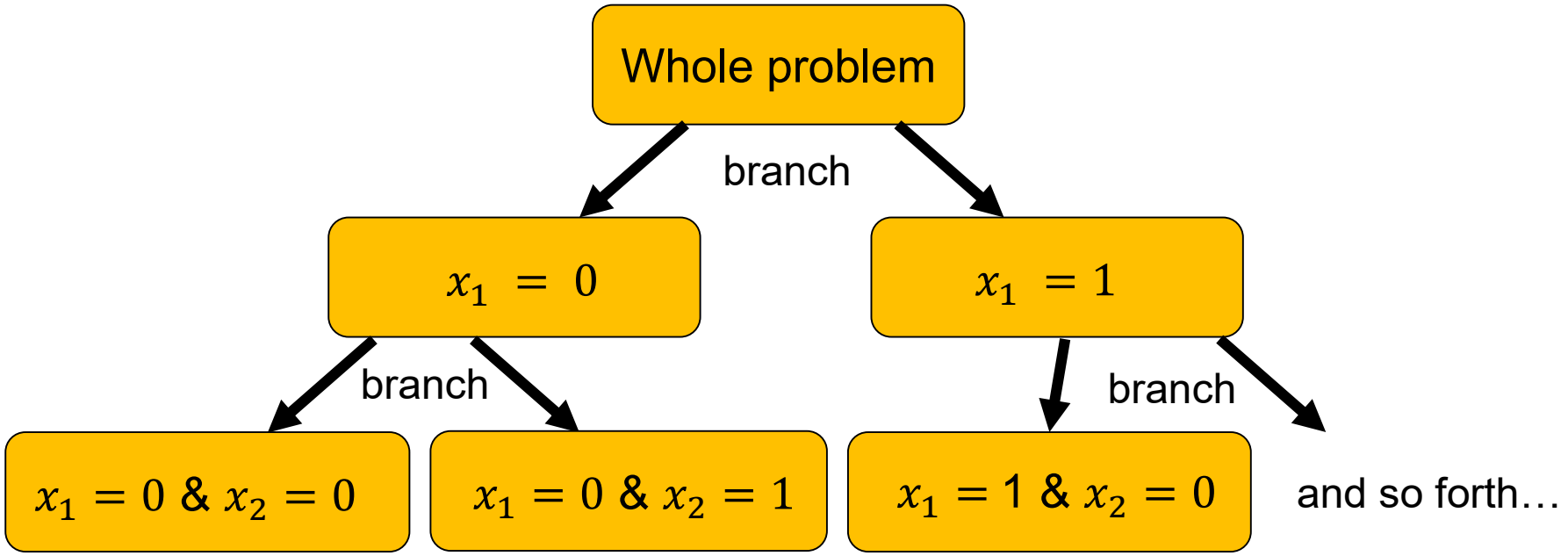
KP: How to Branch?



! order of variables plays an important role

optimally, the subproblems don't overlap

KP: How to Bound?



Maximization, so LB by greedy approach for example:

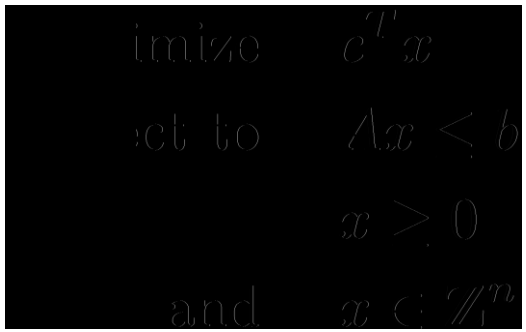
Choose items in decreasing profit/weight ratio until knapsack full

UB by relaxation of constraints (on the variables here):

Use greedy algorithm and pack add. item partially if there is space

…this variable can be used to branch next

A More General Example: Application to ILPs



The ILP formalization covers many problems such as

- Traveling Salesperson Person (TSP)
- Vertex Cover and other covering problems
- Set packing and other packing problems
- Boolean satisfiability (SAT)

Diffrerent Approaches to Solve an ILP

- Do not restrict the solutions to integers and round the solution of this so-called relaxed problem (=remove the integer constraints) by a continuous solver (e.g. Dantzig or interior point methods)

  → no guarantee to be exact
- Exploiting the instance property of A being total unimodular:

  unimodular matrix: square integer matrix with determinant +1 or −1

  (equivalent: integer matrix that is invertible over the integers)

  total unimodular = every square submatrix is unimodular
  - feasible solutions are guaranteed to be integer in this case
  - algorithms for continuous relaxation can be used (e.g. the simplex algorithm)
- With heuristic methods (typically without any quality guarantee)
  - for example genetic algorithms
- Using exact algorithms such as branch and bound

Branch and Bound for ILPs

Here, we just give an idea instead of a concrete algorithm...

- How to compute upper bounds (assuming maximization)?
- How to split a problem into subproblems (“branching”)?
- Optional: how to compute lower bounds?
- How to decide which next tree node to split?

Branch and Bound for ILPs

How to compute upper bounds (assuming maximization)?

- drop the integer constraints and solve the so-called LP-relaxation
- can be solved by standard LP algorithms such as simplex method by Dantzig

What's then?

- The LP has no feasible solution. Fine. Prune.
- We found an integer solution. Fine as well. Might give us a new lower bound to the overall problem.
- The LP problem has an optimal solution which is worse than the highest lower bound over all already explored subproblems. Fine. Prune.
- Otherwise: Branch on this subproblem: e.g. if optimal solution has $x_i=2.7865$, use $x_i \leq 2$ and $x_i \geq 3$ as new constraints

Branch and Bound for ILPs

How to split a problem into subproblems ("branching")?

- mainly needed if the solution of the LP-relaxation is not integer
- branch on a variable which is rational

Not discussed here in depth due to time:

- Optional: how to compute lower bounds?
- How to decide which next tree node to split?
  - seems to be good choice: subproblem with largest upper bound of LP-relaxation
- Advanced algorithms such as branch and cut (cut part: add specific constraints aka "cutting planes" that ensure integer solutions)

Conclusions

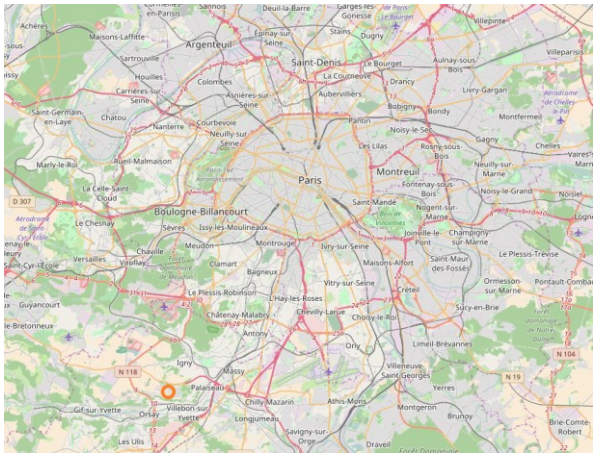
I hope it became clear...

...what the algorithmic ideas behind branch and bound are

...and for which problem types it is supposed to be suitable

Internships/Master's Theses in Blackbox Optimization

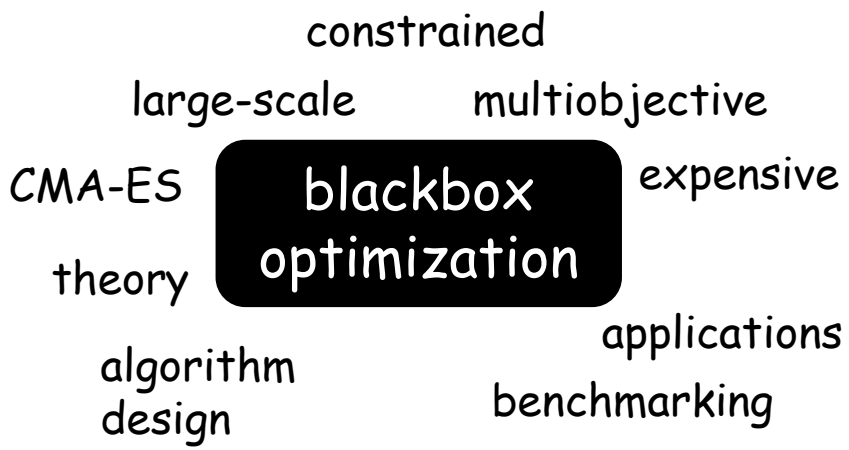
RandOpt team
Inria and Ecole Polytechnique



Permanent members:
Anne Auger, Dimo Brockhoff, Nikolaus Hansen
https://team.inria.fr/randopt/team-members/

3 (soon 4) PhD students

Interests:



Thank you all!

Don’t forget:

- send your group project’s report this Friday
  as PDF to dimo.brockhoff@inria.fr
- be prepared for the final exam on December 15 (in 2 weeks)