

Benchmarking Blackbox Optimization Algorithms

July 5, 2017

CEA/EDF/Inria summer school "Numerical Analysis"
Université Pierre-et-Marie-Curie, Paris, France

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Inria Saclay – Ile-de-France
CMAP, Ecole Polytechnique



Overview of the Remaining Lectures & Exercises

Introduction to (Evolutionary) Multiobjective Optimization (now)

- difference to single-objective optimization, the basics
- algorithms and their design principles; MO-CMA-ES

Benchmarking Optimization Algorithms (this morning)

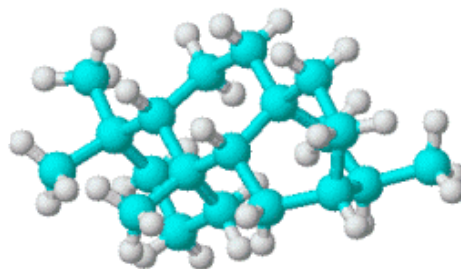
- performance assessment
- automated benchmarking with the COCO platform

Exercise around COCO (this afternoon)

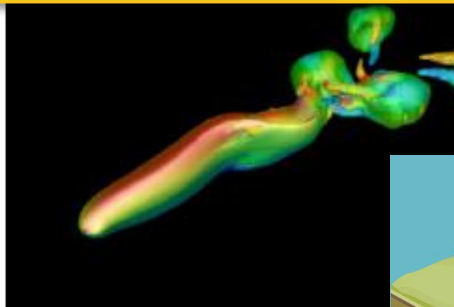
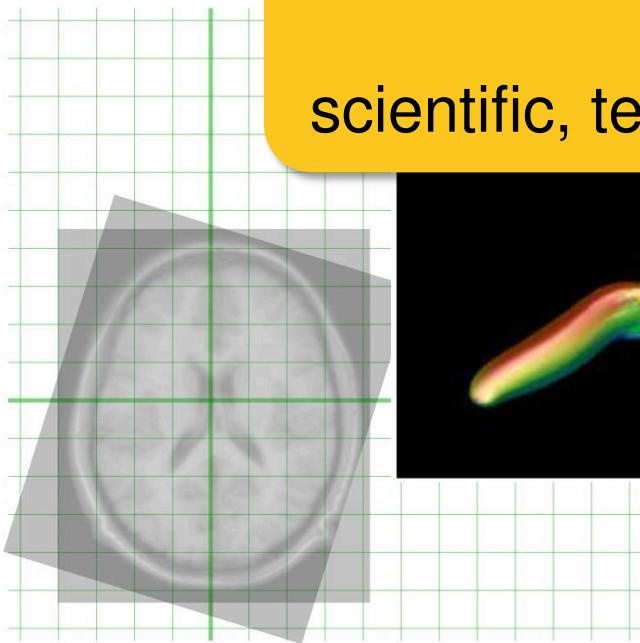
- interpreting available COCO data
- if time allows: looking critically at published results

Exercise on Anne's part (tomorrow afternoon)

- The (1+1)-ES, running CMA-ES and interpreting its output, ...

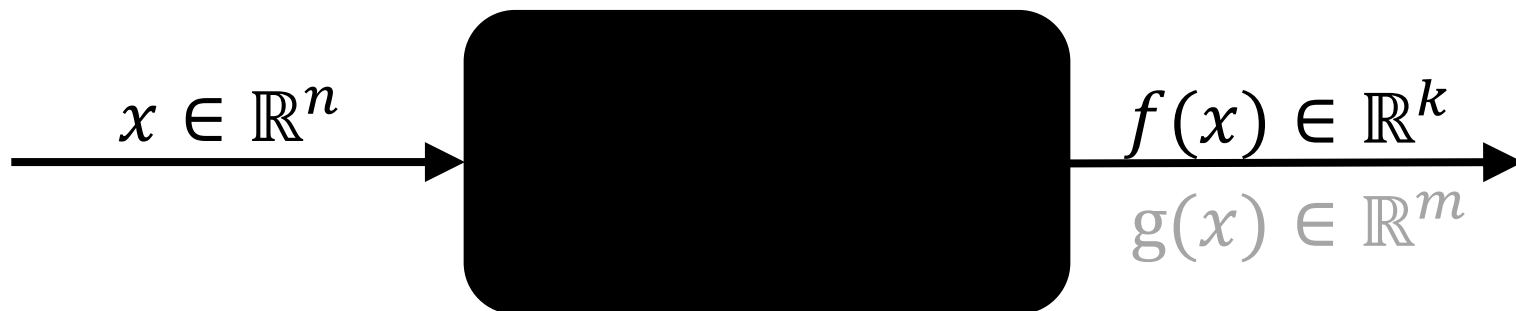


challenging optimization problems
appear in many
scientific, technological and industrial domains



Numerical Blackbox Optimization

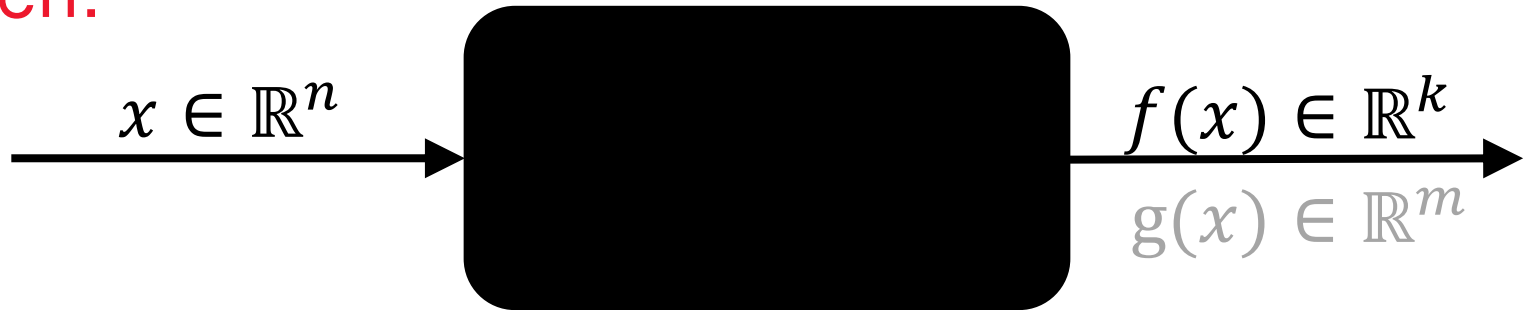
Minimize $f: \Omega \subset \mathbb{R}^n \mapsto \mathbb{R}^k$



derivatives not available or not useful

Practical Blackbox Optimization

Given:



Not clear:

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

Numerical Blackbox Optimizers

Deterministic Algorithms

- Quasi-Newton with estimation of gradient (BFGS) [Broyden et al. 1970]
- Simplex downhill [Nelder & Mead 1965]
- Pattern search [Hooke and Jeeves 1961]
- Trust-region methods (NEWUOA, BOBYQA) [Powell 2006, 2009]

Stochastic (Randomized) Search Methods

- Evolutionary Algorithms (continuous domain)
- Differential Evolution [Storn & Price 1997]
- Particle Swarm Optimization [Kennedy & Eberhart 1995]
- **Evolution Strategies, CMA-ES**
[Rechenberg 1965, Hansen & Ostermeier 2001]
- Estimation of Distribution Algorithms (EDAs) [Larrañaga & Lozano 2001]
- Cross Entropy Method (same as EDA) [Rubinstein 1999]
- Genetic Algorithms [Holland 1975, Goldberg 1989]
- Simulated annealing [Kirkpatrick et al. 1983]
- Simultaneous perturbation stochastic approx. (SPSA) [Spall 2000]

Numerical Blackbox Optimizers

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[Rechenberg 1965, Hansen & Ostermeier 2001]

best choice typically not immediately clear

although practitioners often have knowledge about which difficulties a problem has (e.g. multi-modality or non-separability)

Simultaneous perturbation stochastic approximation (SPSA) [Spall 2000]

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

that's where COCO comes into play

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

automatized benchmarking

How to benchmark algorithms with COCO?

numbbo / coco

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brockho committed on GitHub Merge pull request #1352 from numbbo/development Latest commit 4b1497a on 20 Apr

code-experiments	A little more verbose error message when suite regression test fails	a month ago
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code-preprocessing	Fixed preprocessing to work correctly with the extended biobjective s...	3 months ago
howtos	Update create-a-suite-howto.md	4 months ago
.clang-format	raising an error in bbob2009_logger.c when best_value is NULL. Plus s...	2 years ago
.hgignore	raising an error in bbob2009_logger.c when best_value is NULL. Plus s...	2 years ago
AUTHORS	small correction in AUTHORS	a year ago
LICENSE	Update LICENSE	11 months ago

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Use Git or checkout with SVN using the web URL.

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README.md

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This code reimplements the original Comparing Continuous 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

The screenshot shows a web browser window with the URL `https://github.com/numbbo/coco`. The browser's address bar and tabs are visible at the top. Below the browser window, the GitHub repository page is shown. It features a list of recent commits with their titles and dates. The main content area displays the README for the repository, which is titled "numbbo/coco: Comparing Continuous Optimizers". The README text describes the project as a platform for benchmarking and comparing continuous optimizers, rewritten in ANSI C. It lists supported languages: C/C++, Java, MATLAB/Octave, and Python. It also mentions that contributions to link further languages are welcome and provides links to benchmarking guidelines and the COCO experimental setup description.

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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

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- see the [bbob-biobj](#) and [bbob-biobj-ext](#) [COCO multi-objective functions testbed](#) documentation and the [specificities of the performance assessment for the bi-objective testbeds](#).
- consult the [BBOB workshops series](#),
- consider to [register here](#) for news,
- see the [previous COCO home page here](#) and
- see the [links below](#) to learn more about the ideas behind CoCO.

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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
```

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
```

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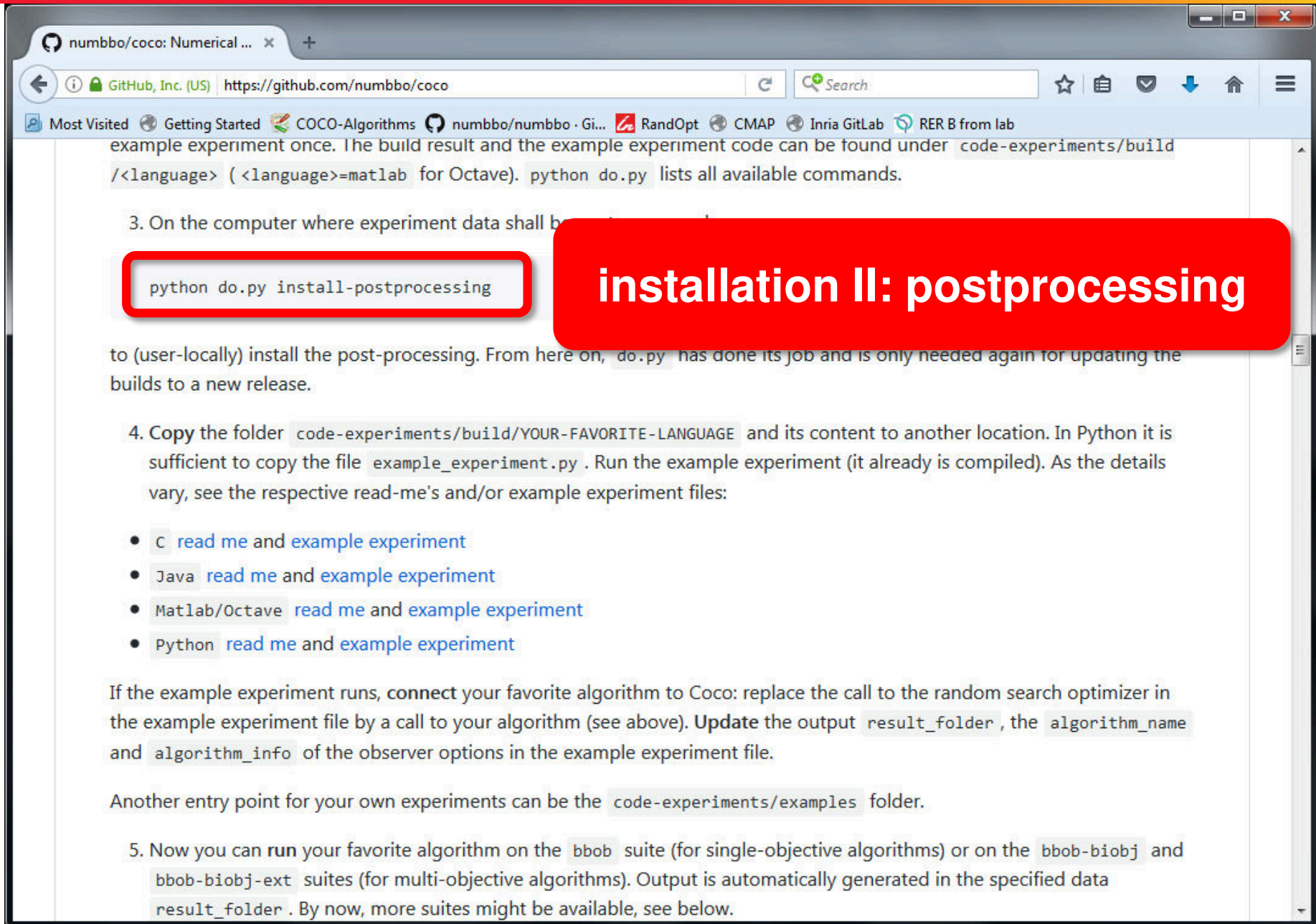
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installation I: experiments



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(user-locally) install the post-processing. From here on, `do.py` has done its job and is only needed again for updating the builds to a new release.

4. Copy the folder `code-experiments/build/YOUR-FAVORITE-LANGUAGE` and its content to another location. In Python it is sufficient to copy the file `example_experiment.py`. Run the example experiment (it already is compiled). As the details vary, see the respective read-me's and/or example experiment files:

- 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](#)

If the example experiment runs, connect your favorite algorithm to Coco: replace the call to the random search optimizer in the example experiment file by a call to your algorithm (see above). Update the output `result_folder`, the `algorithm_name` and `algorithm_info` of the observer options in the example experiment file.

Another entry point for your own experiments can be the `code-experiments/examples` folder.

5. Now you can run your favorite algorithm on the `bbob` suite (for single-objective algorithms) or on the `bbob-biobj` and `bbob-biobj-ext` suites (for multi-objective algorithms). Output is automatically generated in the specified data `result_folder`. By now, more suites might be available, see below.

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coupling algo + COCO

exampleexperiment.m (slightly simplified)

```
while true
    problem = cocoSuiteGetNextProblem(suite, observer);
    dimension = cocoProblemGetDimension(problem);
    i = -1; % count number of independent restarts
    while (BUDGET_MULTIPLIER*dimension > (cocoProblemGetEvaluations(problem) + ...
        cocoProblemGetEvaluationsConstraints(problem)))

        i = i+1;
        doneEvalsBefore = cocoProblemGetEvaluations(problem) + ...
            cocoProblemGetEvaluationsConstraints(problem);
        % start algorithm with remaining number of function evaluations:
        my_optimizer(problem,...
            cocoProblemGetSmallestValuesOfInterest(problem), ...
            cocoProblemGetLargestValuesOfInterest(problem), ...
            BUDGET_MULTIPLIER*dimension - doneEvalsBefore);
        % check whether experiment is over:
        doneEvalsAfter = cocoProblemGetEvaluations(problem) + ...
            cocoProblemGetEvaluationsConstraints(problem);
        if cocoProblemFinalTargetHit(problem) == 1 || ...
            doneEvalsAfter >= BUDGET_MULTIPLIER * dimension
            break;
        end
        if (i >= NUM_OF_INDEPENDENT_RESTARTS)
            break;
        end
    end
    doneEvalsTotal = doneEvalsTotal + doneEvalsAfter;
end
```


numbbo/coco at develop... x +

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6. Postprocess the data from the results folder by typing

```
python -m cocopp [-o OUTPUT_FOLDERNAME] YOURDATA
```

Any subfolder in the folder arguments will be searched for... on different folders collected under a single "root" `YOURDATAFOLDER` folder. We can also compare more than one algorithm by specifying several data result folders generated by different algorithms.

A folder, `ppdata` by default, will be generated, which contains all output from the post-processing, including an `index.html` file, useful as main entry point to explore the result with a browser. Data might be overwritten, it is therefore useful to change the output folder name with the `-o OUTPUT_FOLDERNAME` option.

A summary pdf can be produced via LaTeX. The corresponding templates can be found in the `code-postprocessing/latex-templates` folder. Basic html output is also available in the result folder of the postprocessing (file `templateBBOBarticle.html`).

7. Once your algorithm runs well, increase the budget in your experiment script, if necessary implement randomized independent restarts, and follow the above steps successively until you are happy.

8. The experiments can be parallelized with any re-distribution of single problem instances to batches (see `example_experiment.py` for an example). Each batch must write in a different target folder (this should happen automatically). Results of each batch must be kept under their separate folder as is. These folders then must be

running the experiment

Another entry point for your own experiments can be the `code-experiments/examples` folder.

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6. Postprocess the data from the results folder by typing

```
python -m cocopp [-o OUTPUT_FOLDERNAME] YOURDATAFOLDER [MORE_DATAFOLDERS]
```

Any subfolder in the folder arguments will be searched for logged data. That is, experiments from different batches can be in different folders collected under a single "root" `YOURDATAFOLDER`. You can also specify several data result folders generated by different algorithms.

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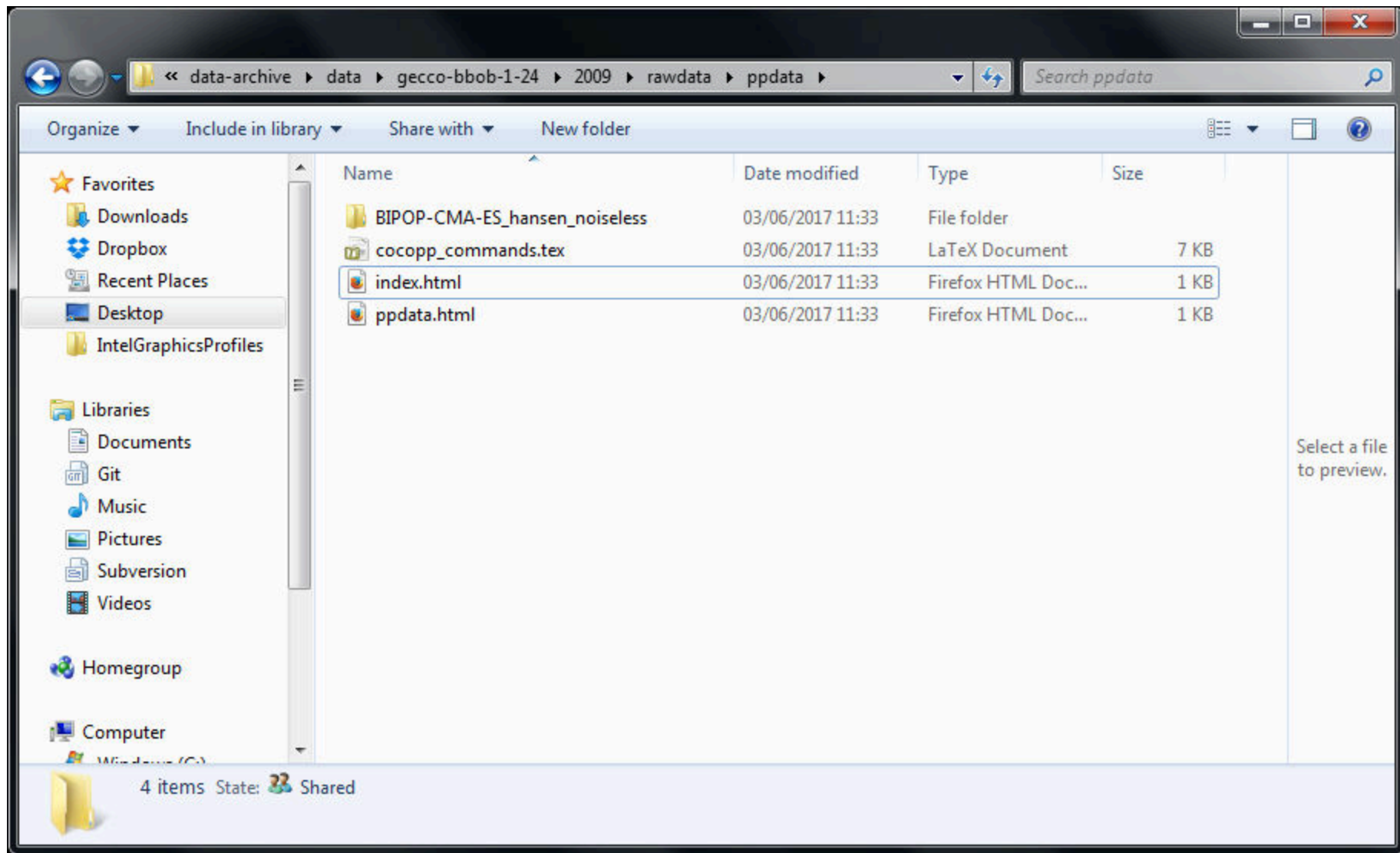
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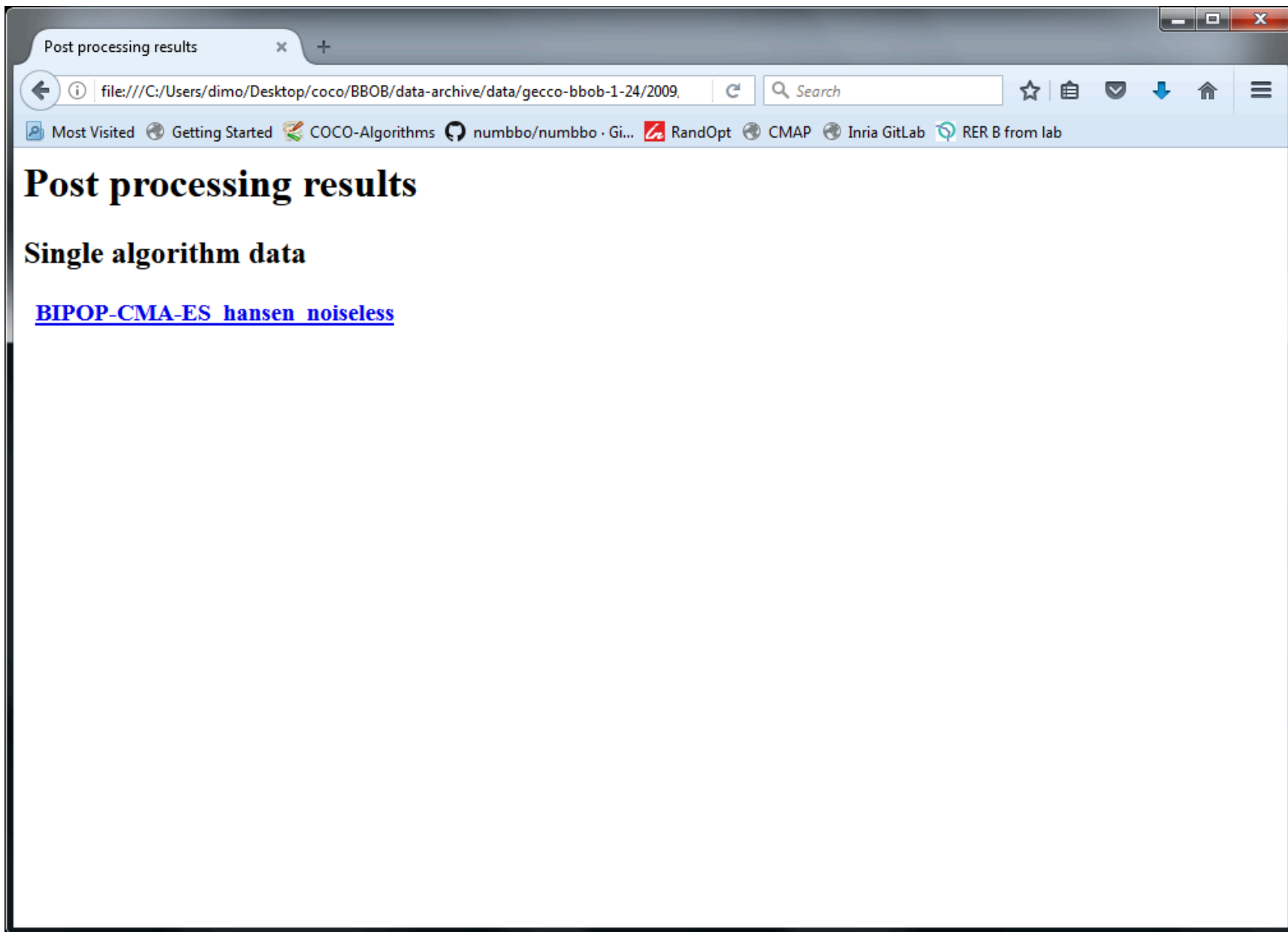
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postprocessing

Result Folder



Automatically Generated Results



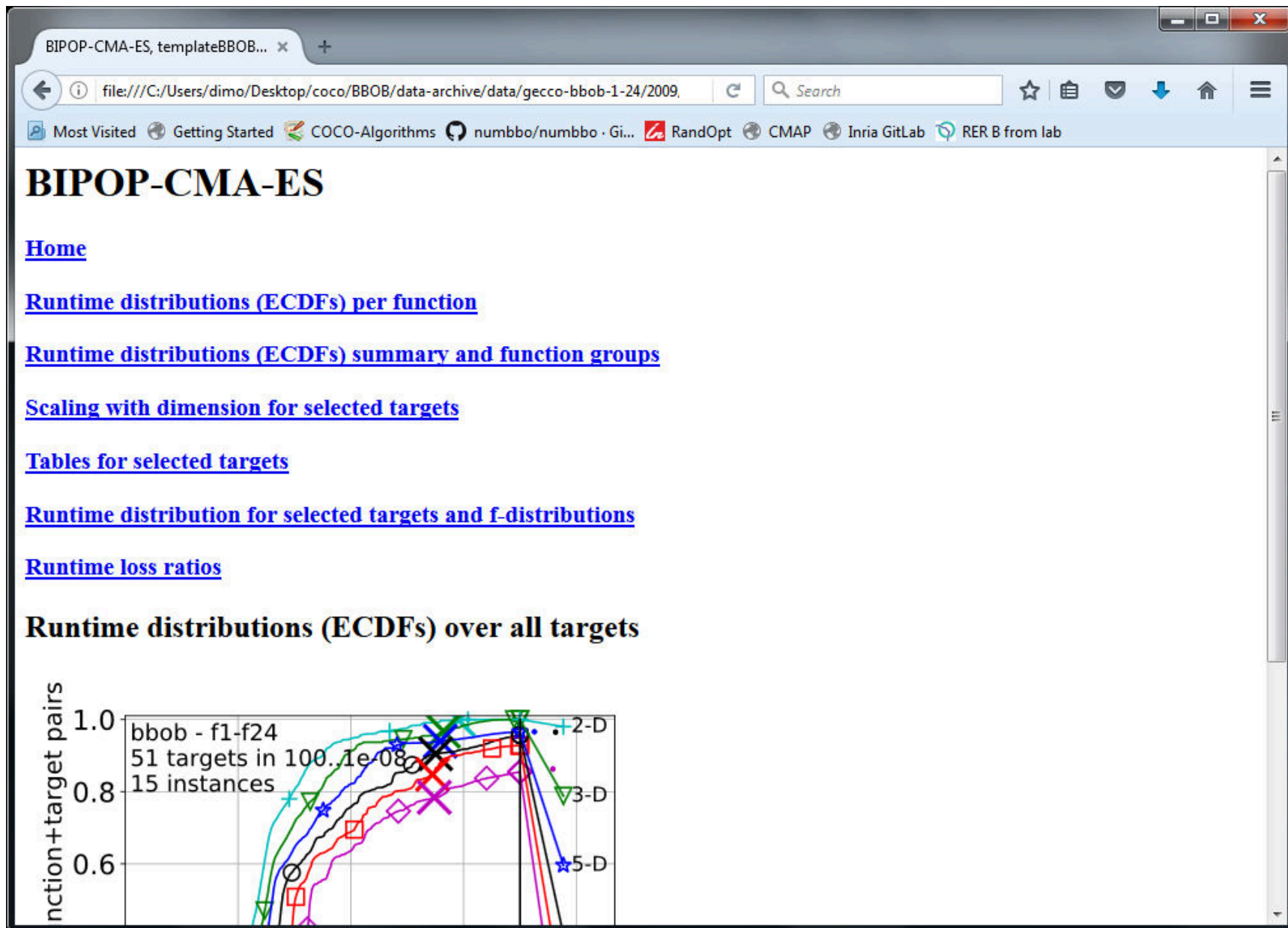
The screenshot shows a web browser window with a single tab titled "Post processing results". The address bar contains the file path: `file:///C:/Users/dimo/Desktop/coco/BBOB/data-archive/data/gecco-bbob-1-24/2009.`. The browser's bookmark bar is visible, showing several links including "Most Visited", "Getting Started", "COCO-Algorithms", "numbbo/numbbo · Gi...", "RandOpt", "CMAP", "Inria GitLab", and "RER B from lab". The main content area of the browser displays the following text:

Post processing results

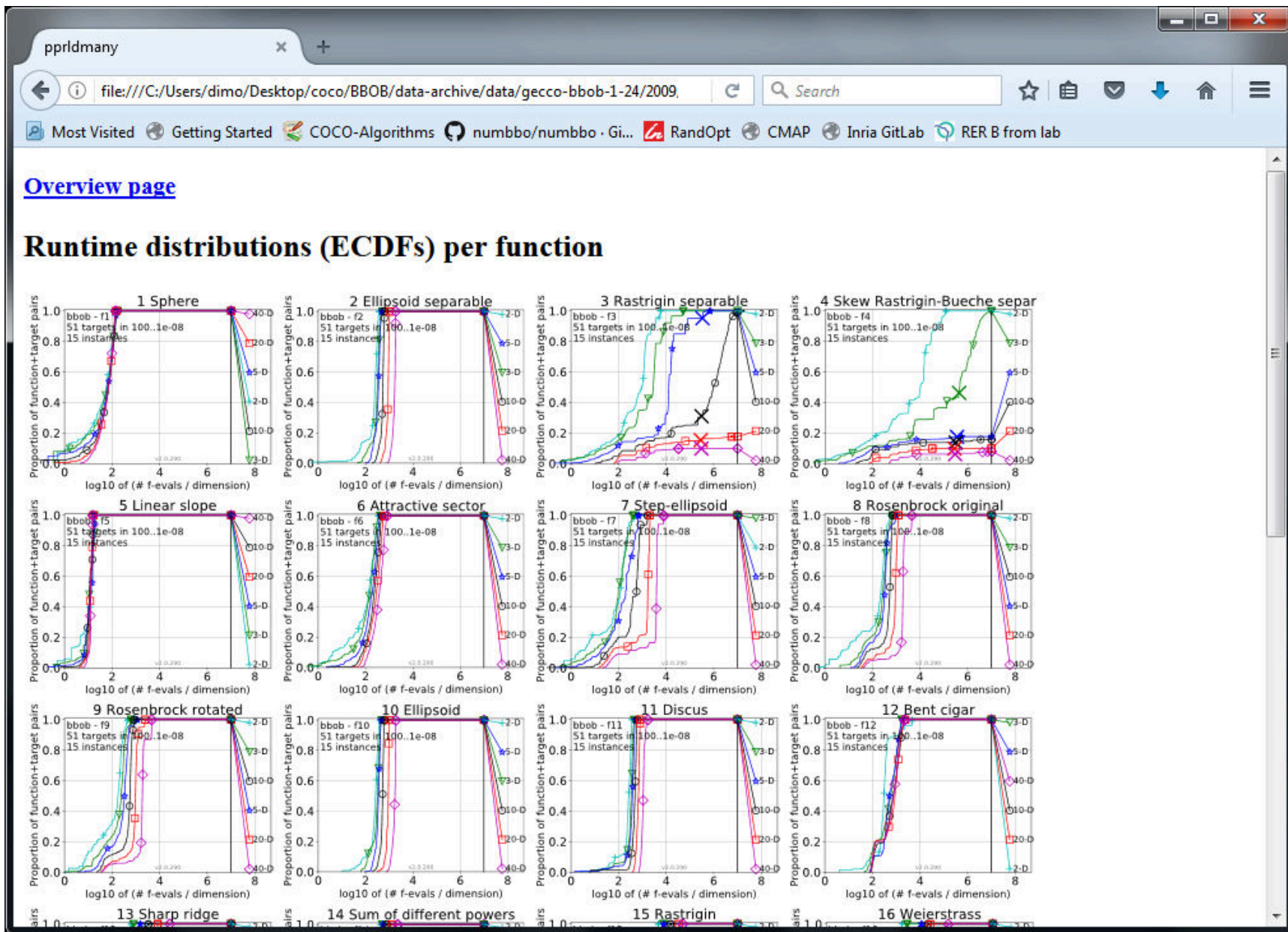
Single algorithm data

[BIPOP-CMA-ES hansen noiseless](#)

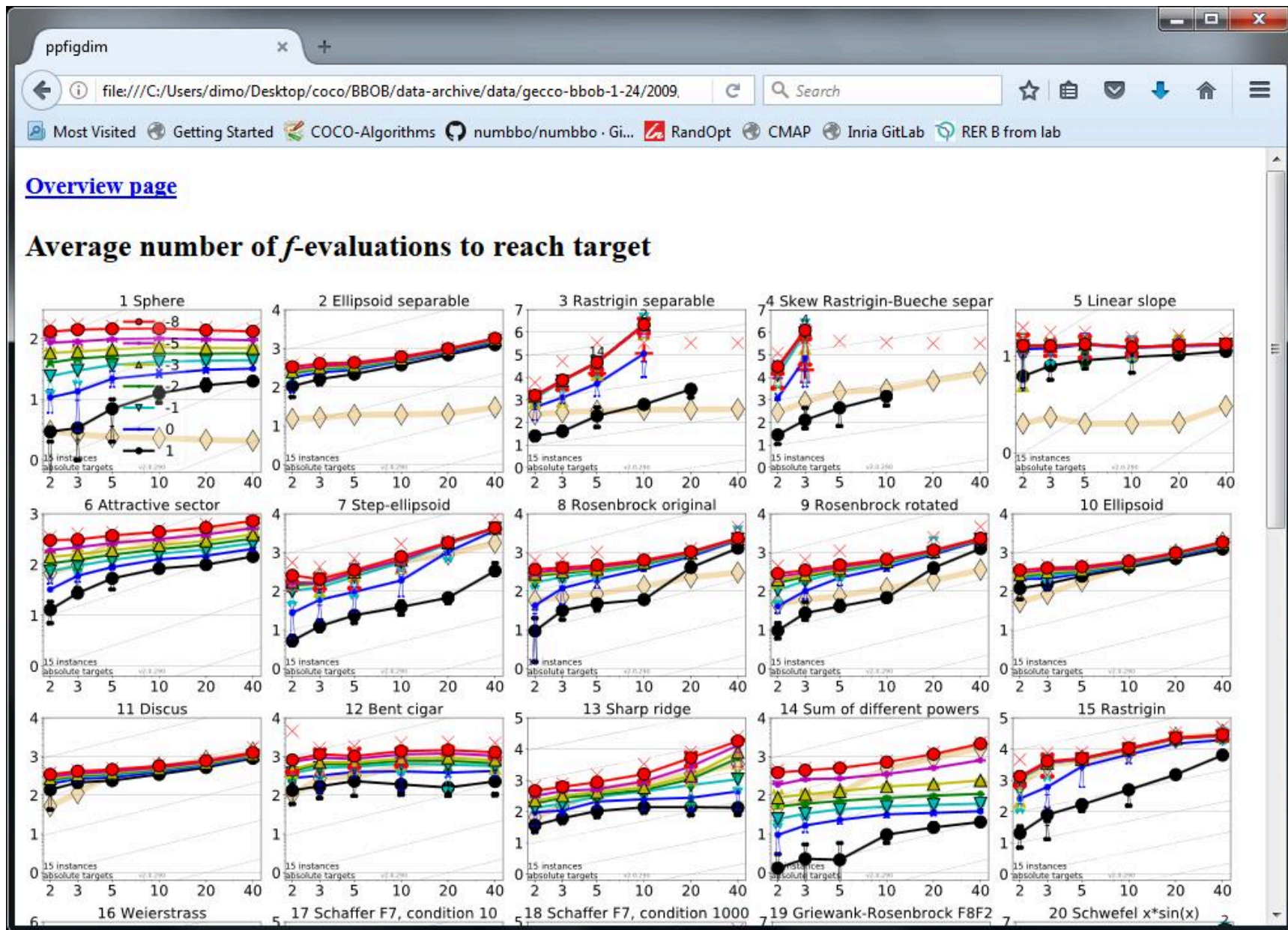
Automatically Generated Results



Automatically Generated Results



Automatically Generated Results



doesn't look too complicated, does it?

[the devil is in the details 😊]

so far:

data for about 170 algorithm variants
(some of which on noisy or multiobjective test functions)
145 workshop papers
by 93 authors from 25 countries

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	140+ algo data sets
▪ bbob-noisy	30 noisy fcts	40+ algo data sets
▪ bbob-biobj	55 bi-objective fcts	16 algo data sets

Under development:

- an extended biobjective suite
- a large-scale version of the bbob suite
- a constrained test suite

Long-term goals:

- combining difficulties
- almost real-world problems
- real-world problems

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?

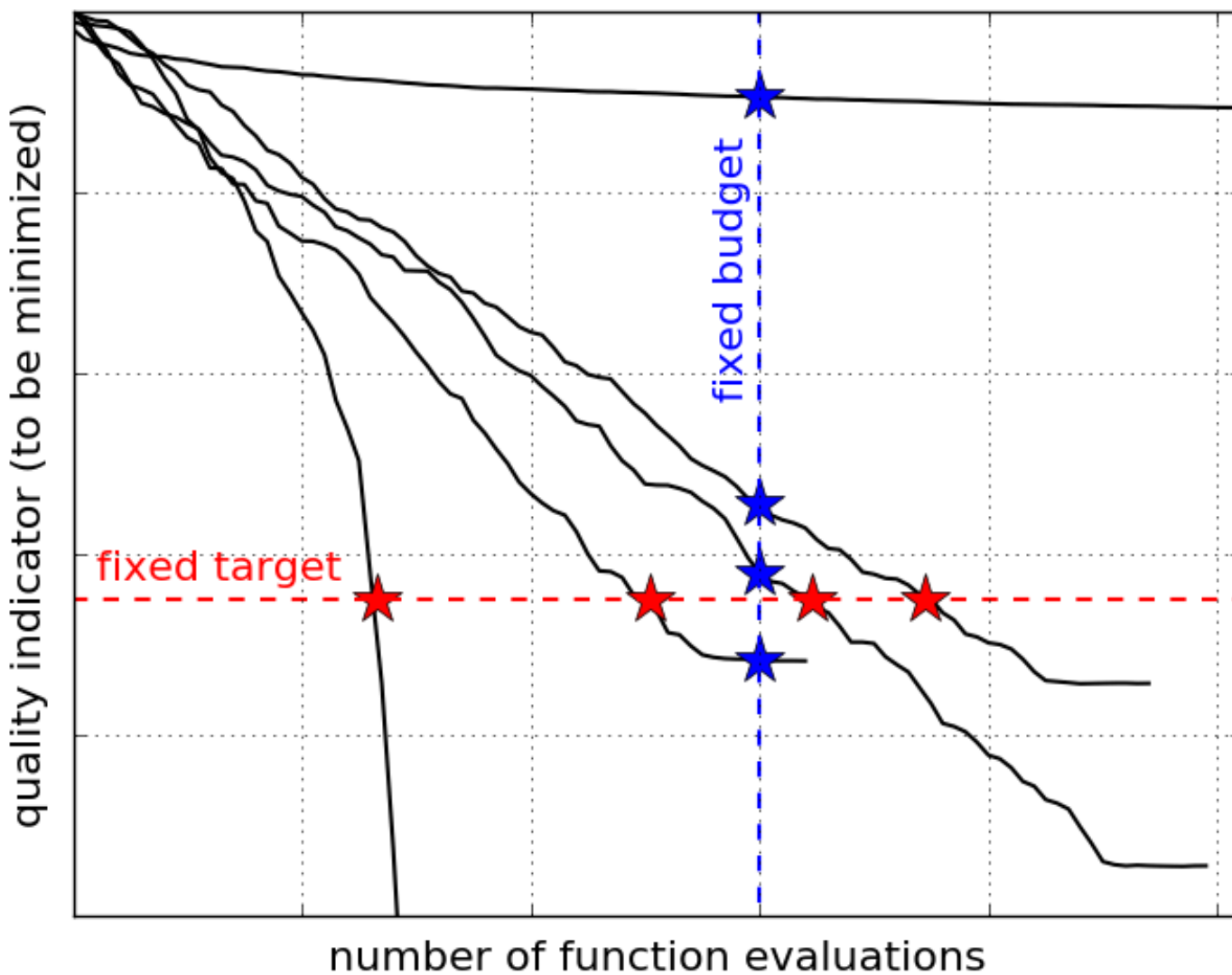
Two objectives:

- 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...

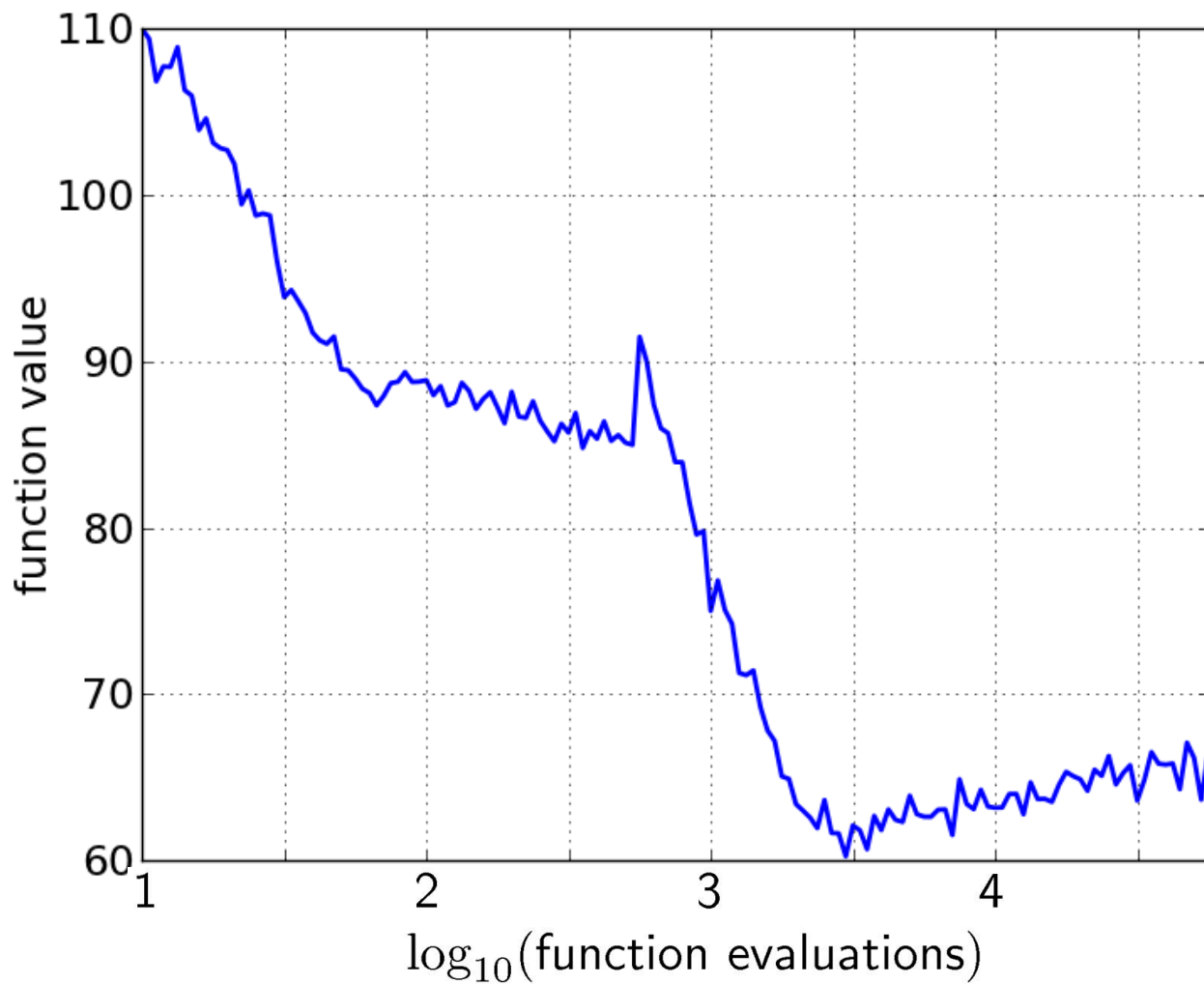


ECDF:

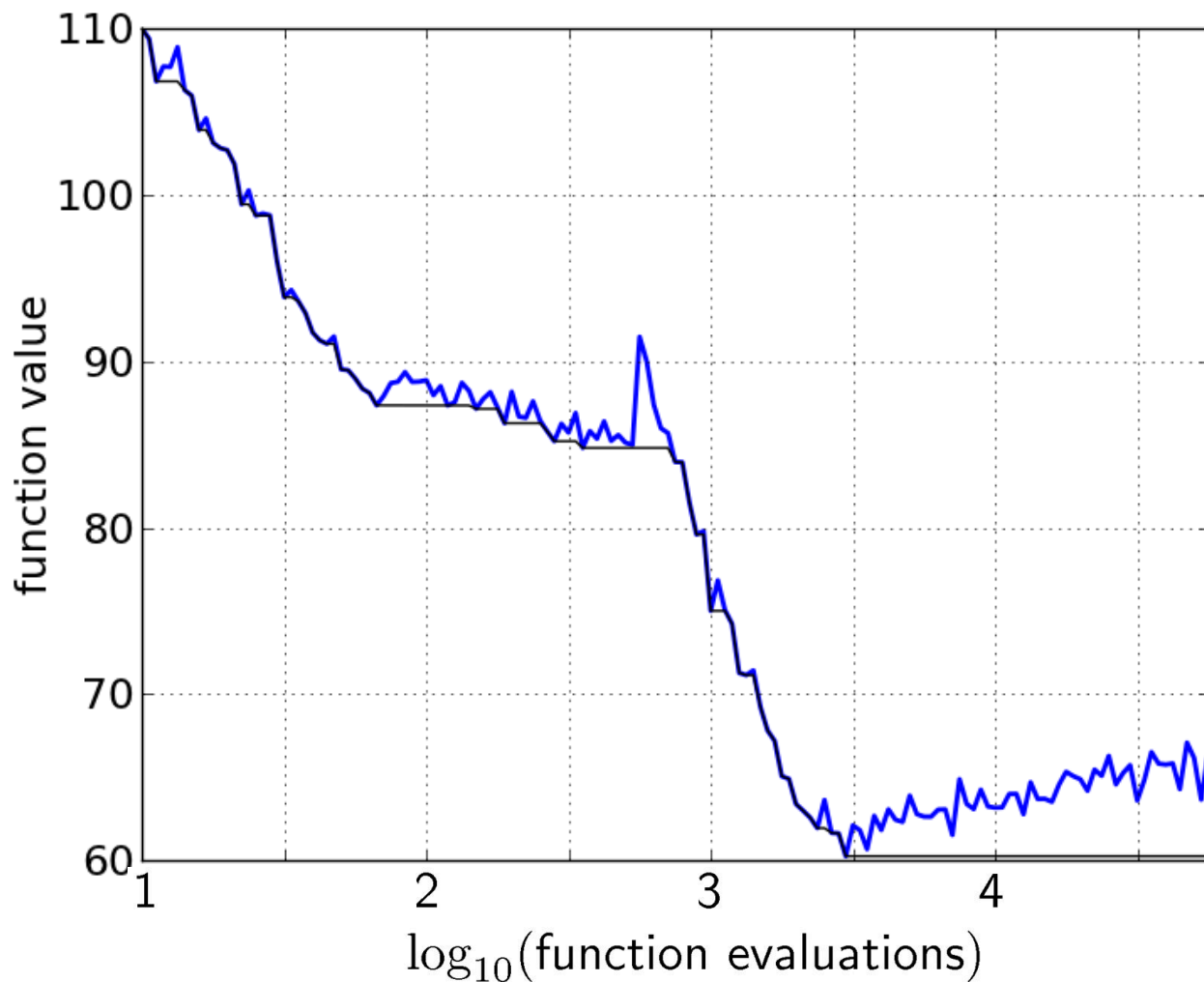
Empirical Cumulative Distribution Function of the
Runtime

[aka data profile]

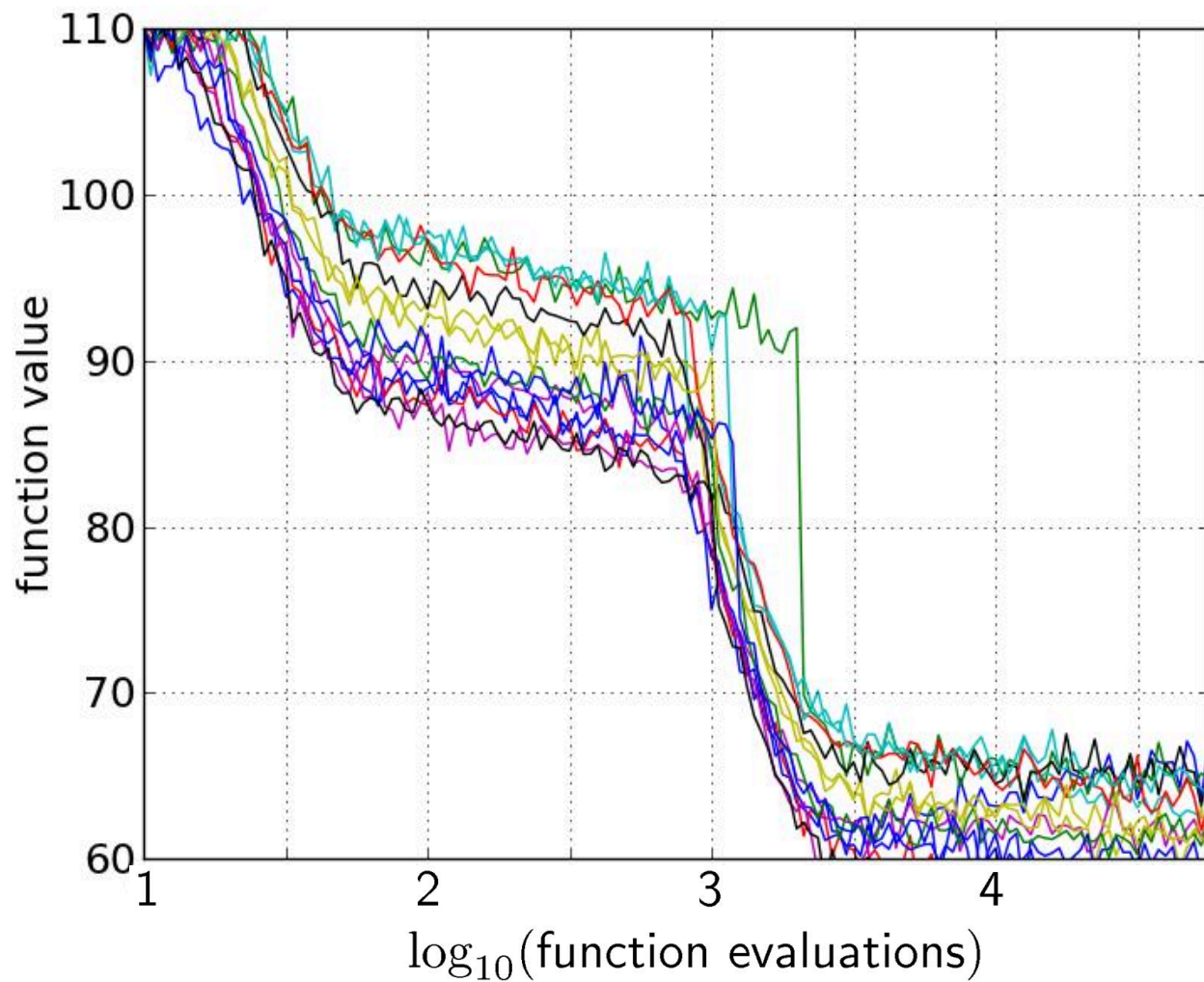
A Convergence Graph



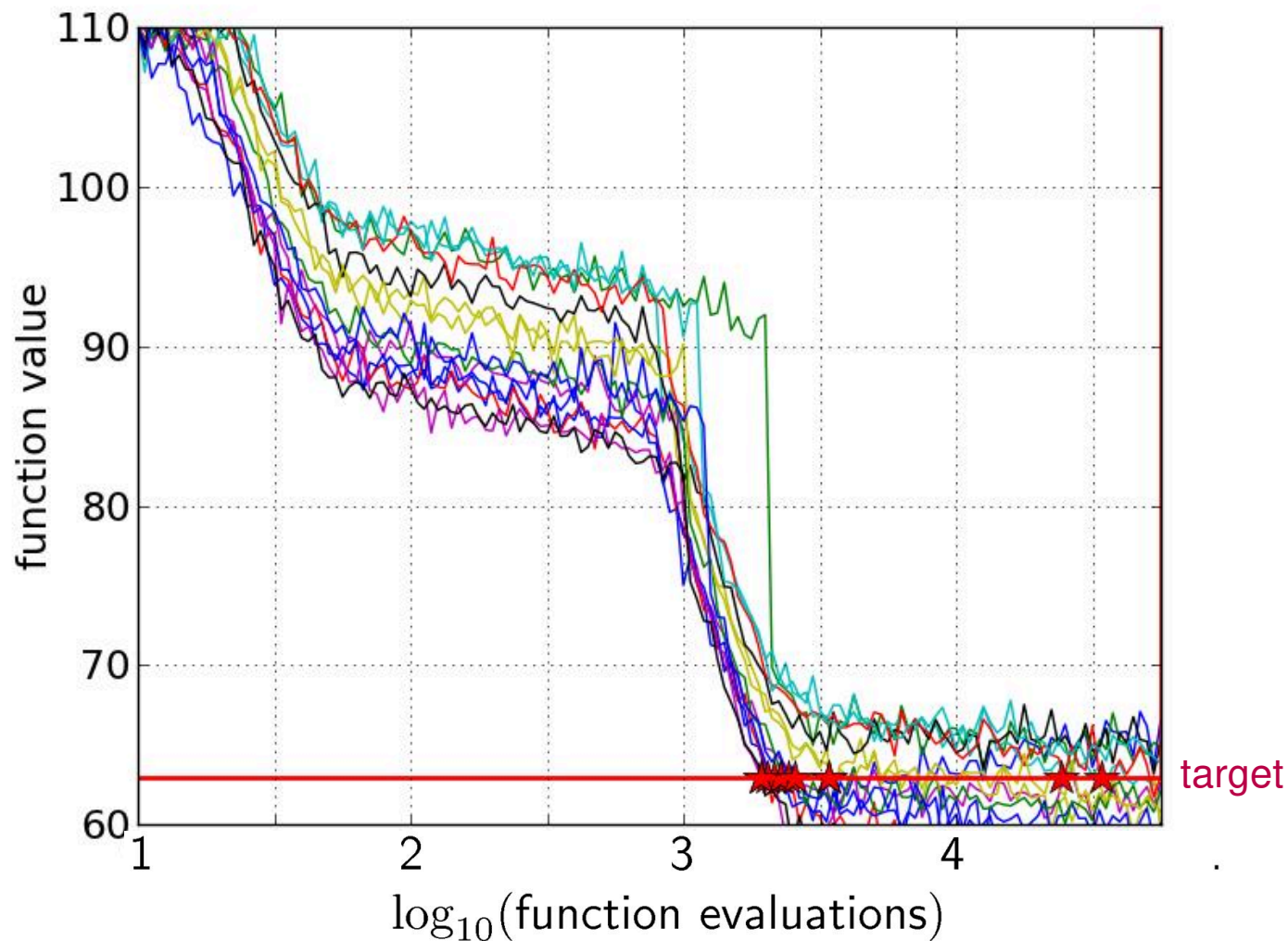
First Hitting Time is Monotonous



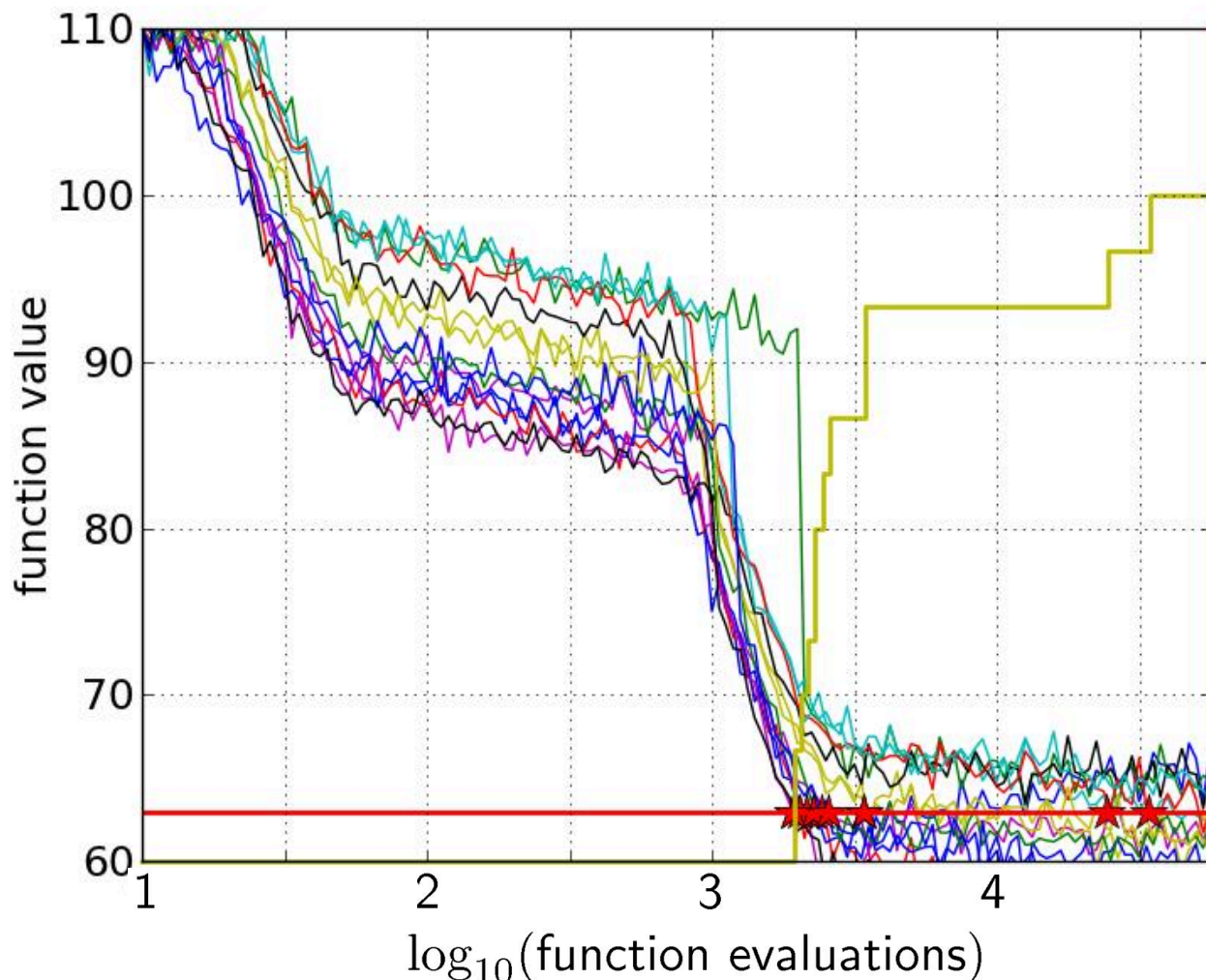
15 Runs



15 Runs \leq 15 Runtime Data Points



Empirical Cumulative Distribution Function (ECDF)



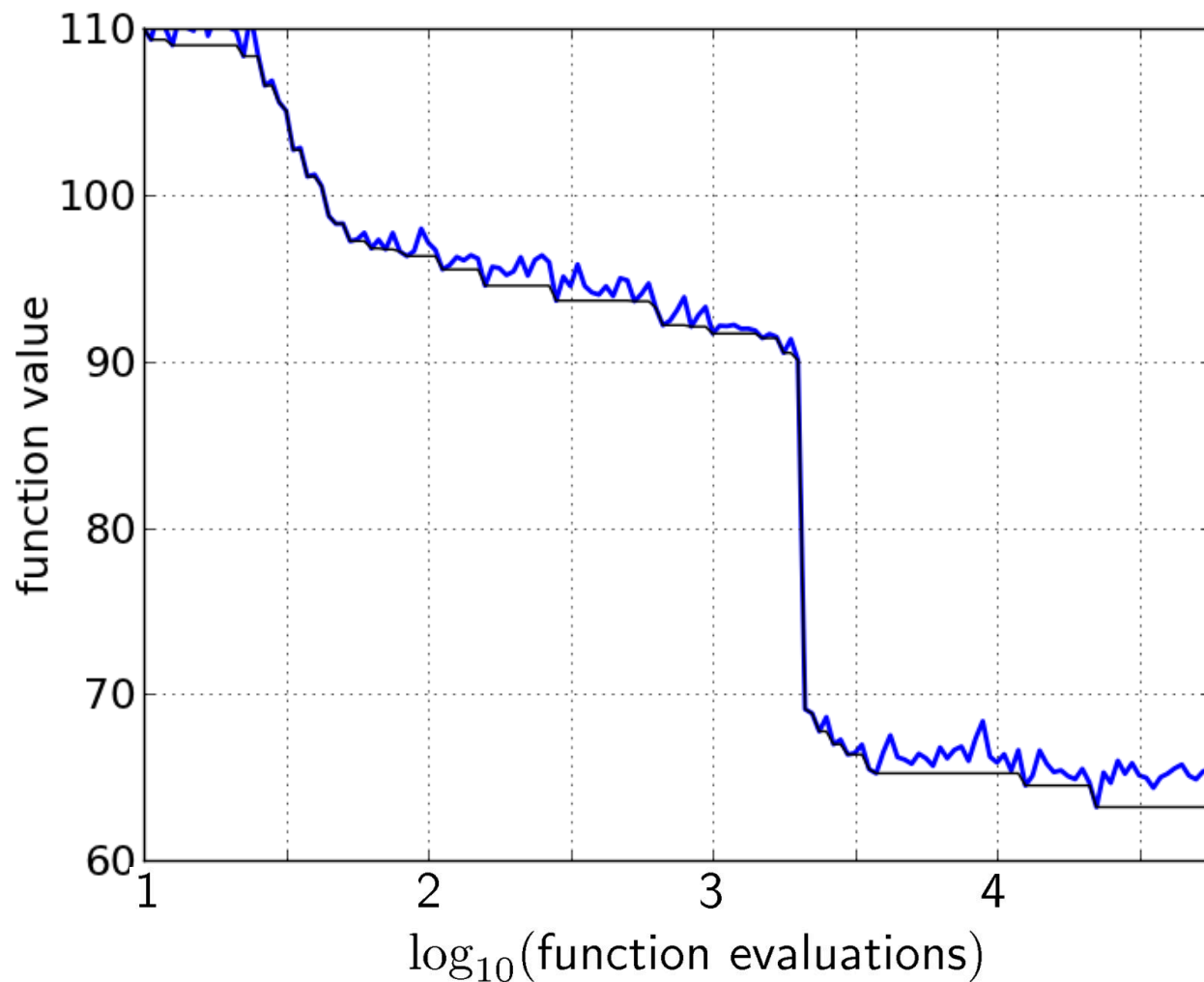
the **ECDF** of run lengths to reach the target

- has for each data point a **vertical step of constant size**

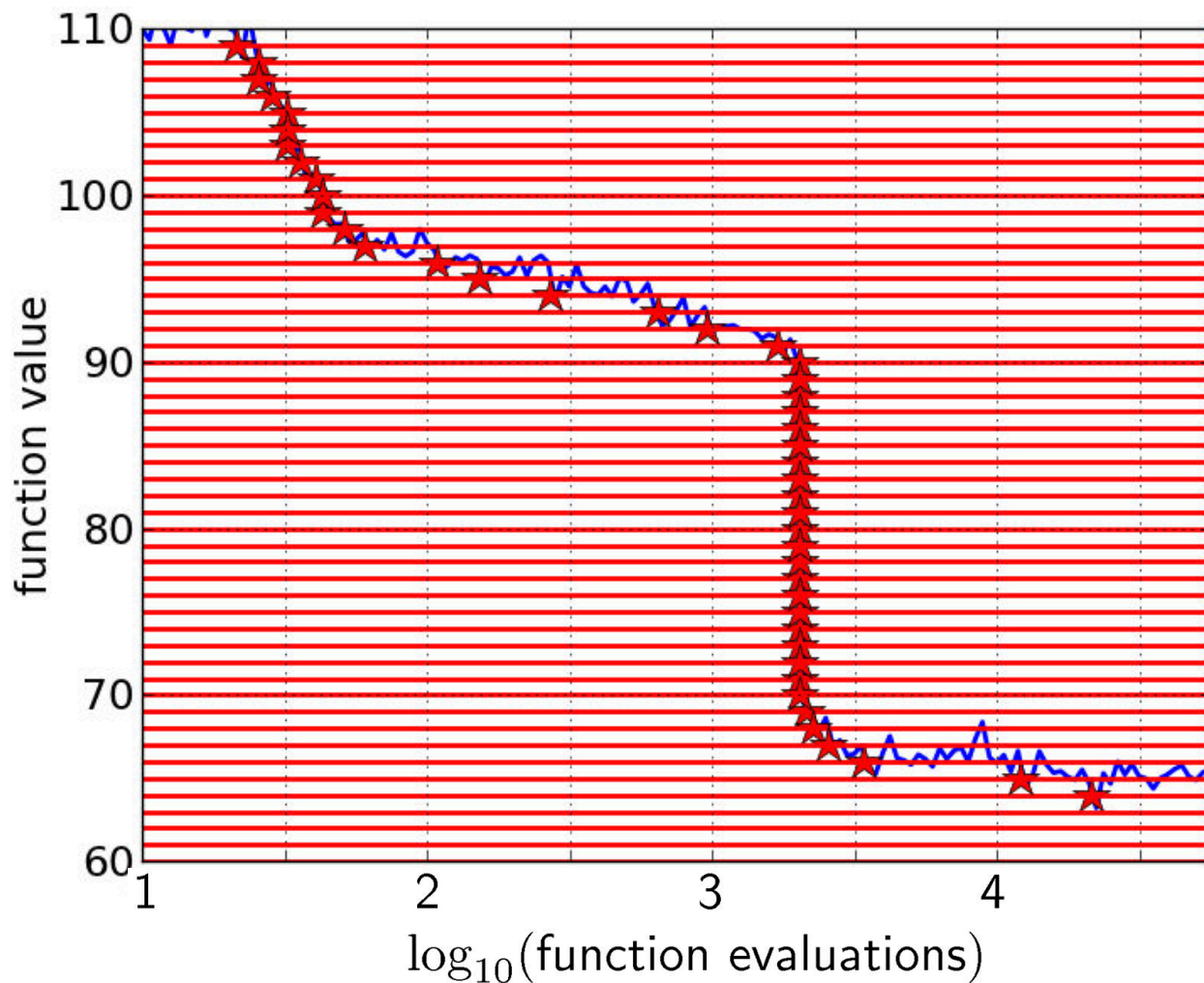
- displays for each x-value (budget) the count of observations to the left (first hitting times)

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

Reconstructing A Single Run

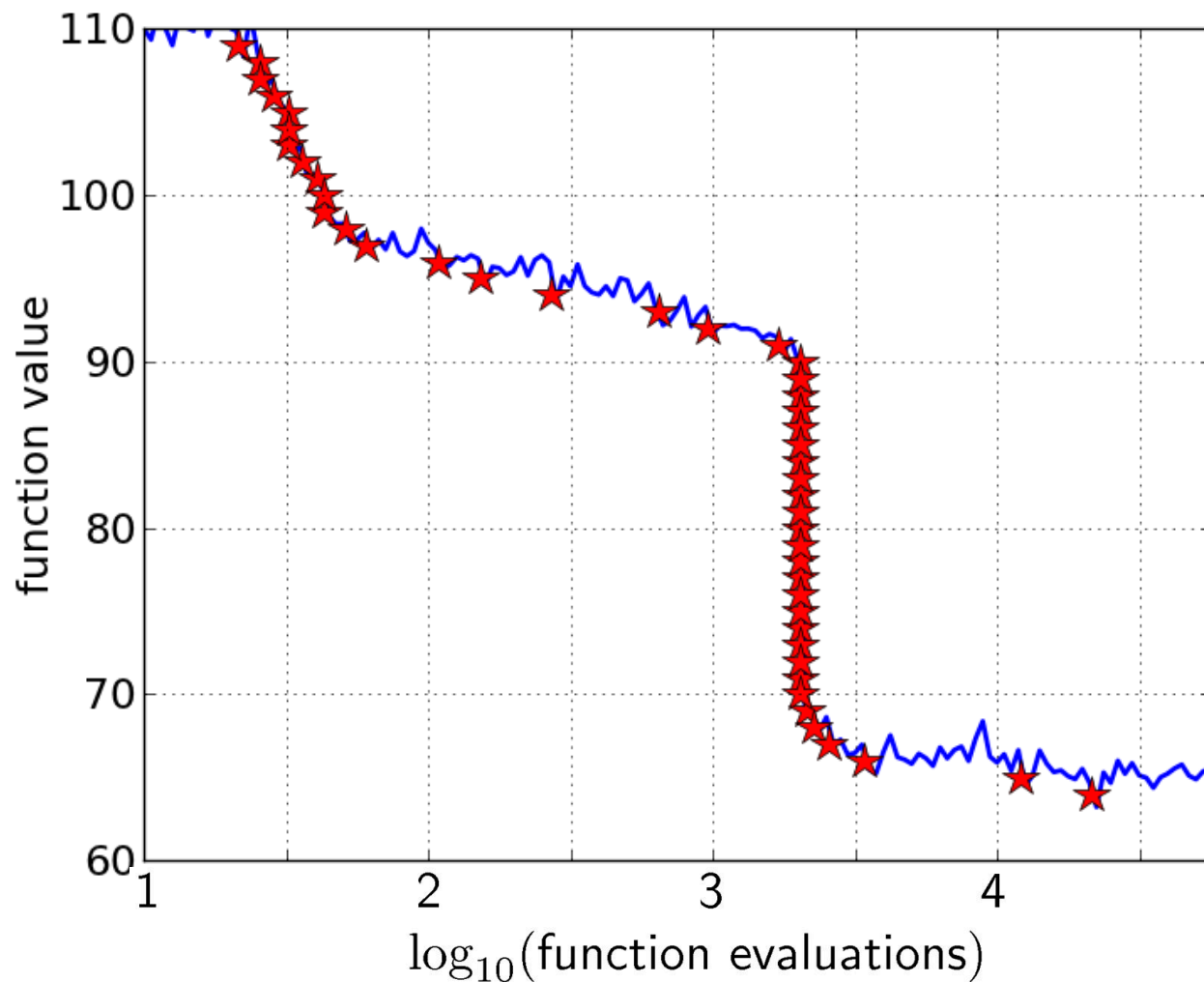


Reconstructing A Single Run

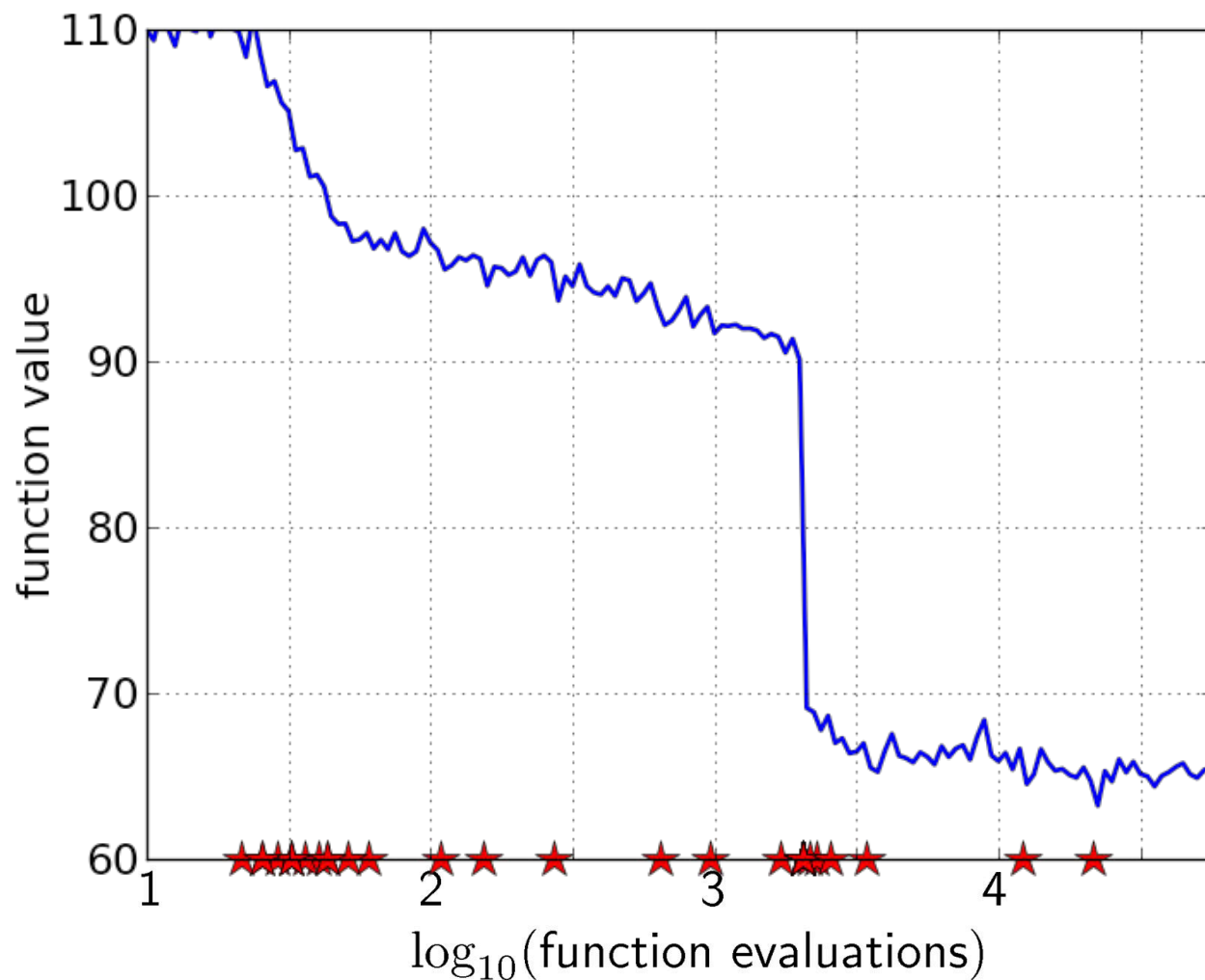


50 equally spaced targets

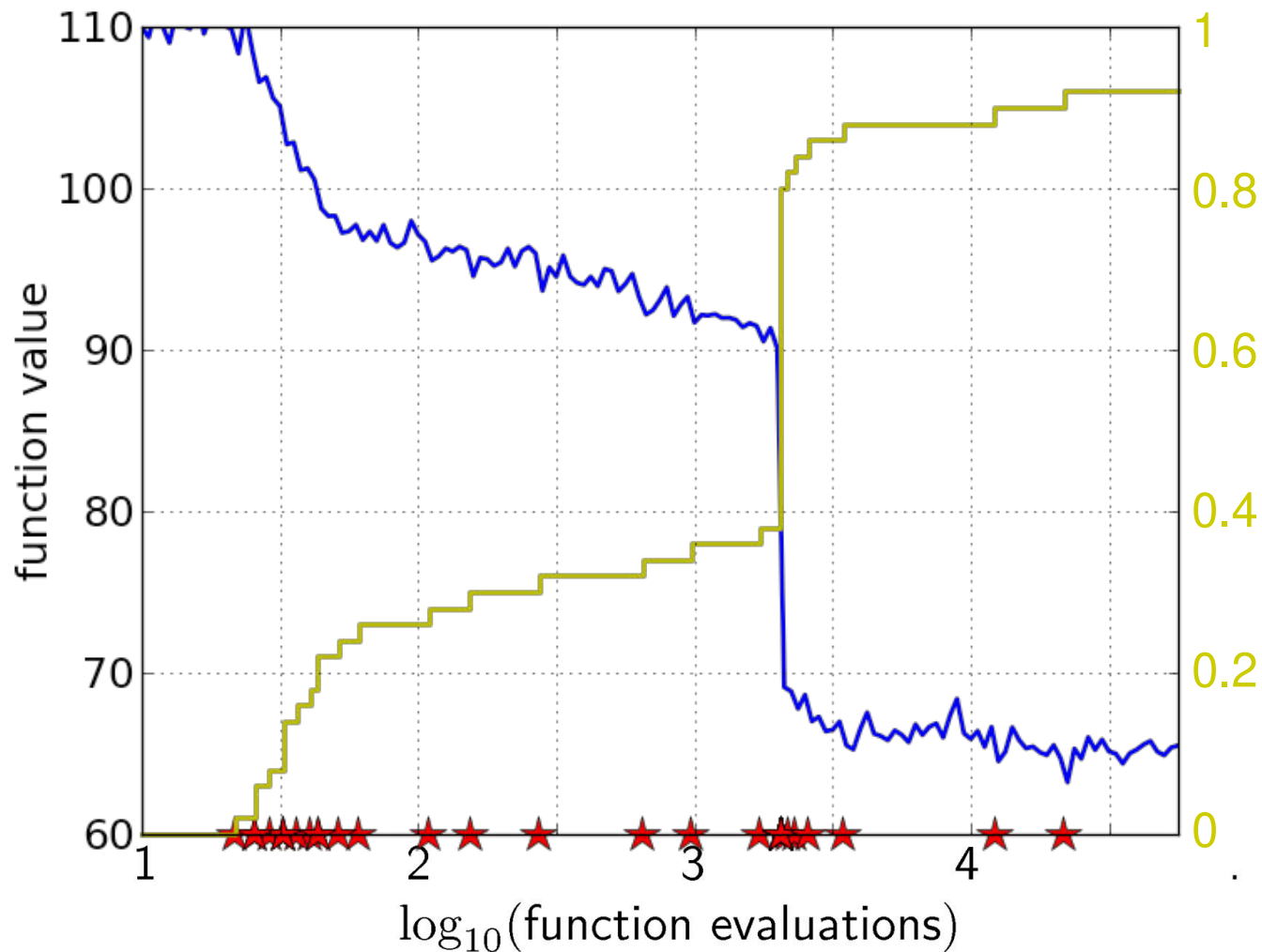
Reconstructing A Single Run



Reconstructing A Single Run

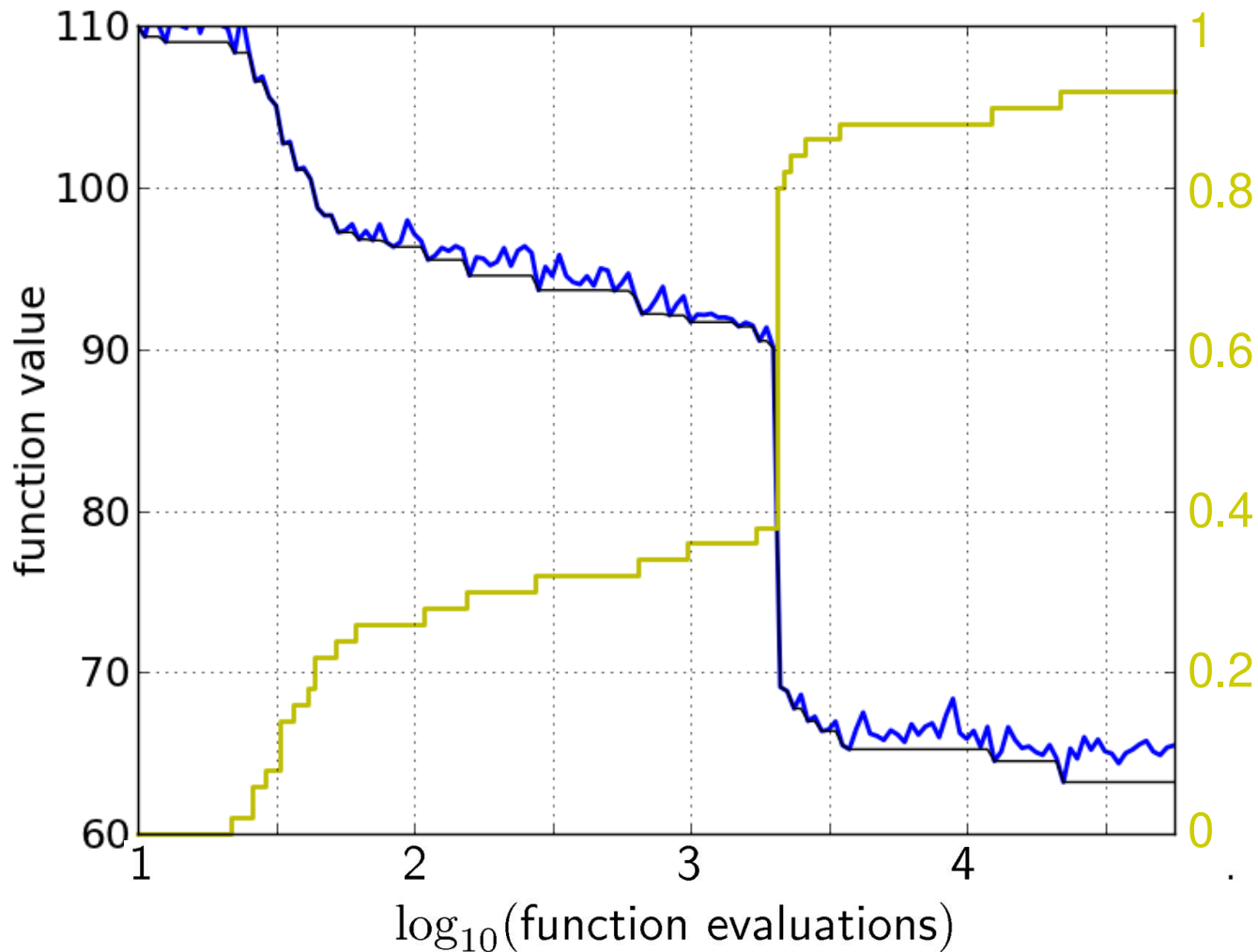


Reconstructing A Single Run



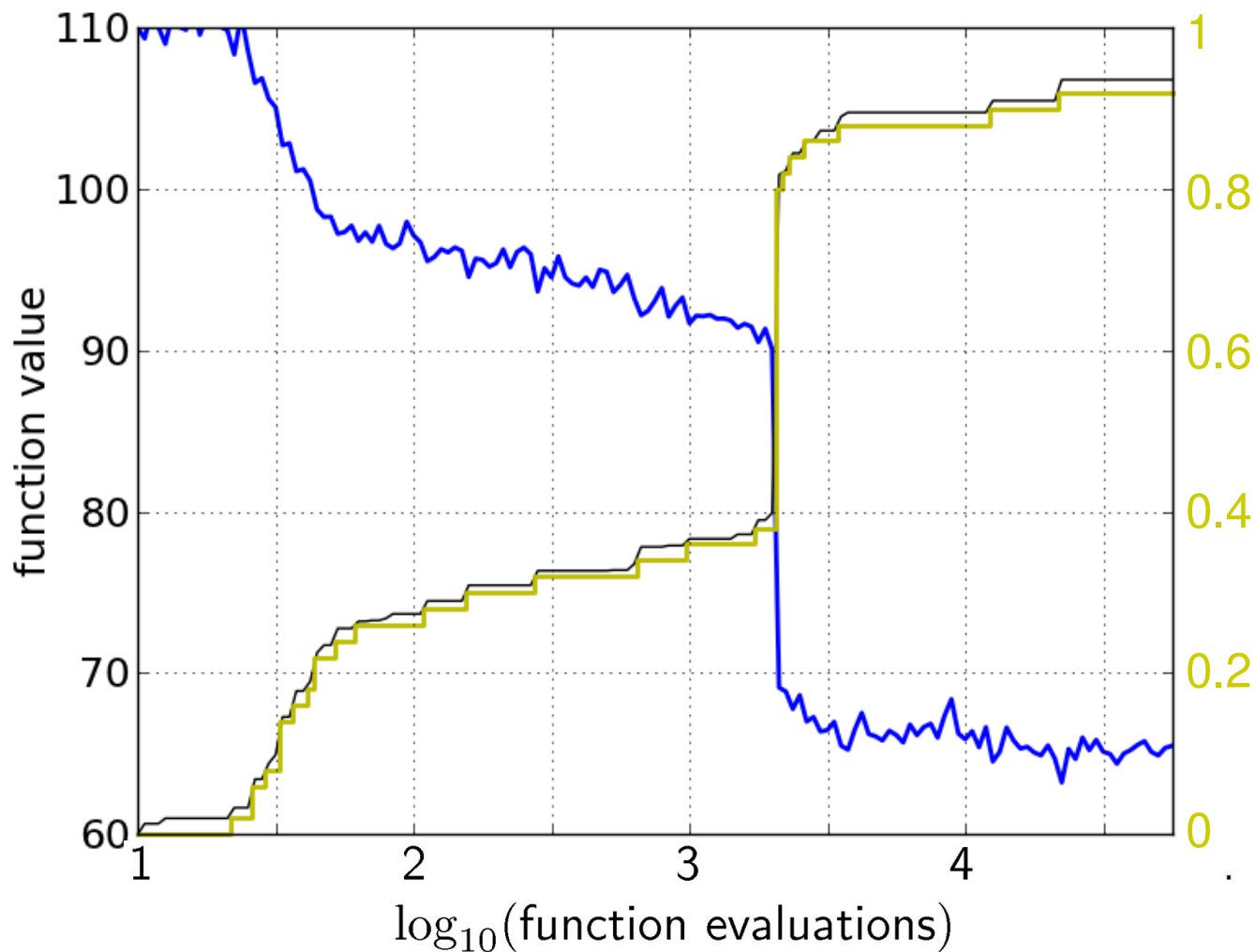
the empirical CDF makes a step for each star, is monotonous and displays for each budget the fraction of targets achieved within the budget

Reconstructing A Single Run



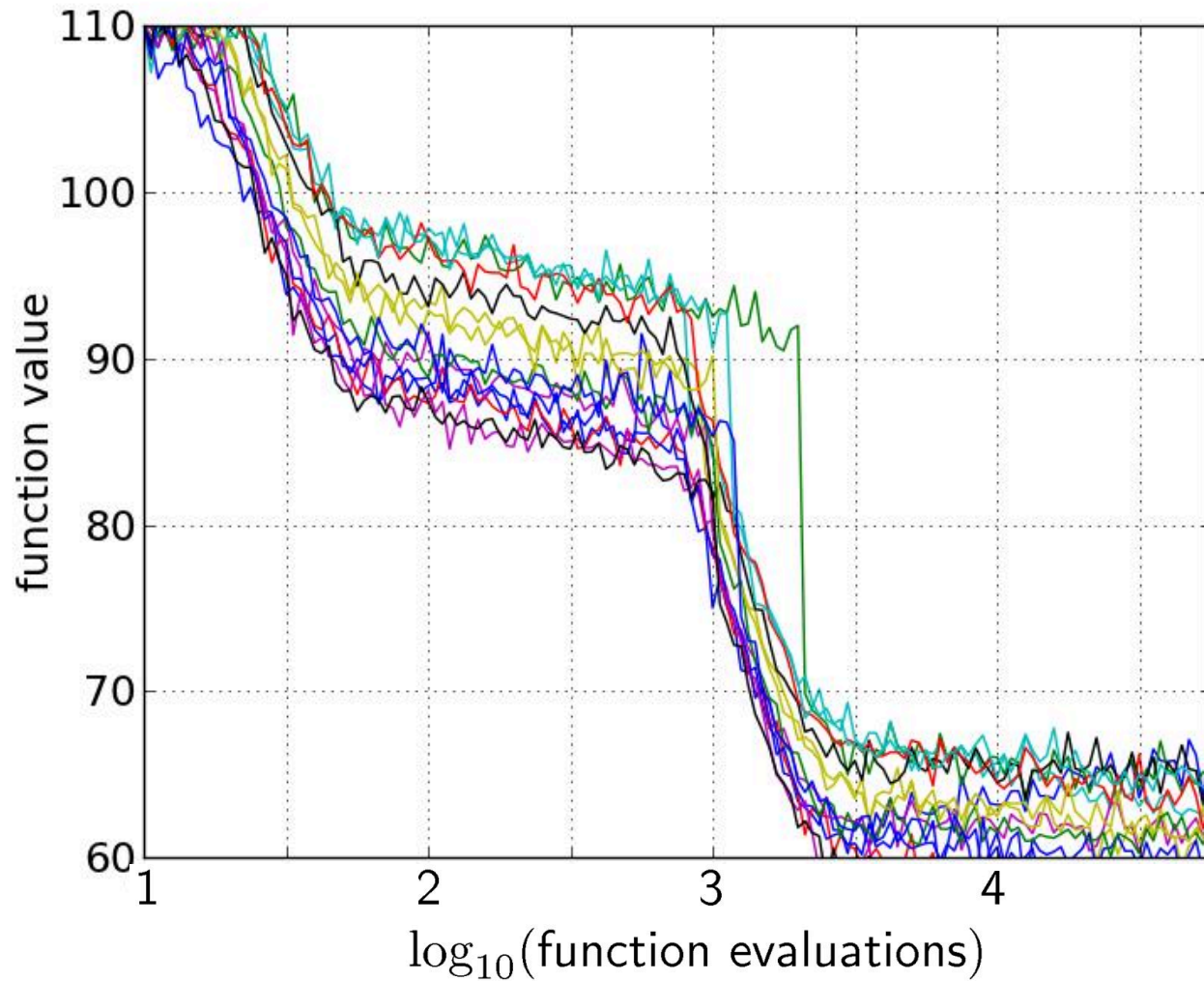
the ECDF
recovers the
monotonous
graph,
discretised
and flipped

Reconstructing A Single Run

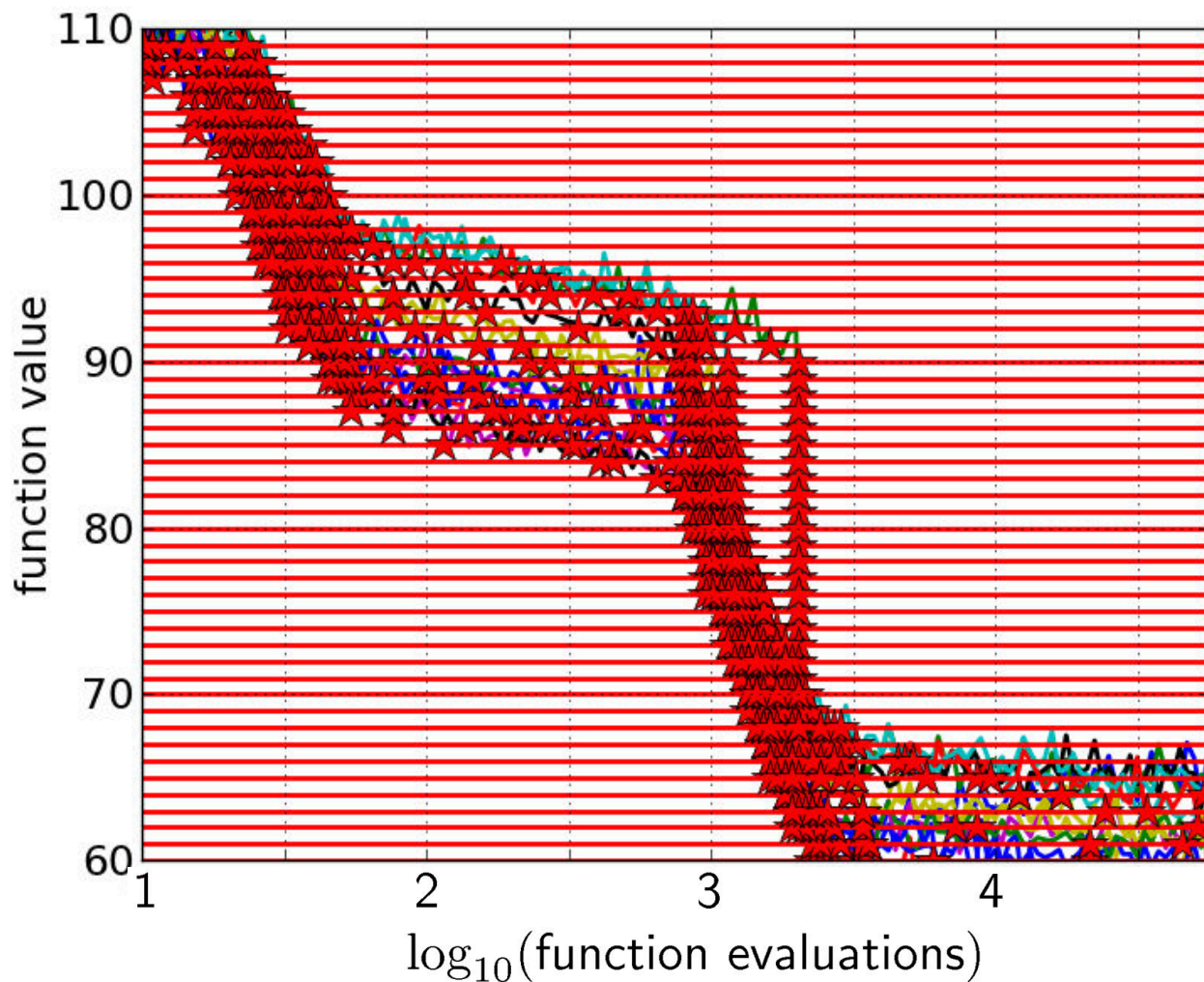


the ECDF
recovers the
monotonous
graph,
discretised
and flipped

Aggregation



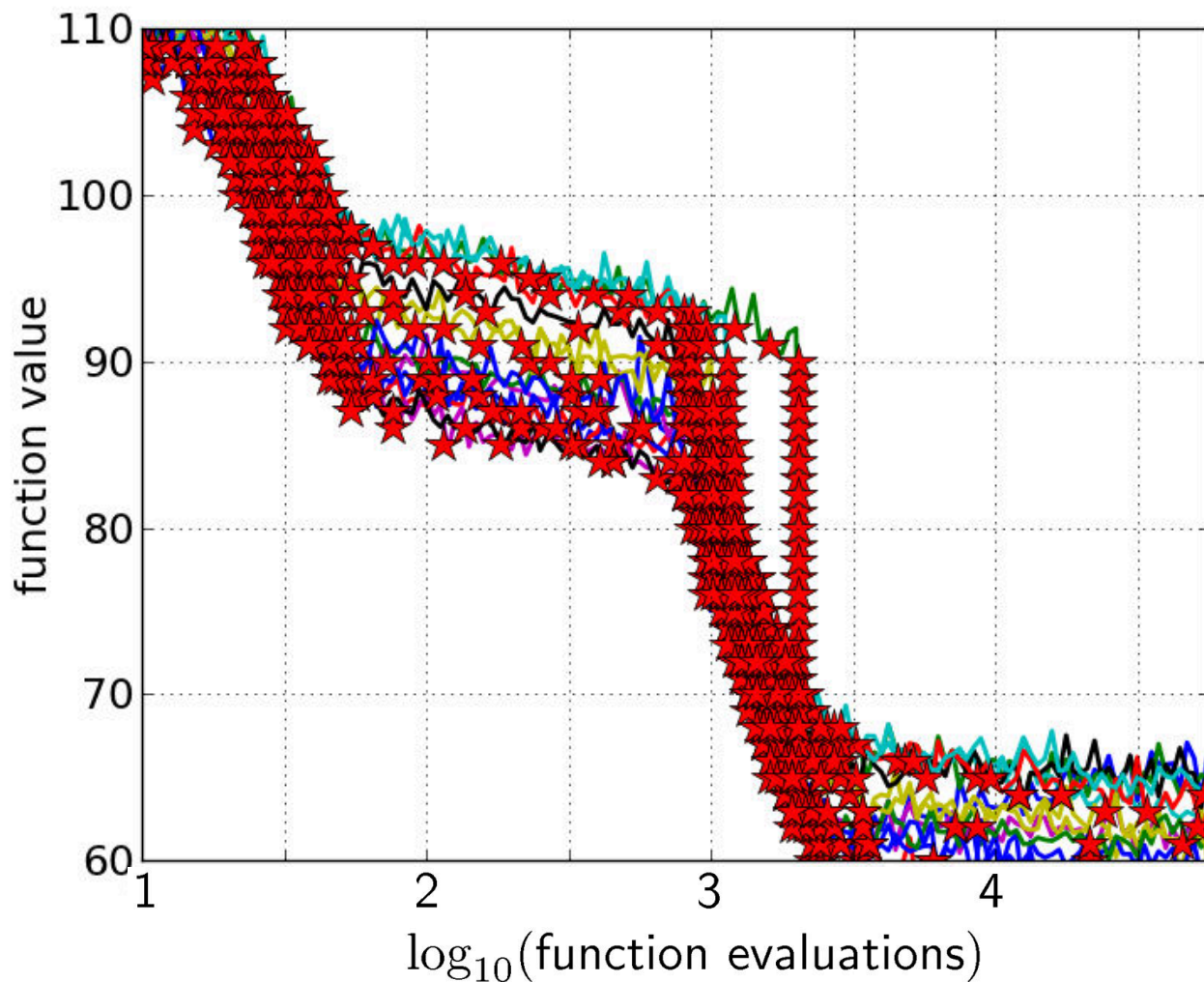
Aggregation



15 runs

50 targets

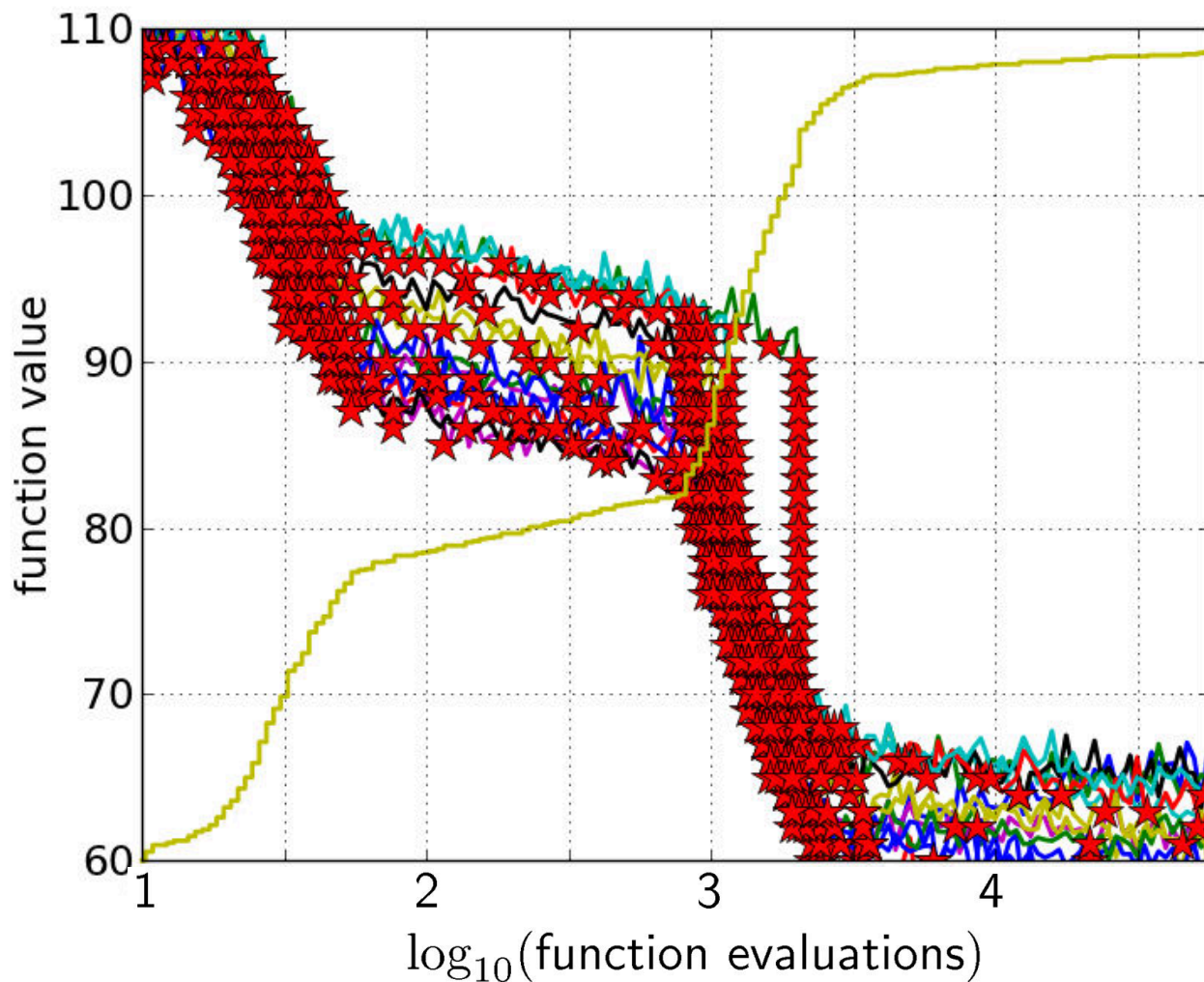
Aggregation



15 runs

50 targets

Aggregation

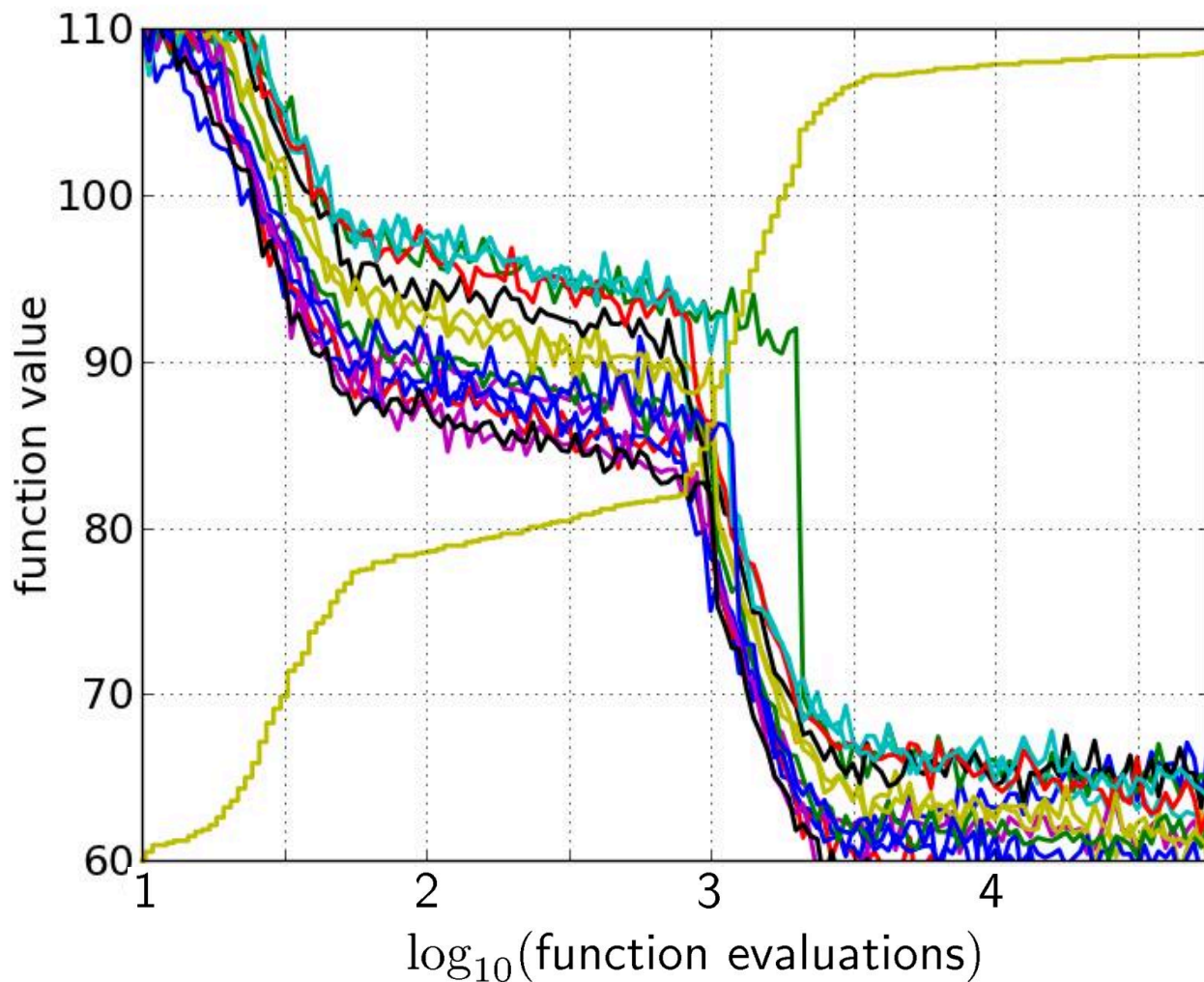


15 runs

50 targets

ECDF with
750 steps

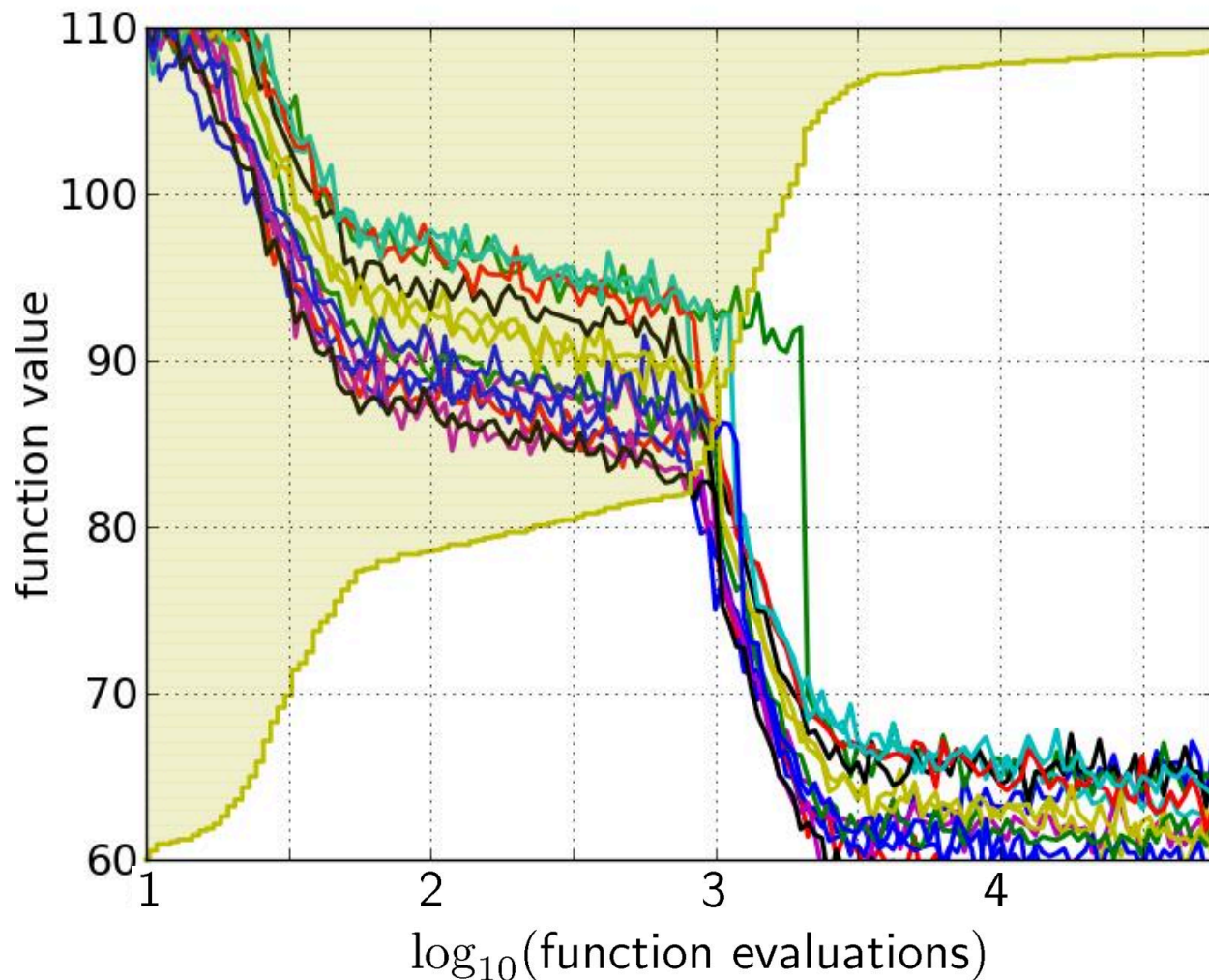
Aggregation



50 targets from
15 runs

...integrated in a
single graph

Interpretation



50 targets from
15 runs

...integrated in a
single graph

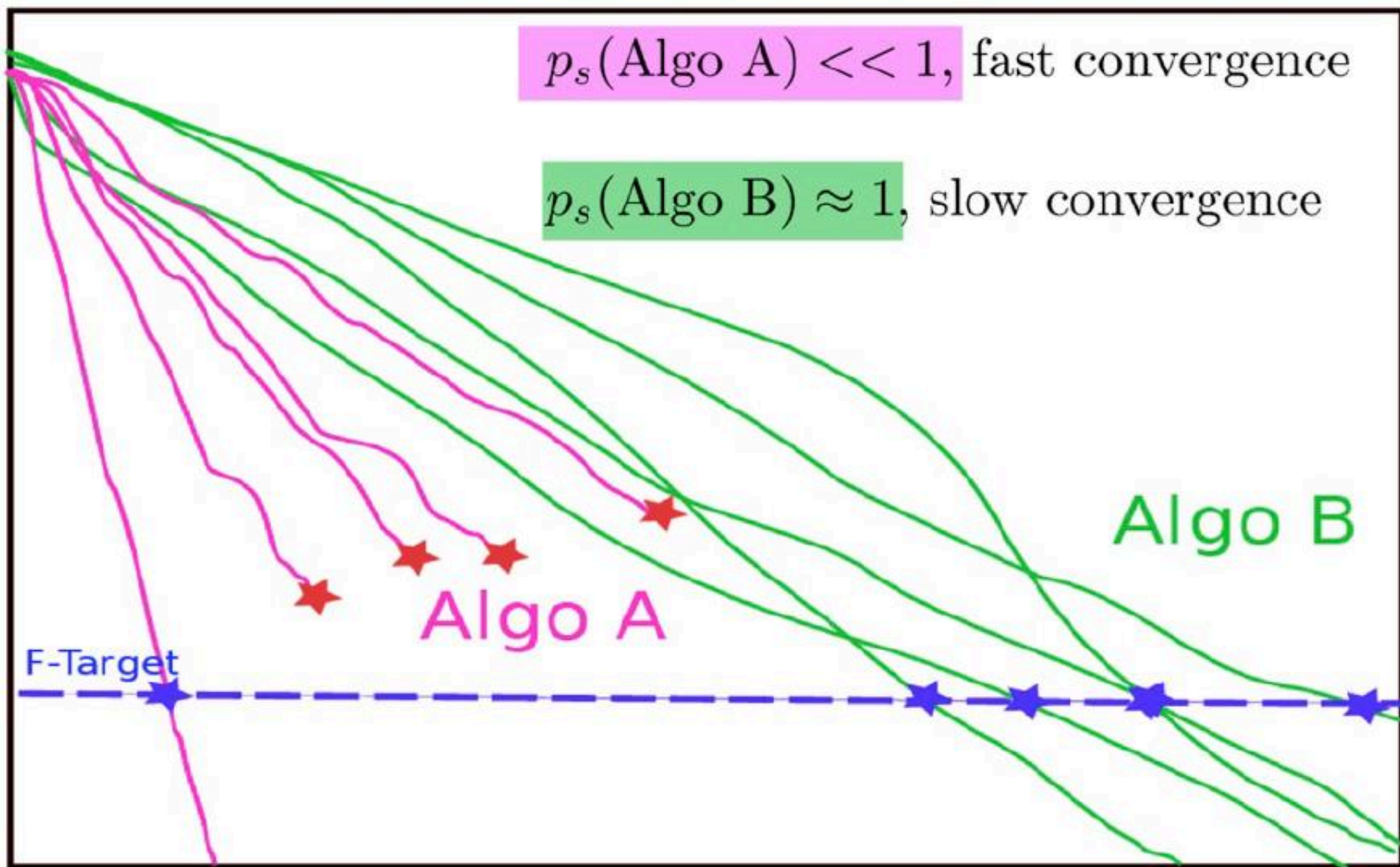
area over the
ECDF curve

=

average log
runtime

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

Fixed-target: Measuring Runtime



Fixed-target: Measuring Runtime of Restarted Algo

- Algo Restart A:



- Algo Restart B:



Fixed-target: Measuring Runtime of Restarted Algo

- 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):

$$\hat{p}_s = \frac{\#successes}{\#runs}$$

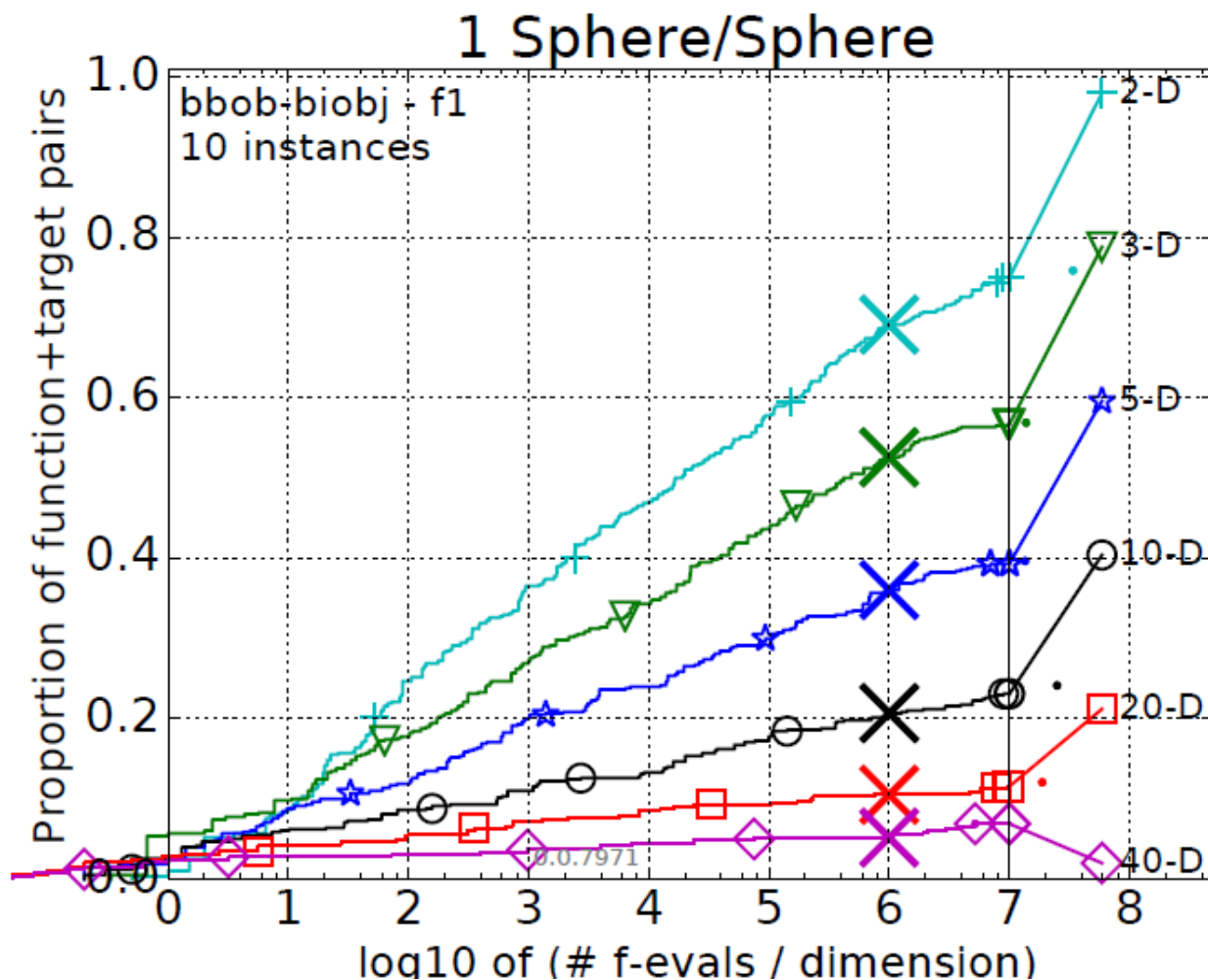
\widehat{RT}_{unsucc} = Average evals of unsuccessful runs

\widehat{RT}_{succ} = Average evals of successful runs

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

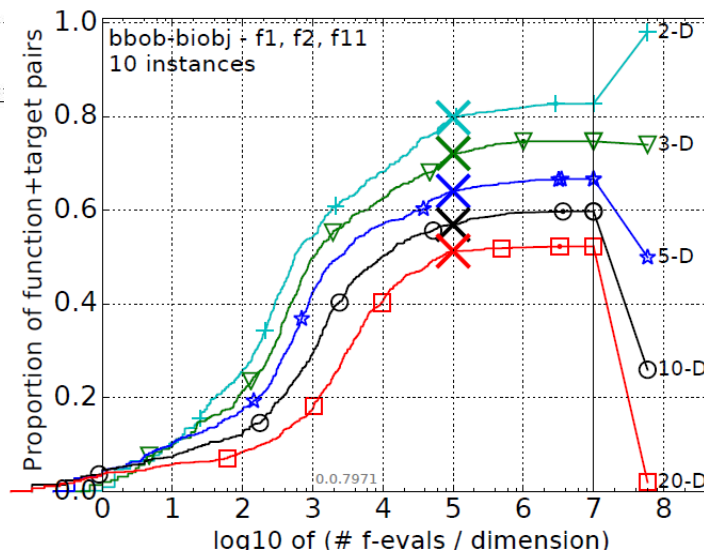
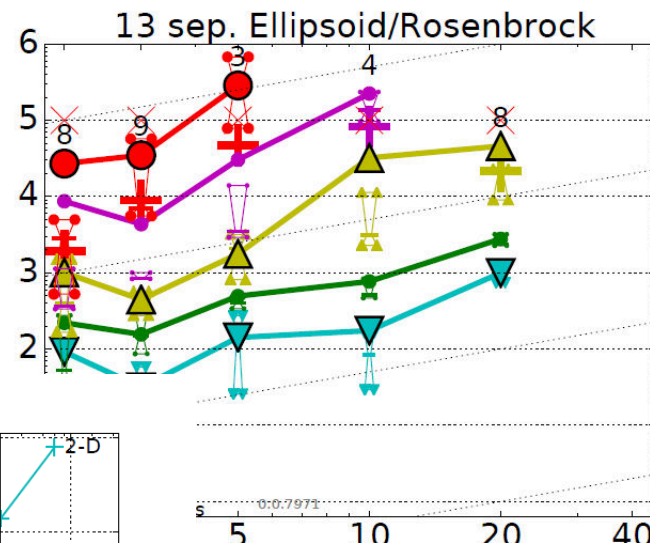
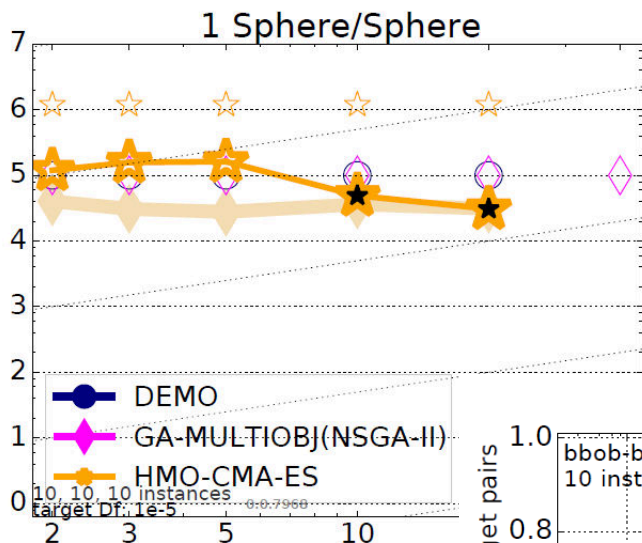
ECDFs with Simulated Restarts

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



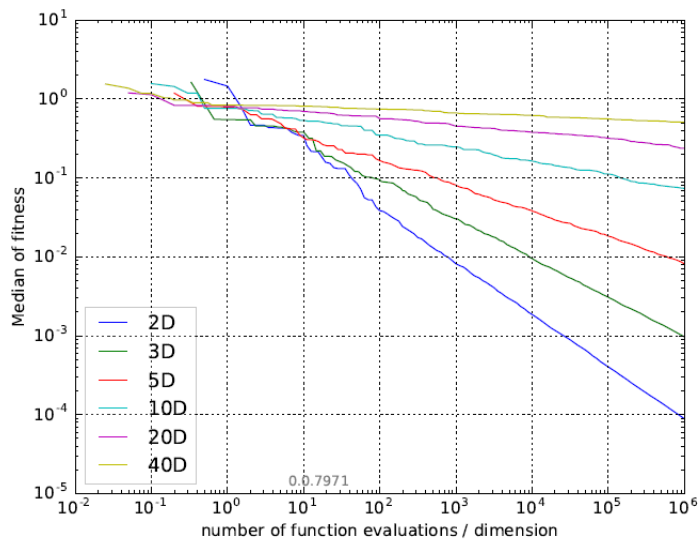
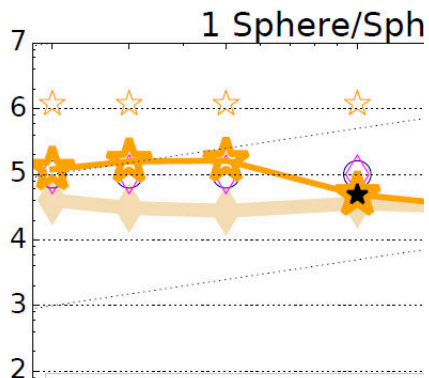
More Automated Plots...

...might come back to it in detail later today

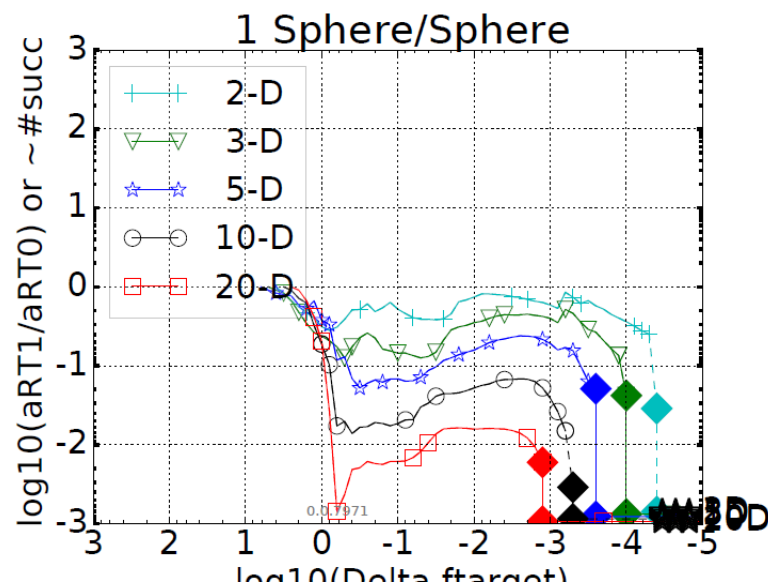
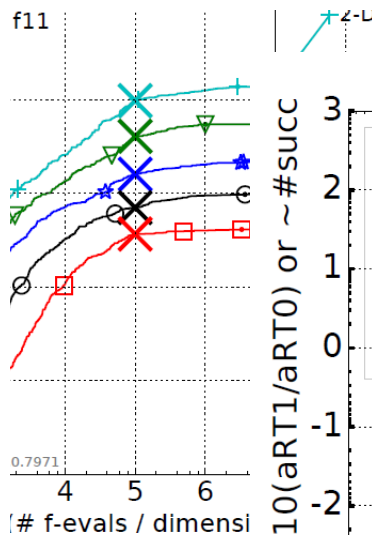
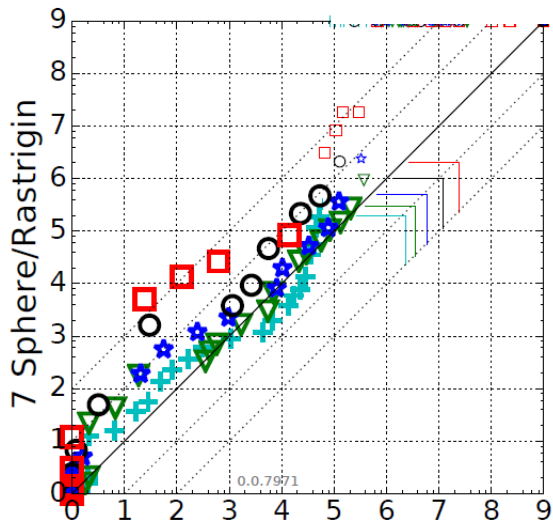
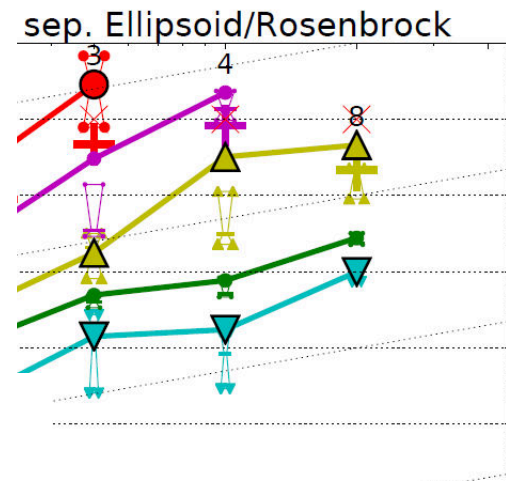


More Automated Plots...

...might come



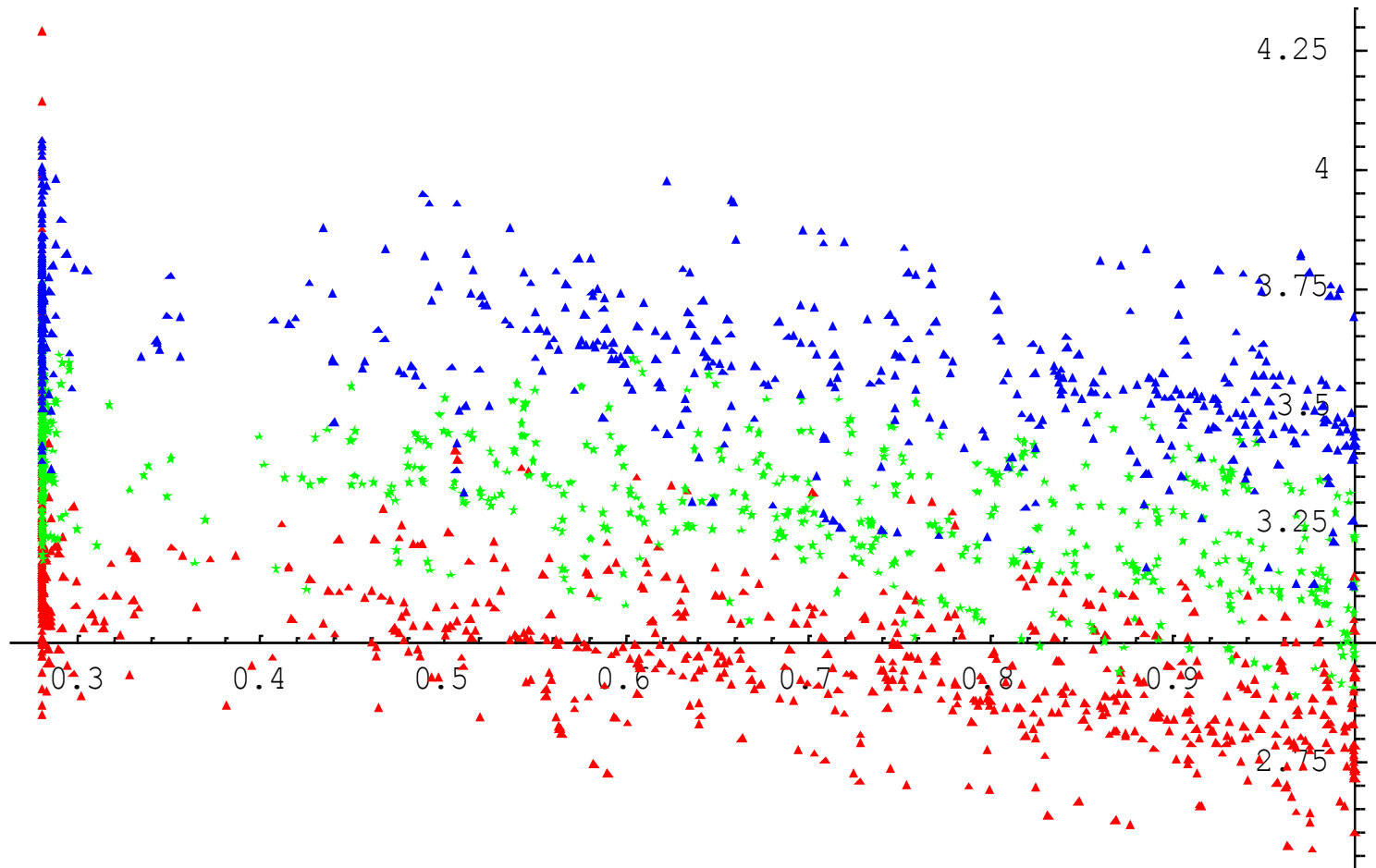
today



how to do benchmarking in the
multiobjective case?

Once Upon a Time...

... multiobjective EAs were mainly compared visually:

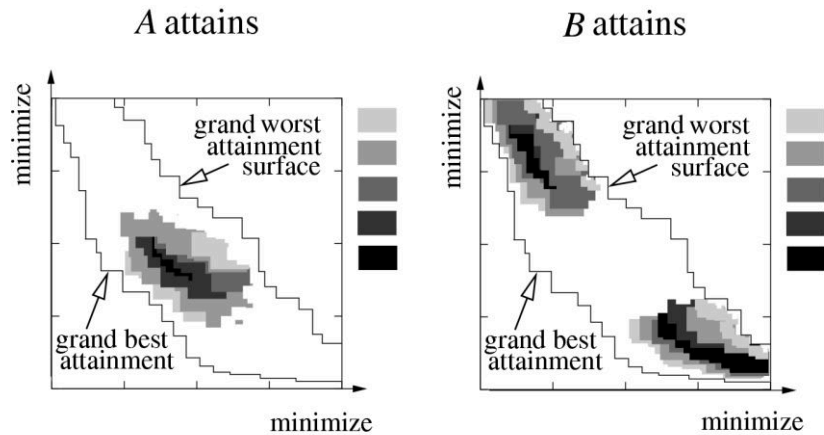


ZDT6 benchmark problem: **IBEA**, **SPEA2**, **NSGA-II**

Two Main Approaches for Empirical Studies

Attainment function approach

- applies statistical tests directly to the approximation set
- detailed information about how and where performance differences occur



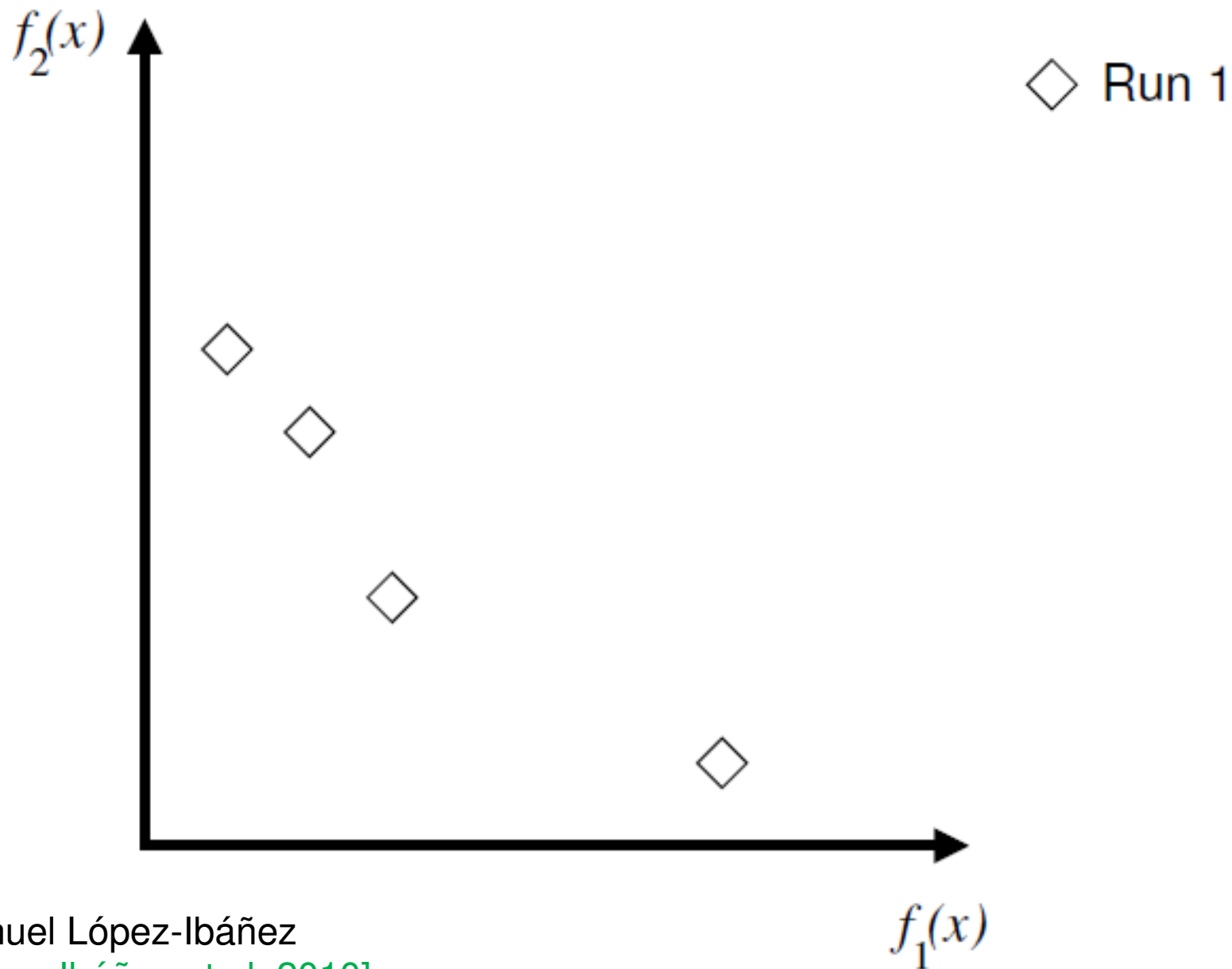
Quality indicator approach

- reduces each approximation set to a single quality value
- applies statistical tests to the quality values

<i>Indicator</i>	A	B
Hypervolume indicator	6.3431	7.1924
ϵ -indicator	1.2090	0.12722
R_2 indicator	0.2434	0.1643
R_3 indicator	0.6454	0.3475

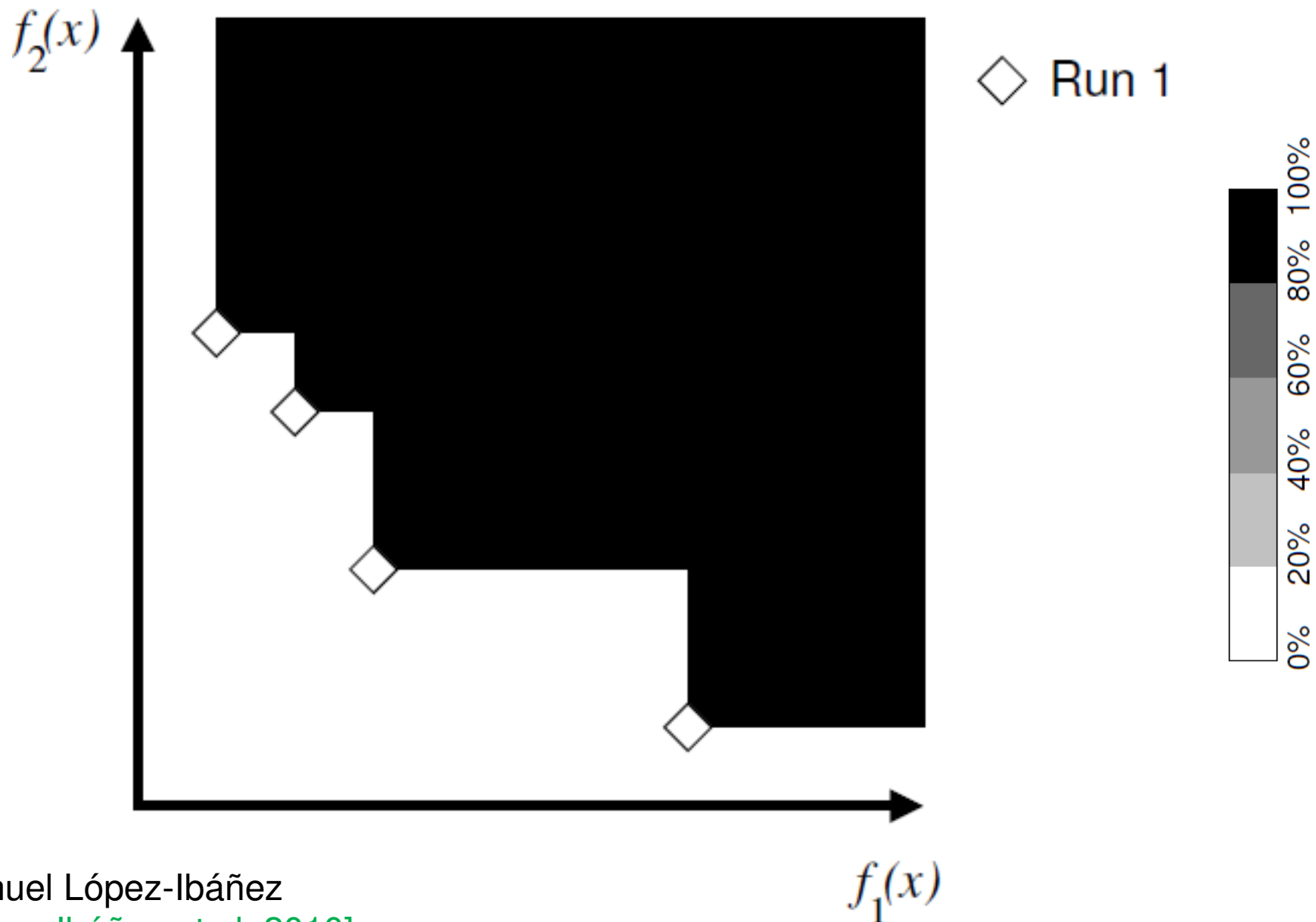
see e.g. [Zitzler et al. 2003]

Empirical Attainment Functions: Idea



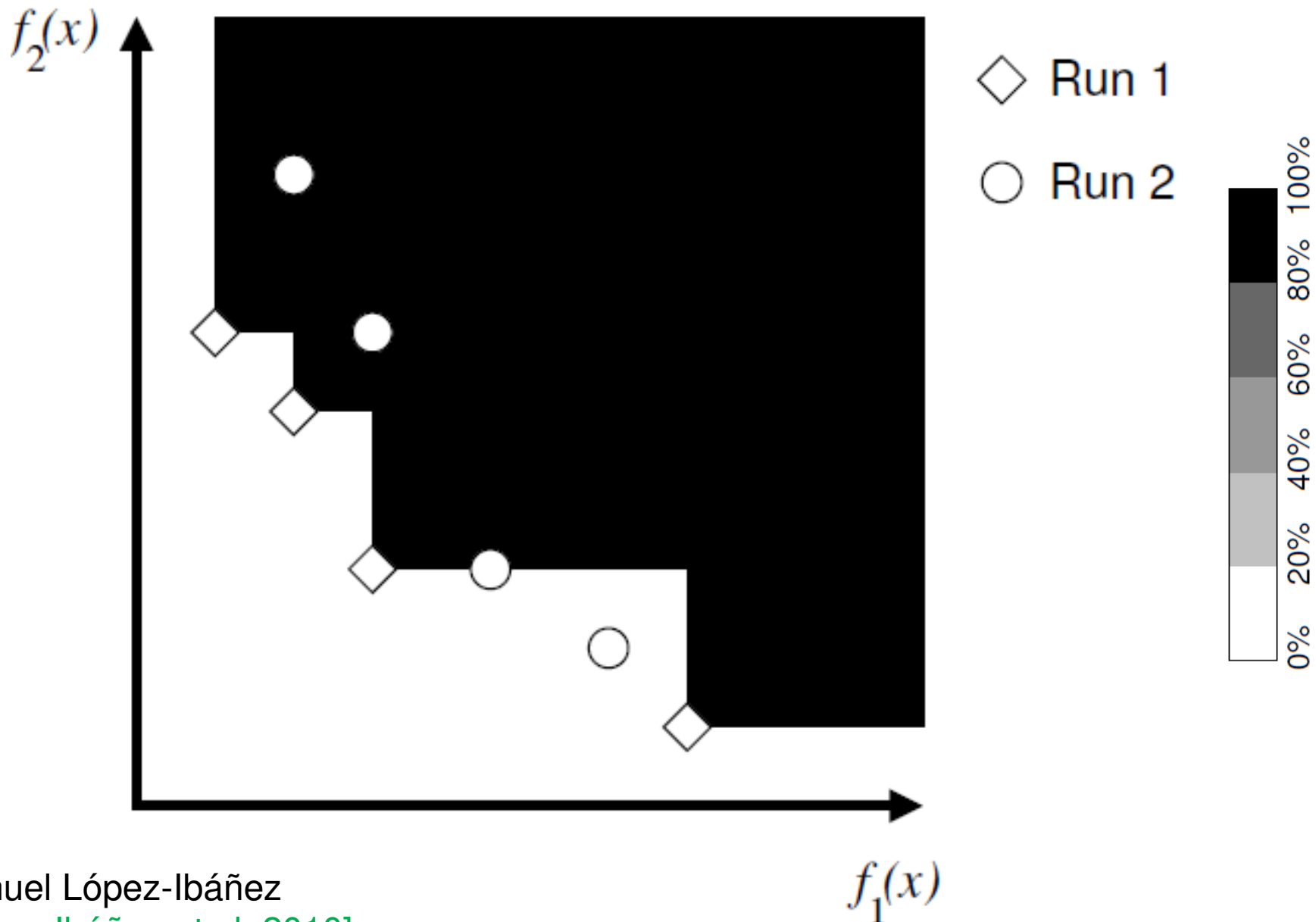
© Manuel López-Ibáñez
[López-Ibáñez et al. 2010]

Empirical Attainment Functions: Idea



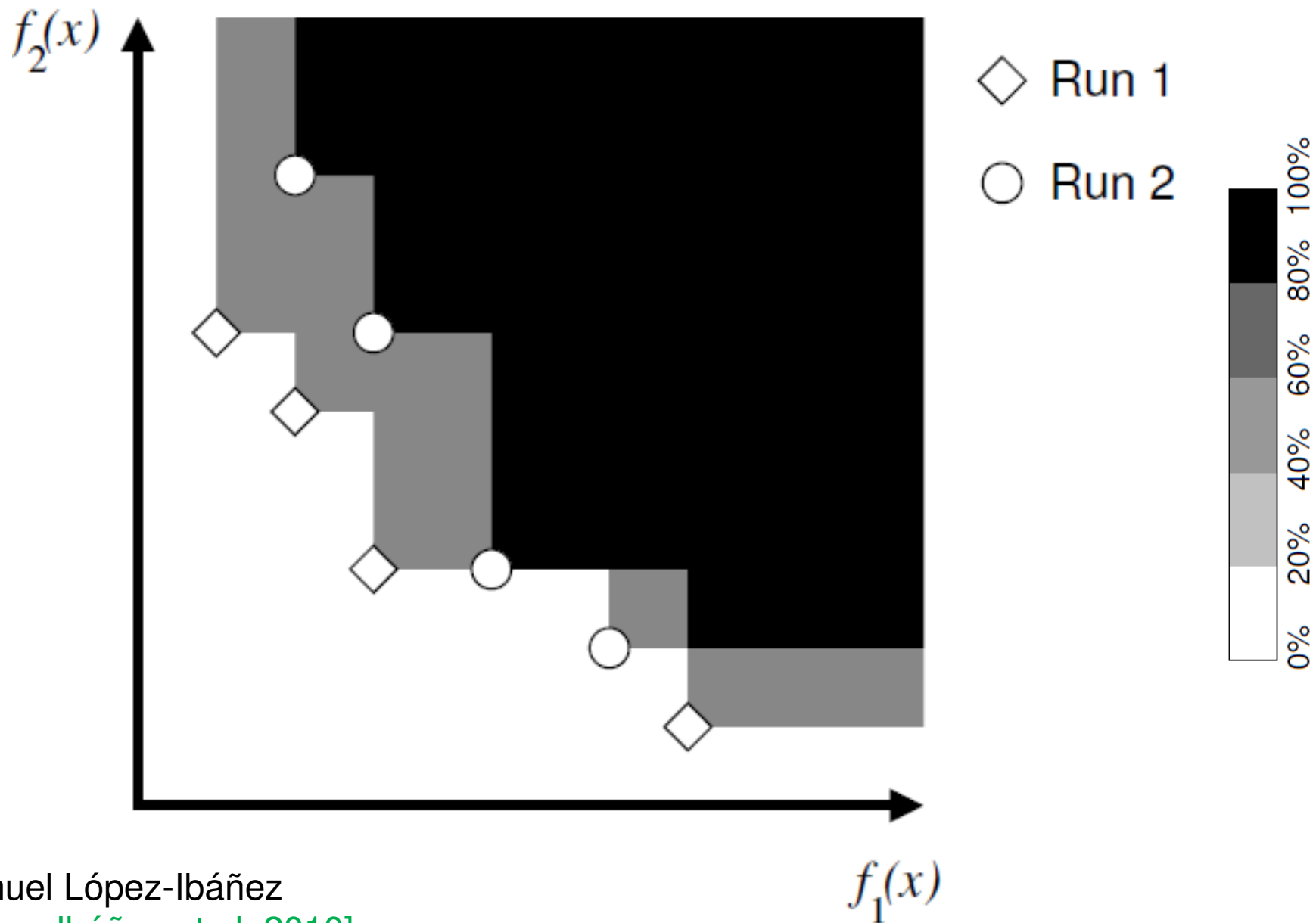
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[López-Ibáñez et al. 2010]

Empirical Attainment Functions: Idea



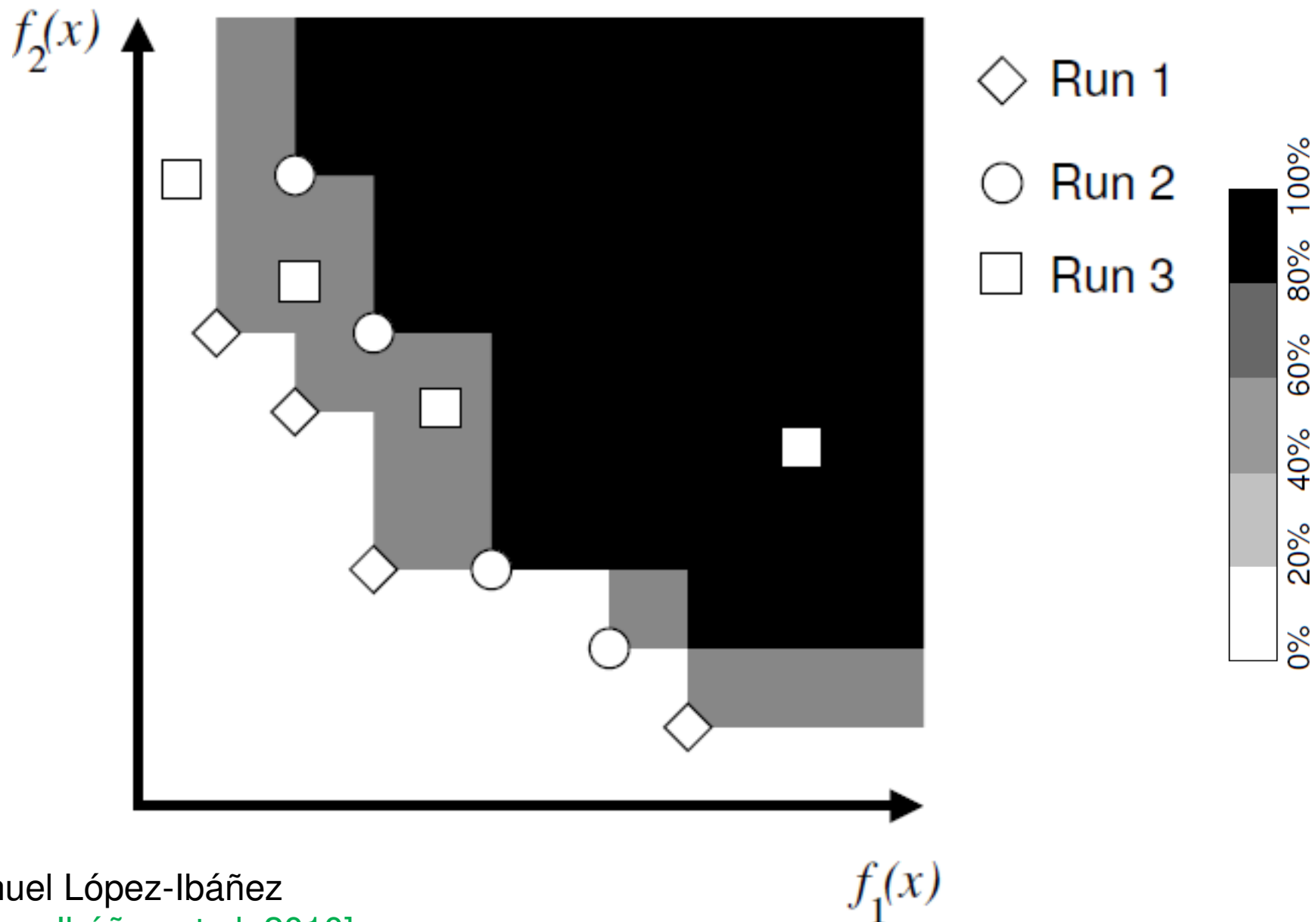
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[López-Ibáñez et al. 2010]

Empirical Attainment Functions: Idea



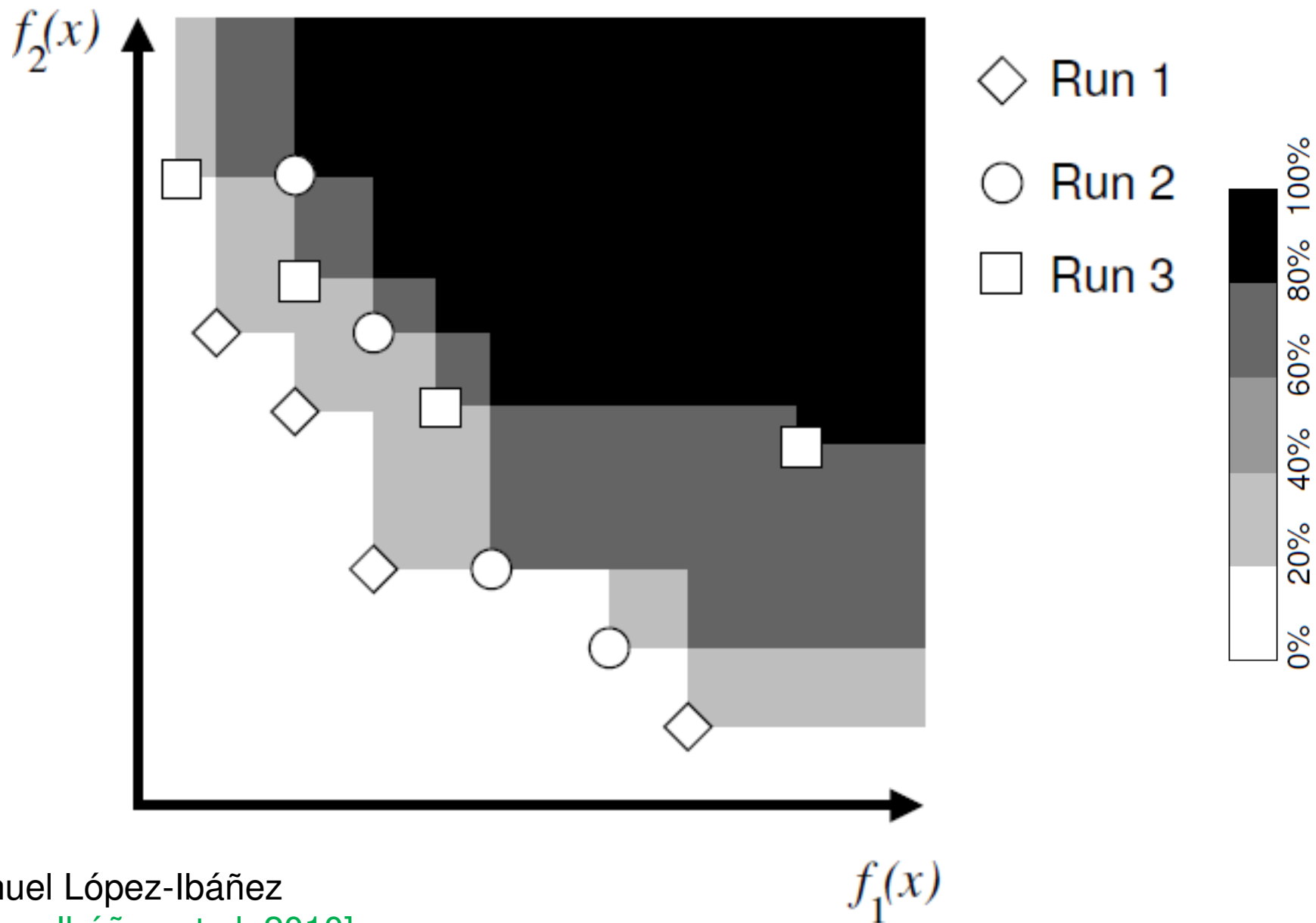
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[López-Ibáñez et al. 2010]

Empirical Attainment Functions: Idea



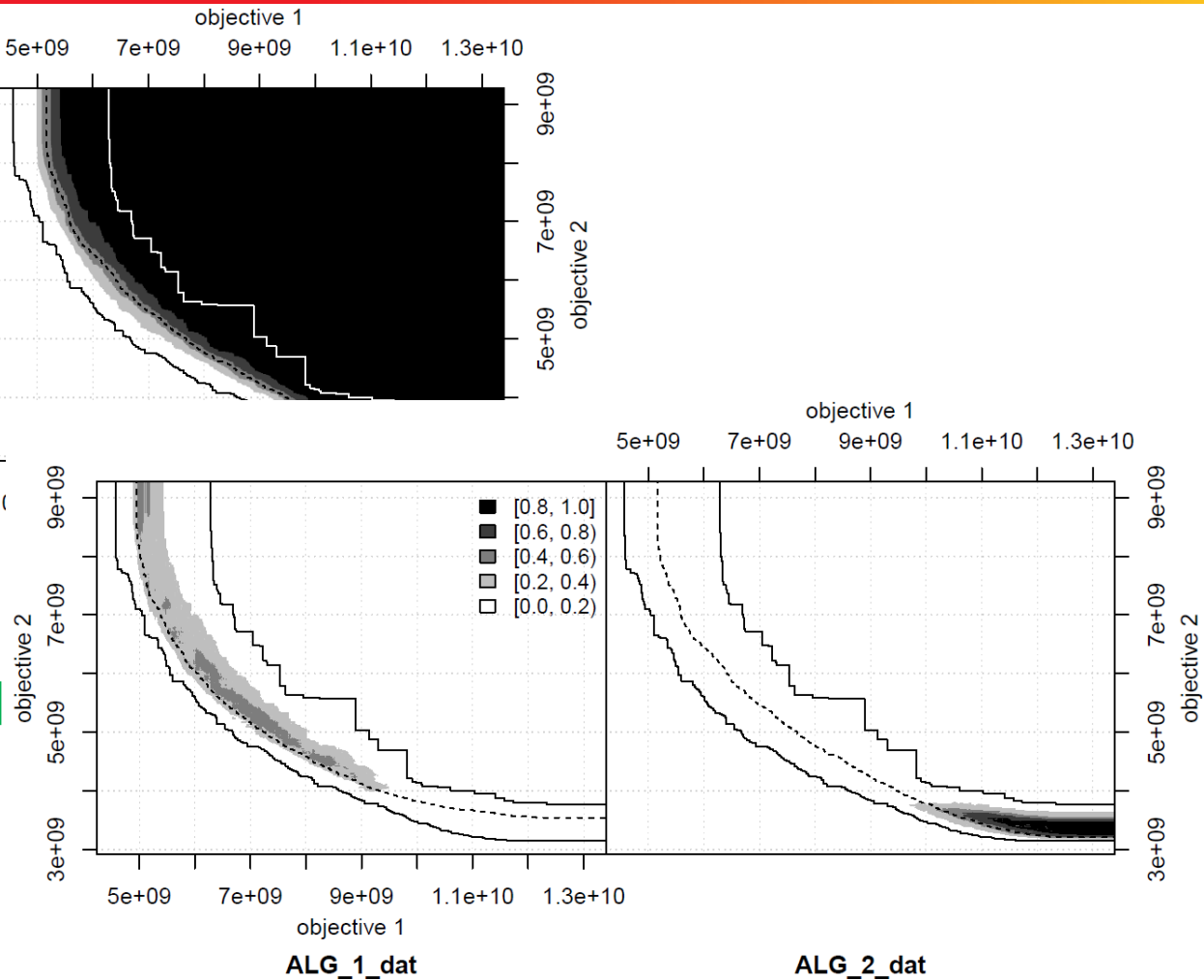
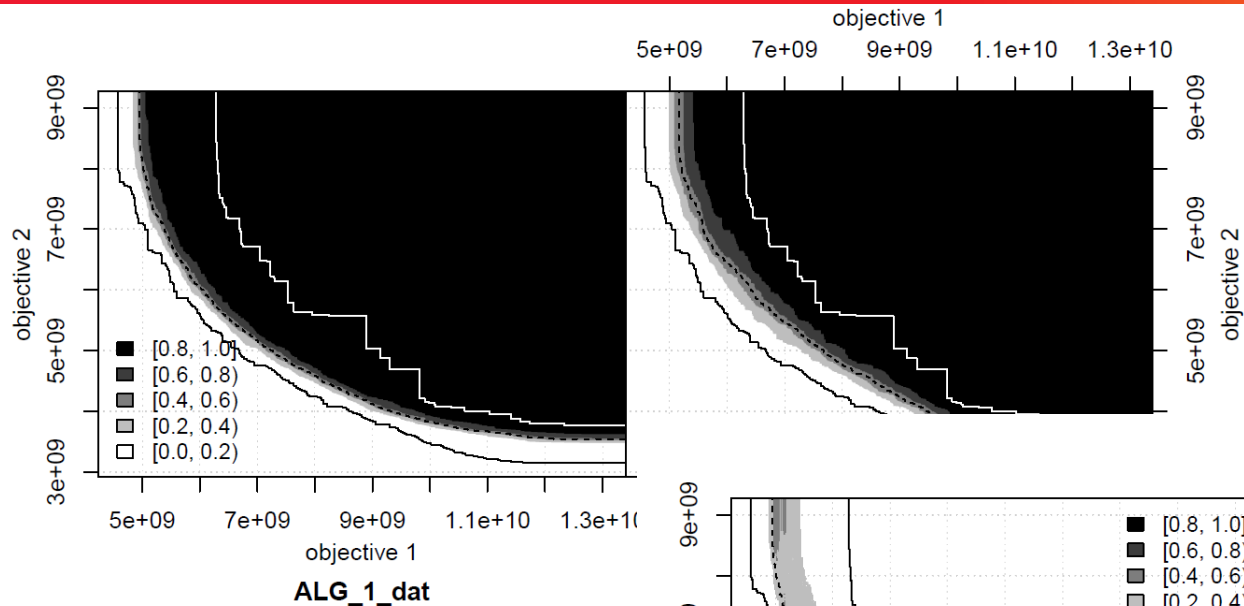
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[López-Ibáñez et al. 2010]

Empirical Attainment Functions: Idea



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[López-Ibáñez et al. 2010]

Attainment Plots in Practice

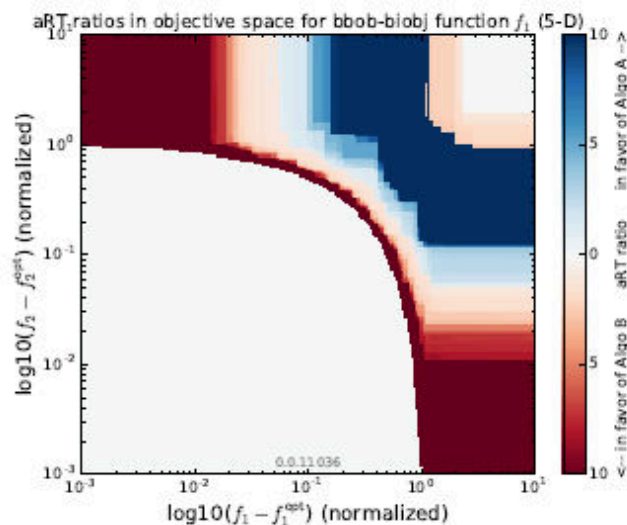
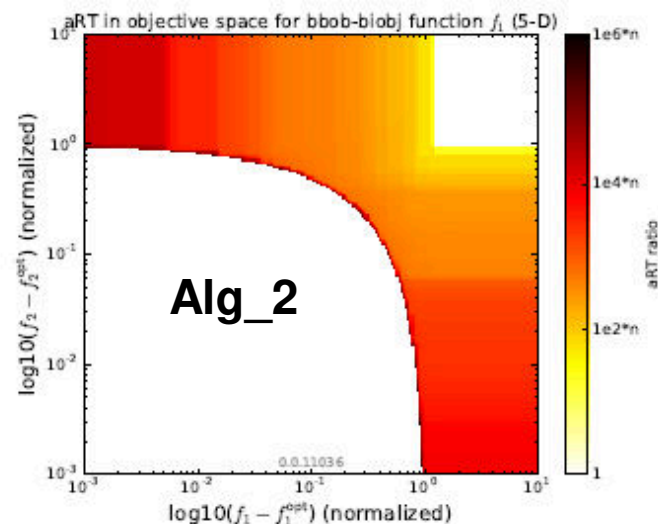
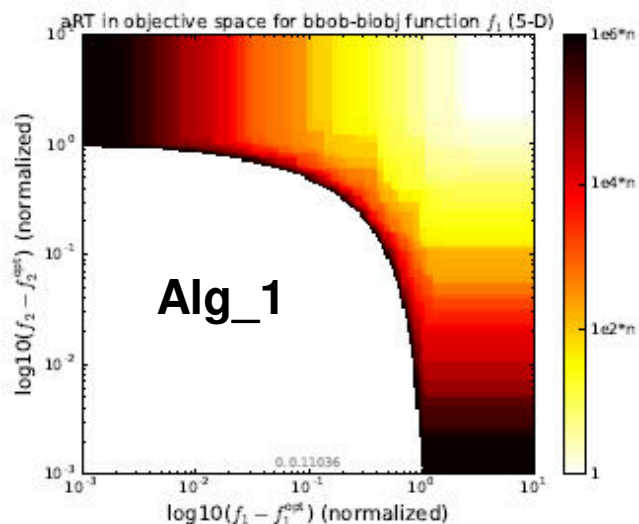


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[López-Ibáñez et al. 2010]

latest implementation online at
<http://eden.dei.uc.pt/~cmfonsec/software.html>
R package: <http://lopez-ibanez.eu/eaftools>
see also [López-Ibáñez et al. 2010, Fonseca et al. 2011]

Average Runtime Attainment Plots

...display not only the success probabilities, but the **average runtime** to attain points in objective space:



[Brockhoff et al. 2017]

Most Used Approach: Quality Indicators

A quality indicator

- maps a solution set to a real number
- can be used with standard performance assessment
 - report median, variance, ...
 - boxplots
 - statistical tests
- should optimally refine the dominance relation on sets

Recommendation:

- use hypervolume (refinement, i.e. it does not contradict the dominance relation)
- or epsilon indicator or R2 indicator (are weak refinements)

Also important:

- interpretation of the results (by knowing theoretical properties of the used indicator)

Quality Indicator Approach

Idea:

- transfer multiobjective problem into a set problem
- define an objective function (“quality indicator”) on sets
- use the resulting total (pre-)order (on the quality values)

Question:

Can any total (pre-)order be used or are there any requirements concerning the resulting preference relation?

⇒ Underlying dominance relation should be reflected!

$$A \preceq B :\Leftrightarrow \forall y \in B \exists x \in A x \leq_{par} y$$

Refinements and Weak Refinements

① \succsim^{ref} **refines** a preference relation \succsim iff

$$A \succsim B \wedge B \not\succeq A \Rightarrow A \succsim^{\text{ref}} B \wedge B \not\succeq^{\text{ref}} A \quad (\text{better} \Rightarrow \text{better})$$

\Rightarrow fulfills requirement

② \succsim^{ref} **weakly refines** a preference relation \succsim iff

$$A \succsim B \wedge B \not\succeq A \Rightarrow A \succsim^{\text{ref}} B \quad (\text{better} \Rightarrow \text{weakly better})$$

\Rightarrow does not fulfill requirement, but \succsim^{ref} does not contradict \succsim

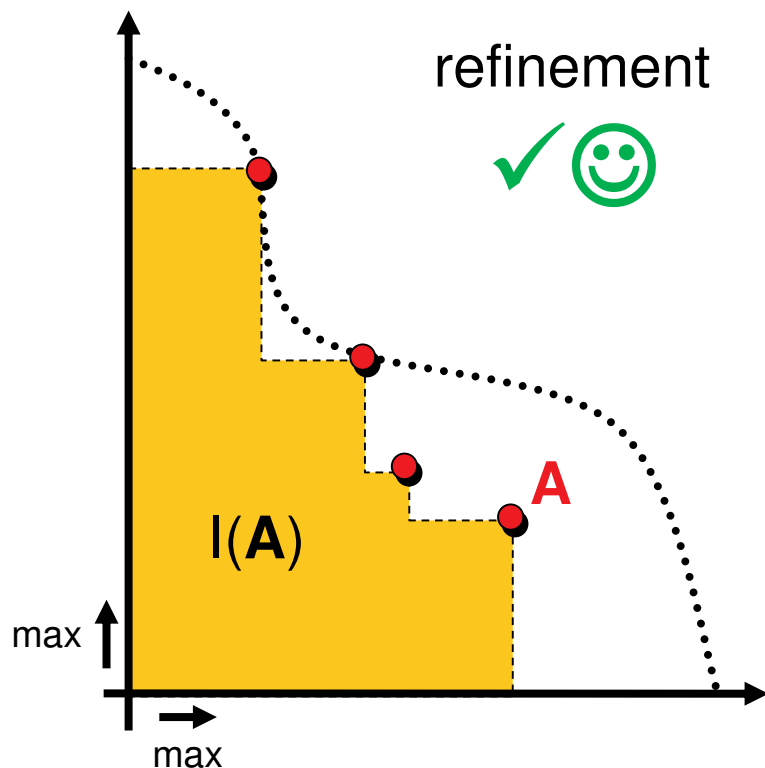
! sought are total refinements...

[Zitzler et al. 2010]

Example: Refinements Using Indicators

$$A \stackrel{\text{ref}}{\preceq} B :\Leftrightarrow I(A) \geq I(B)$$

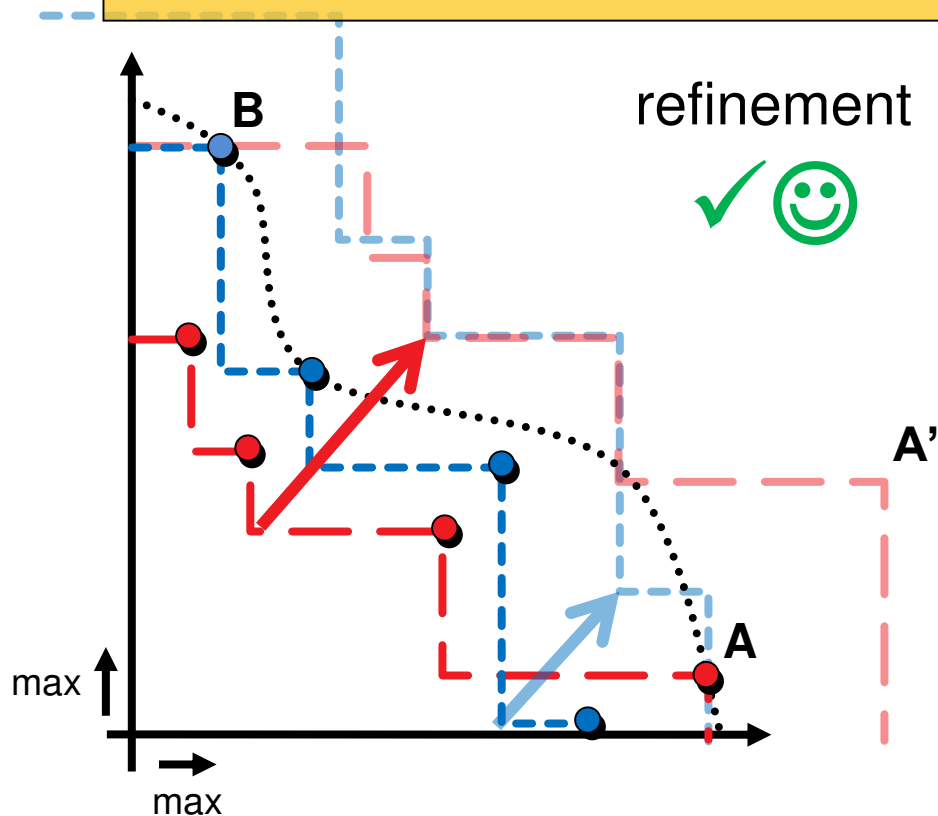
$I(A)$ = volume of the weakly dominated area in objective space



unary hypervolume indicator

$$A \stackrel{\text{ref}}{\preceq} B :\Leftrightarrow I(A,B) \leq I(B,A)$$

$I(A,B)$ = how much needs A to be moved to weakly dominate B



binary epsilon indicator

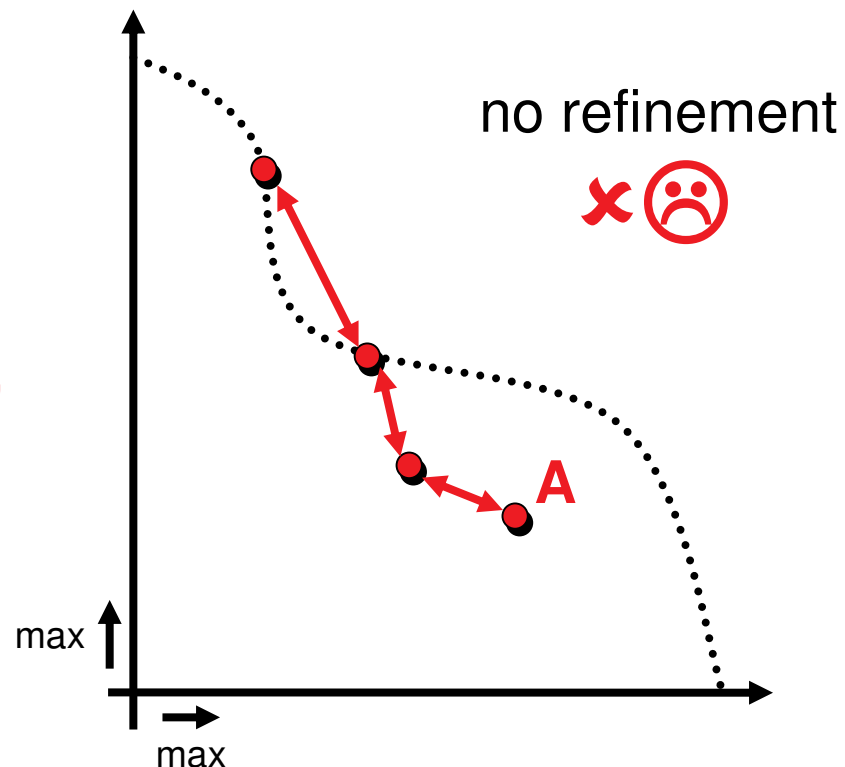
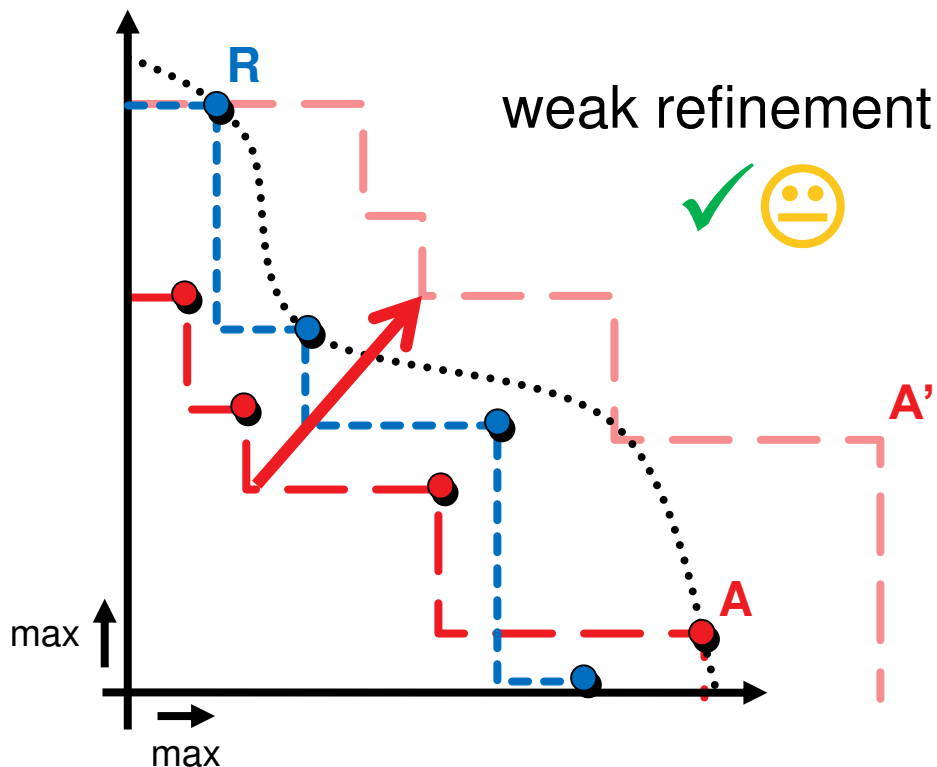
Example: Weak Refinement / No Refinement

$$A \stackrel{\text{ref}}{\preceq} B \Leftrightarrow I(A, R) \leq I(B, R)$$

$$A \stackrel{\text{ref}}{\preceq} B \Leftrightarrow I(A) \leq I(B)$$

$I(A, R)$ = how much needs A to be moved to weakly dominate R

$I(A)$ = variance of pairwise distances

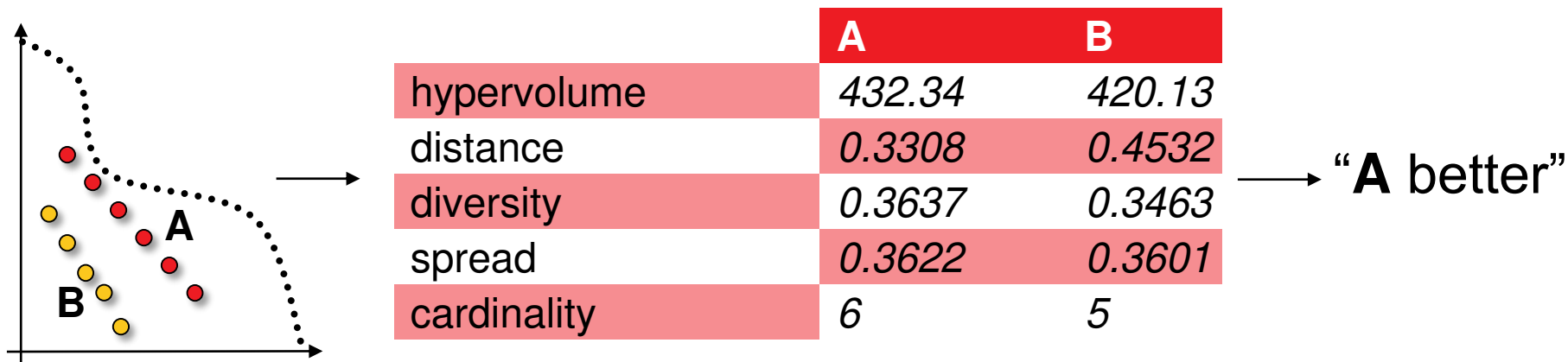


unary epsilon indicator

unary diversity indicator

Quality Indicator Approach

Goal: compare two Pareto set approximations A and B



Comparison method C = quality measure(s) + Boolean function

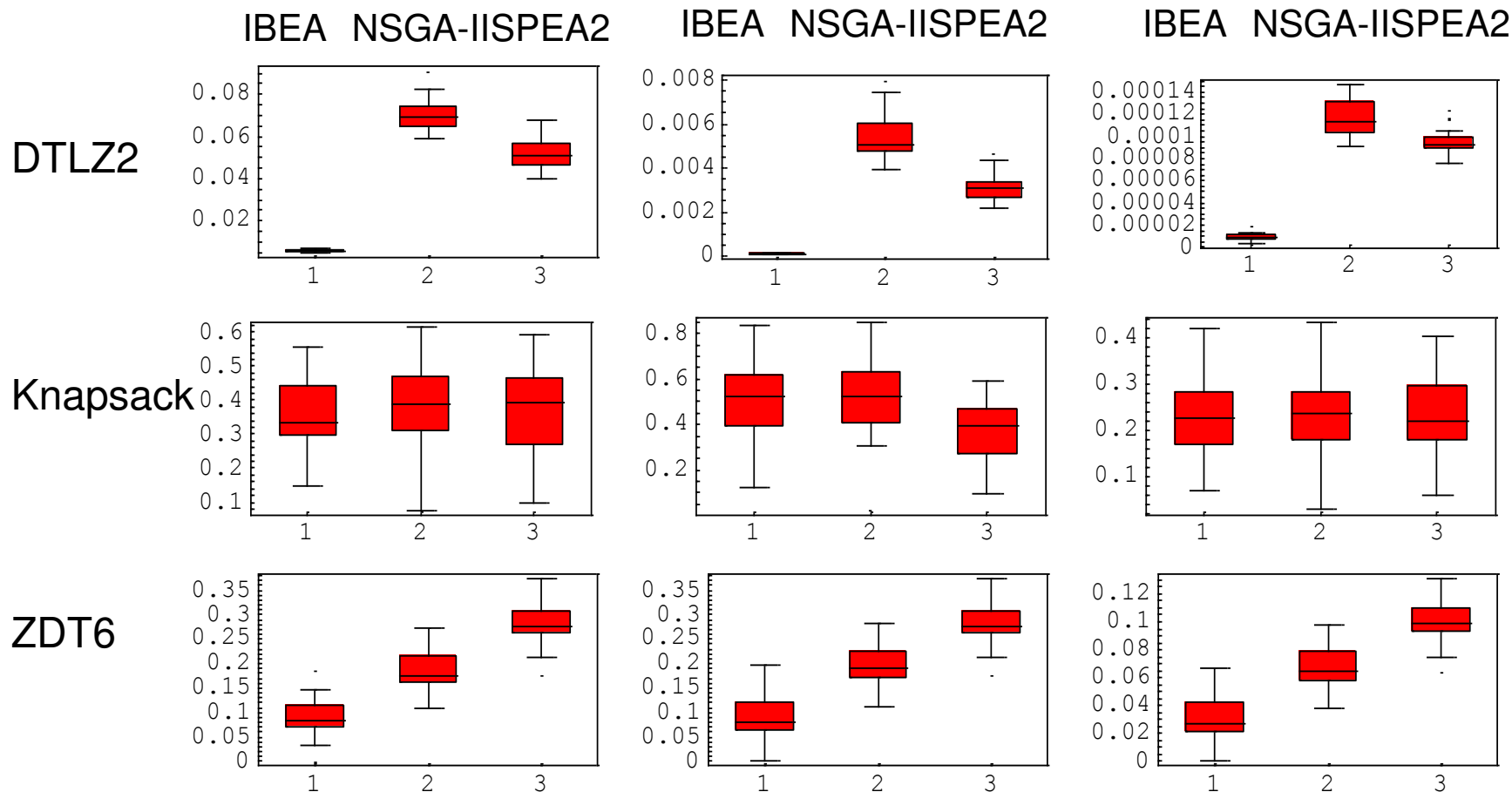


Example: Box Plots

epsilon indicator

hypervolume

R indicator



Statistical Assessment (Kruskal Test)

ZDT6 Epsilon

is better
than

	IBEA	NSGA2	SPEA2
IBEA		~0 😊	~0 😊
NSGA2	1		~0 😊
SPEA2	1	1	

Overall p-value = $6.22079e-17$.
Null hypothesis rejected (alpha 0.05)

DTLZ2 R

is better
than

	IBEA	NSGA2	SPEA2
IBEA		~0 😊	~0 😊
NSGA2	1		1
SPEA2	1	~0 😊	

Overall p-value = $7.86834e-17$.
Null hypothesis rejected (alpha 0.05)

Knapsack/Hypervolume: H_0 = No significance of any differences

so what do we do within COCO?

*besides the average runtime attainment plots
in objective space*

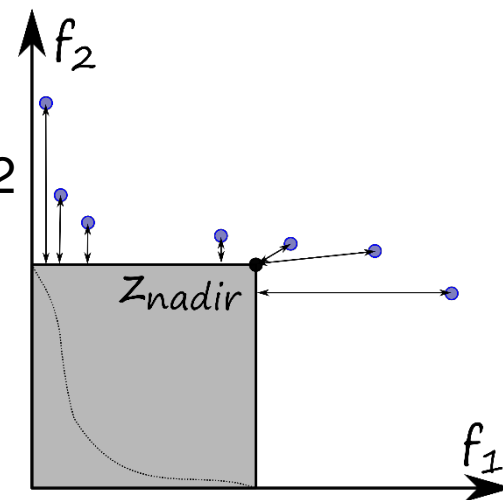
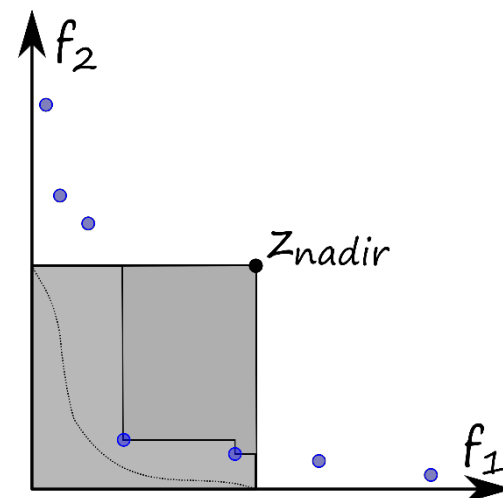
Bi-objective Performance Assessment

algorithm quality =

normalized* hypervolume (HV)
of all non-dominated solutions
if a point dominates nadir

closest normalized* negative
distance to region of interest $[0, 1]^2$
if no point dominates nadir

* such that ideal= $[0,0]$ and nadir= $[1,1]$



[Brockhoff et al. 2016]

Bi-objective Performance Assessment

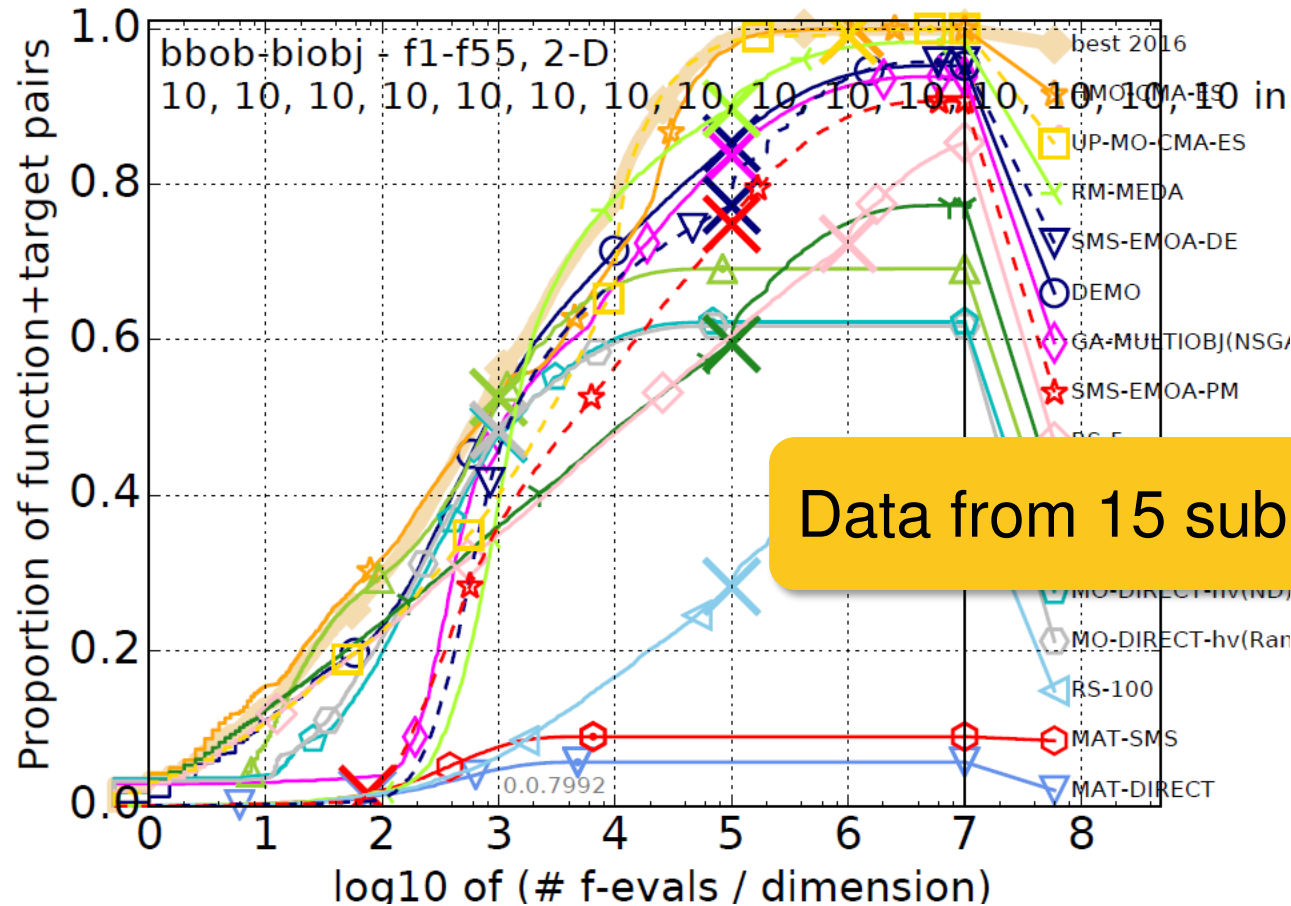
We measure runtimes to reach (HV indicator) targets:

- relative to a **reference set**, given as the best Pareto front approximation known (since exact Pareto set not known)
 - incl. all non-dominated points found by the 15 algos of BBOB-2016
- actual **absolute hypervolume targets** used are

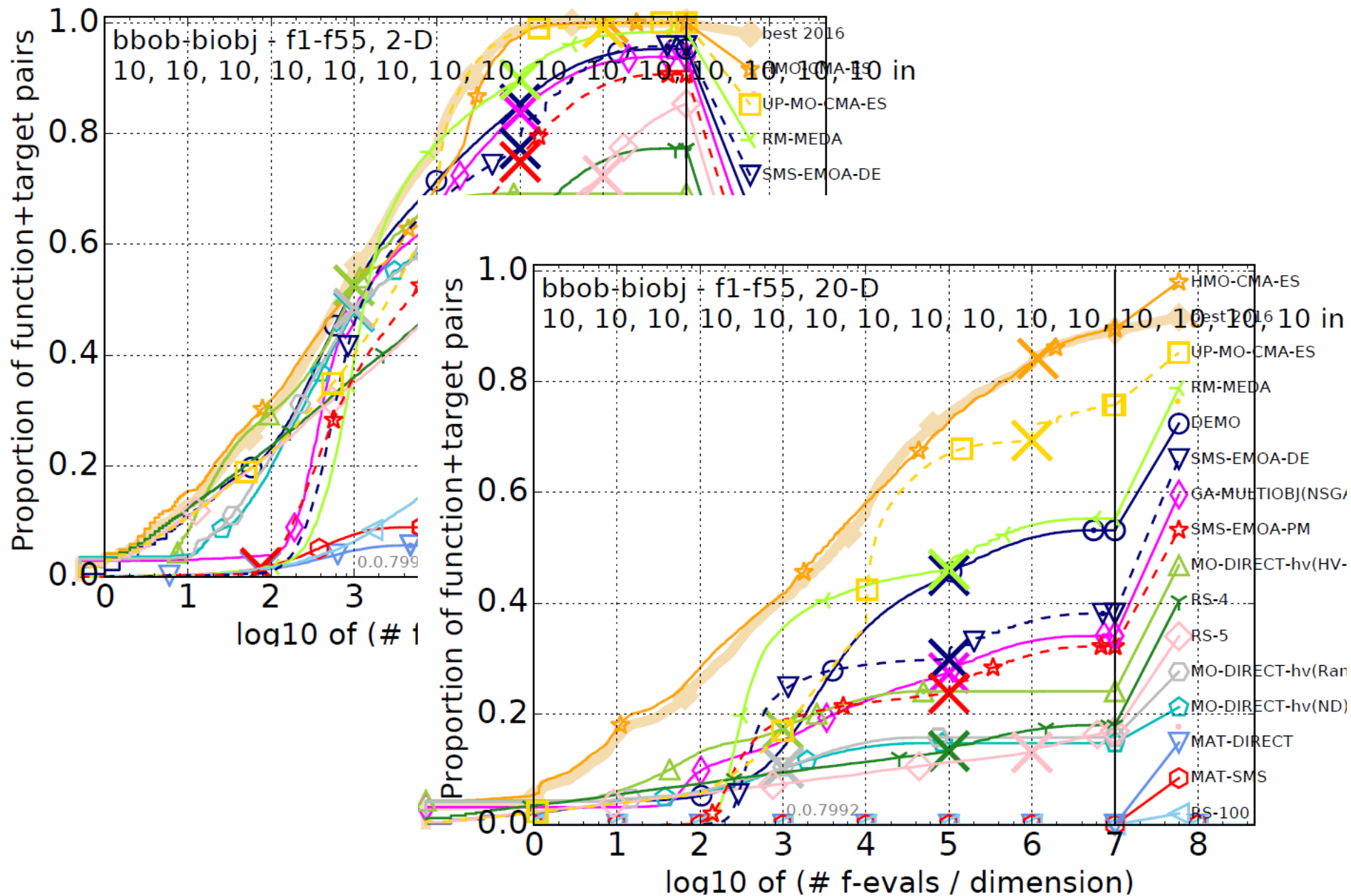
HV(refset) – targetprecision

with 58 **fixed** targetprecisions between 1 and -10^{-4} (same for all functions, dimensions, and instances) in the displays

Exemplary BBOB-2016 Results



Exemplary BBOB-2016 Results



State-of-the-art numerical benchmarking

- fixed target view preferred over fixed budget view
- ECDF plot of collected runtimes most important plot
 - allows for aggregation over targets, functions, and instances
 - but should not aggregate over dimension
 - dimension is "input parameter" to the algorithm
- multiobjective case can be handled the same way by using a quality indicator such as the hypervolume indicator

References

- [Brockhoff et al. 2016] D. Brockhoff, T. Tušar, D. Tušar, T. Wagner, N. Hansen, and A. Auger. Biobjective Performance Assessment with the COCO Platform. arXiv e-print arXiv:1605.01746v1, 2016.
- [Brockhoff et al. 2017] D. Brockhoff, A. Auger, N. Hansen, and T. Tusar. Quantitative Performance Assessment of Multiobjective Optimizers: The Average Runtime Attainment Function. In Conference on Evolutionary Multi-Criterion Optimization (EMO 2017), pages 103–119. Springer, 2017
- [Broyden et al. 1970] this work actually corresponds to a couple of papers:
C. G. Broyden. J Inst Maths Appl 6 (1970) 76.
R. Fletcher. Comp J 13 (1970) 317.
D. Goldfarb. Math. Comp 24 (1970) 23.
D. F. Shanno. Math Comp. 24 (1970) 647
- [Goldberg 1989] D. E. Goldberg. Genetic algorithms in search, optimization and machine learning. Addison-Wesley, Reading, MA. 1989.
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