A Practical Guide to Benchmarking and Experimentation

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- Installing IPython is *not* a prerequisite to follow the tutorial
- for downloading the material, see
  slides: http://www.cmap.polytechnique.fr/~nikolaus.hansen/benchmarking-and-experimentation-gecco17-slides.pdf
  code: http://www.cmap.polytechnique.fr/~nikolaus.hansen/benchmarking-and-experimentation-gecco17-code.tar.gz
  at http://www.cmap.polytechnique.fr/~nikolaus.hansen/invitedtalks.html

Overview

- about experimentation (with demonstrations)

  making quick experiments, interpreting experiments,
  investigating scaling, parameter sweeps,
  invariance, repetitions, statistical significance…

- about benchmarking

  choosing test functions, performance measures,
  the problem of aggregation, invariance,
  a short introduction to the COCO platform…

Why Experimentation?

- The behaviour of many if not most interesting algorithms is
  - not amenable to a (full) theoretical analysis even when applied to simple problems

    calling for an alternative to theory for investigation
  - not fully comprehensible or even predictable without (extensive) empirical examinations

    even on simple problems
    comprehension is the main driving force for scientific progress
- Virtually all algorithms have parameters

  like most (physical/biological/…) models in science
  we rarely have explicit knowledge about the “right” choice
  this is a *big* obstacle in designing and benchmarking algorithms
- We are interested in solving *black-box* optimisation problems

  which may be “arbitrarily” complex

Scientific Experimentation

- What is the aim? *Answer a question*, ideally quickly and comprehensively

consider in advance what the question is and in which
way the experiment can answer the question

- do not (blindly) trust what one needs to rely on (code, claims, …) without *good* reasons

check/test “everything” yourselves, practice stress testing, boosts also understanding
one key element for success
Why Most Published Research Findings Are False [Ioannidis 2005]

- run *rather many than few* experiments, as there are many questions to answer, practice *online experimentation*

to run many experiments they must be *quick to implement and run*
develops a feeling for the effect of setup changes

- run any experiment at least twice

assuming that the outcome is stochastic
get an estimator of variation

- display: *the more* the better, *the better* the better

figures are *intuition pumps* (not only for presentation or publication)
it is hardly possible to overestimate the value of a good figure
data is the only way experimentation can help to answer questions, therefore look at them!

Scientific Experimentation

- don't make minimising CPU-time a primary objective

  avoid spending time in implementation details to tweak performance

- It is usually more important to know why algorithm A performs badly on function f, than to make A faster for unknown, unclear or trivial reasons

  mainly because an algorithm is applied to *unknown* functions
  and the "why" allows to predict the effect of design changes

- *Testing Heuristics: We Have it All Wrong* [Hooker 1995]

  "The emphasis on competition is fundamentally anti-intellectual and does not build the sort of insight that in the long run is conducive to more effective algorithms"

- there are many devils in the details, results or their interpretation may crucially depend on simple or intricate bugs or subtleties

  yet another reason to run many (slightly) different experiments
  check limit settings to give consistent results

- Invariance is a very powerful, almost indispensable tool

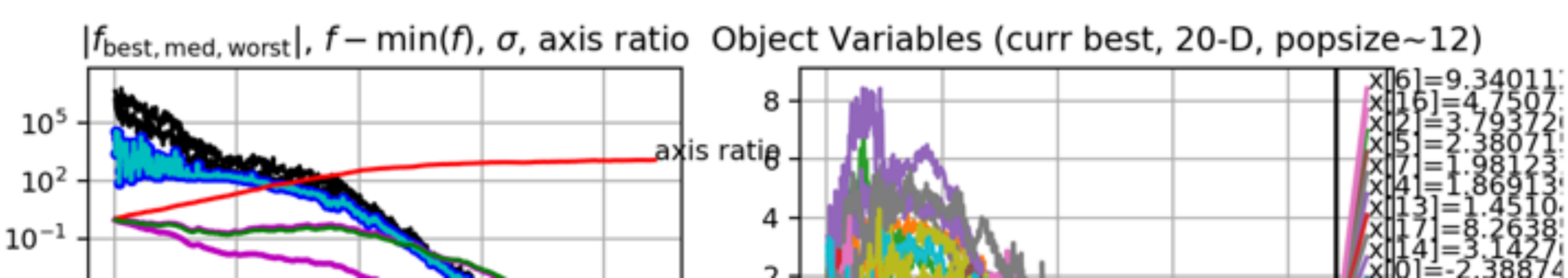
Jupyter IPython notebook

```
%pylab nbagg
import cma
cma.fmin(cma.ff.tablet, 20 * [1], 1);
```

```
Populating the interactive namespace from numpy and matplotlib
(6_w,12)-aCMA-ES (mu_w=3.7,w_1=40%) in dimension 20 (seed=344737, Wed Jul  5 16:09:44 2017)
Iterat #Fevals   function value  axis ratio  sigma  min&max std  t[m:s]
    1     12 2.637846492377813e+03 1.0e+00 9.49e-01  9e-01  1e+00 0:00.0
    2     24 3.858353384747645e+04 1.1e+00 9.13e-01  9e-01  9e-01 0:00.0
    3     36 1.589934793439056e+04 1.2e+00 8.94e-01  9e-01  9e-01 0:00.0
  100   1200 1.805167565570186e+02 6.6e+00 2.52e-01  6e-02  3e-01 0:00.1
  200   2400 9.260486860109009e+01 4.2e+01 2.79e-01  1e-02  4e-01 0:00.3
  300   3600 8.460045942108286e+00 2.0e+02 3.20e-01  4e-03  4e-01 0:00.4
  400   4800 5.352841113616880e-02 5.2e+02 4.71e-02  2e-04  5e-02 0:00.5
  500   6000 1.169838413517761e-04 8.7e+02 2.61e-03  3e-06  2e-03 0:00.7
  600   7200 2.232682824828931e-08 9.9e+02 5.00e-05  4e-08  3e-05 0:00.8
  700   8400 1.483610308401096e-12 1.2e+03 4.61e-07  3e-10  2e-07 0:00.9
  736   8832 2.696542797455203e-14 1.2e+03 1.03e-07  5e-11  5e-08 0:01.0
termination on tolfun=1e-11 (Wed Jul  5 16:09:46 2017)
final/bestever f-value = 1.422957e-14 1.422957e-14
incumbent solution: [ -1.01044748e-11  -3.22608195e-08  -8.75163241e-10  -3.66834969e-08
   2.35485309e-08  -9.59521093e-10   4.23137381e-08   6.92049899e-09 ...]
std deviations: [  5.07976963e-11   4.52415829e-08   4.67529085e-08   4.36659472e-08
   4.04686177e-08   4.38294341e-08   4.65665203e-08   5.01580767e-08 ...]
```

```
cma.plot()
```

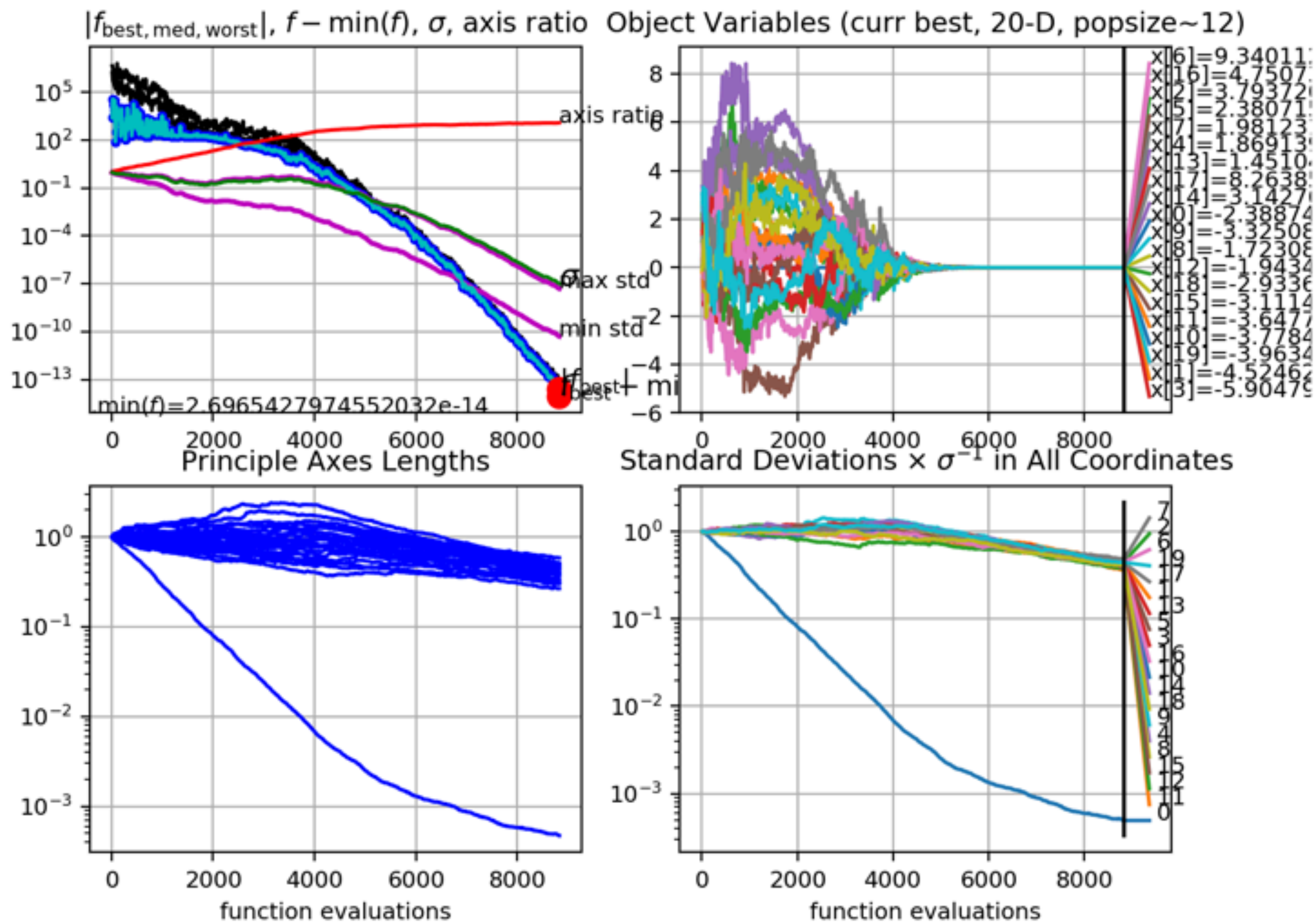
Figure 328



```
4.04686177e-08   4.38294341e-08   4.65665203e-08   5.01580767e-08 ...]
```

```
cma.plot()
```

Figure 328



Jupyter IPython notebook

```
# download&install anaconda python
# shell cmd "conda create" in case a different Python version is needed
# shell cmd "pip install cma" to install a CMA-ES module (or see github)
# shell cmd "jupyter-notebook" and click on compact-ga.ipynb
from __future__ import division, print_function
%pylab nbagg
```

```
Populating the interactive namespace from numpy and matplotlib
```

- Demonstration

Canonical GA: Experimentation Summary

Parameters: learning granularity K, boundaries on the mean

Methodology:

- display, display, display
- utility of empirical cumulative distribution functions, ECDF
- test on simple functions with (rather) predictable outcome

in particular the random function

Results:

- invariant behaviour on a random function points to an intrinsic scaling of the granularity parameter K with the dimension
- same invariance on onemax?
- sweep hints to optimal setting for K on onemax
- scaling with dimension on onemax is almost indistinguishable from *linear with dimension only for the above setting of K*

Invariance: onemax

- Assigning 0/1 is an "arbitrary" and "trivial" encoding choice
- Does not change the function "structure"
  - affine linear transformation $x_i \mapsto -x_i + 1$

    the same transformation in each transformed variable
    continuous domain: isotropic transformation
  - all level sets $\{x \mid f(x) = \text{const}\}$ have the same size (number of elements, same volume)
  - no variable dependencies
  - same neighbourhood
- Instead of 1 function, we now consider 2**n different but equivalent functions

  2**n is non-trivial, it is the size of the search space itself

Invariance

The grand aim of all science is to cover the greatest number of empirical facts by logical deduction from the smallest number of hypotheses or axioms.
— Albert Einstein

- Empirical performance results
  - from benchmark functions
  - from solved real world problems

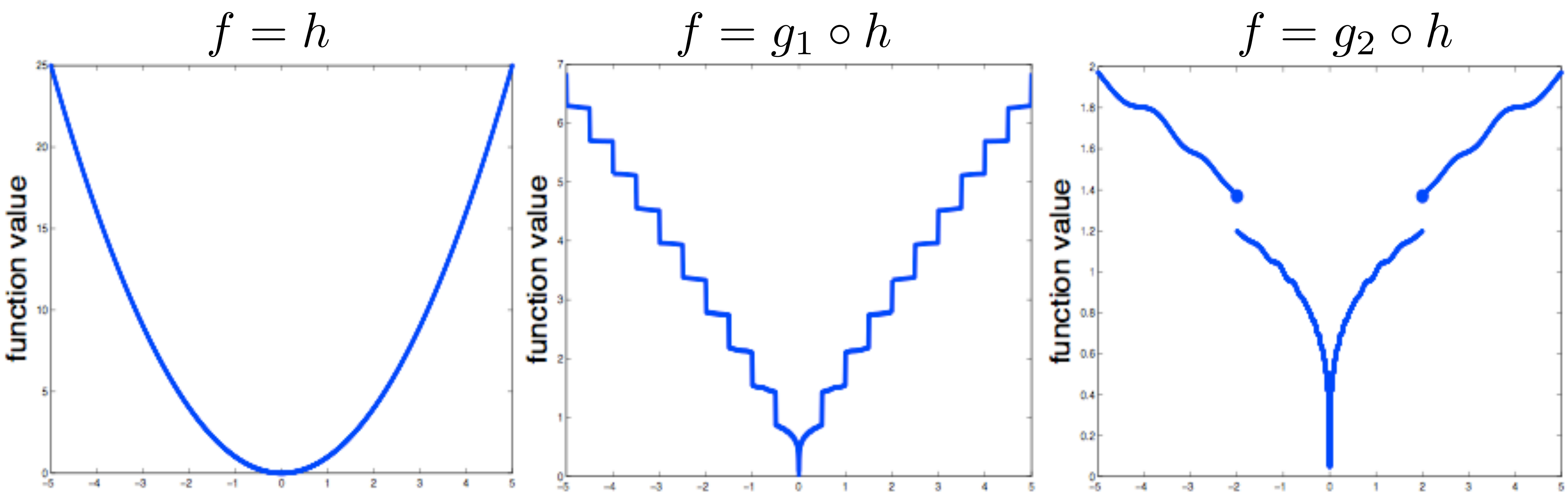
  are only useful if they do generalize to other problems

- Invariance is a strong non-empirical statement about generalization

  generalizing (identical) performance from a single function to a whole class of functions

Consequently, invariance is of greatest importance for the assessment of search algorithms.

Invariance Under Order Preserving Transformations



Three functions belonging to the same equivalence class

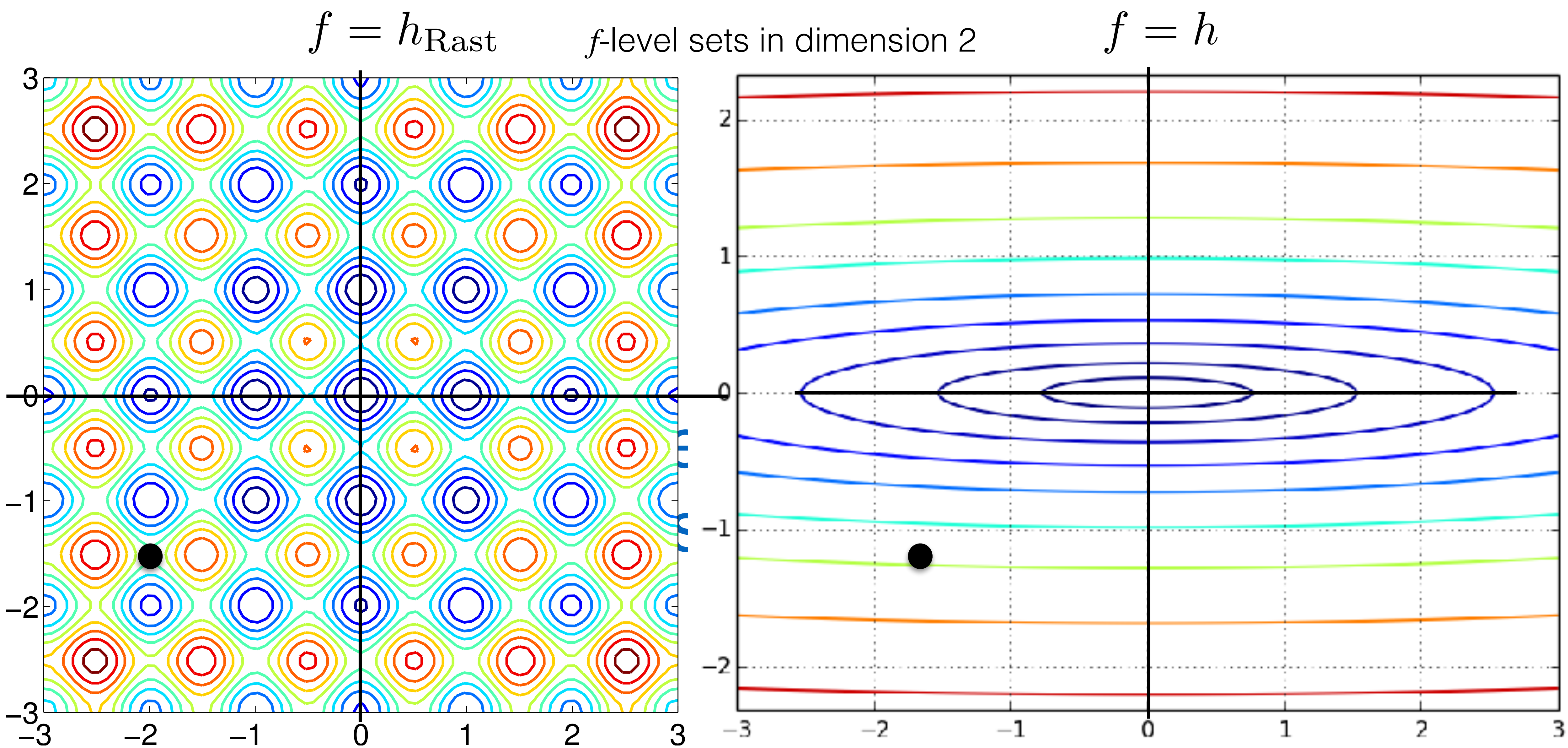
A *function-value free search algorithm* is invariant under the transformation with any order preserving (strictly increasing) g.

Invariances make

- observations meaningful
- algorithms predictable and/or "robust"

as a rigorous notion of generalization

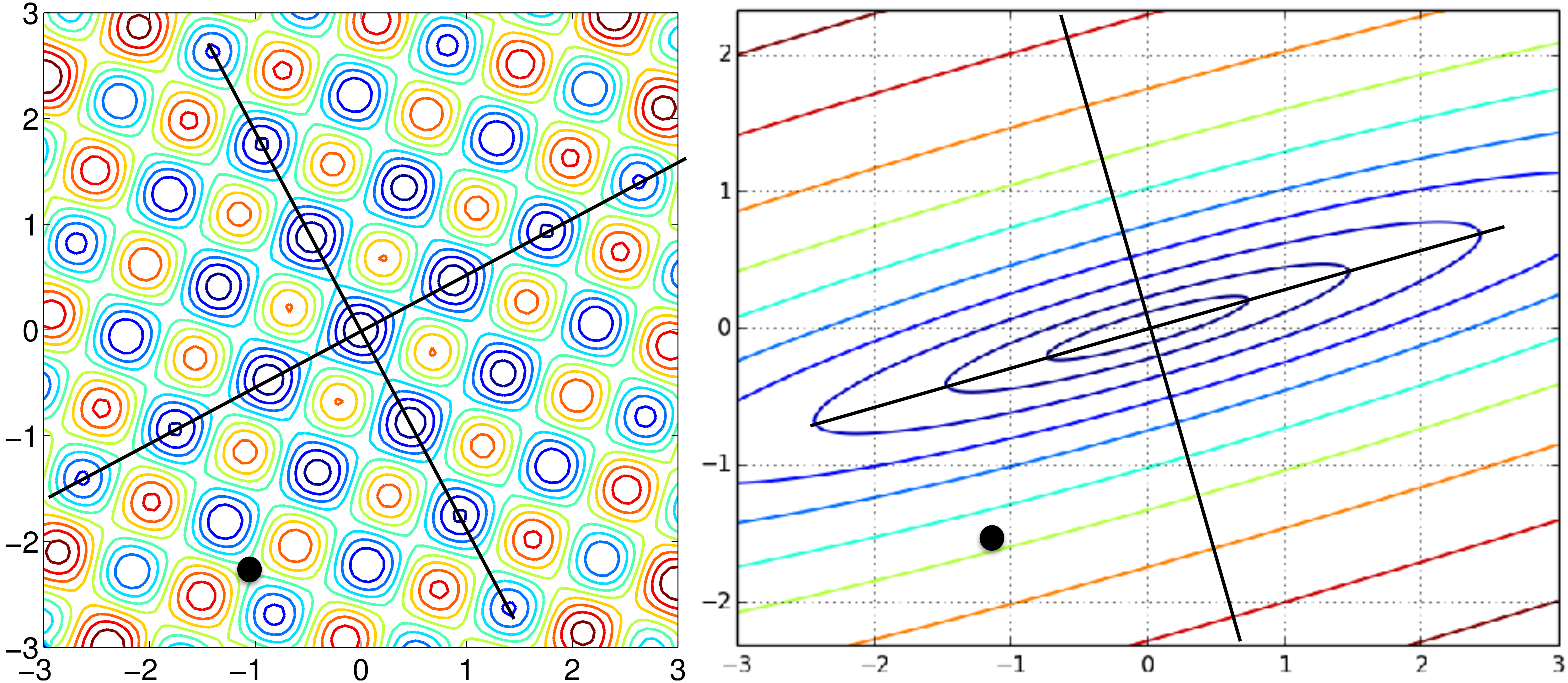
Invariance Under Rigid Search Space Transformations



for example, invariance under search space rotation
(separable vs non-separable)

Invariance Under Rigid Search Space Transformations

$f = h_{\mathrm{Rast}} \circ R$ f-level sets in dimension 2 $f = h \circ R$



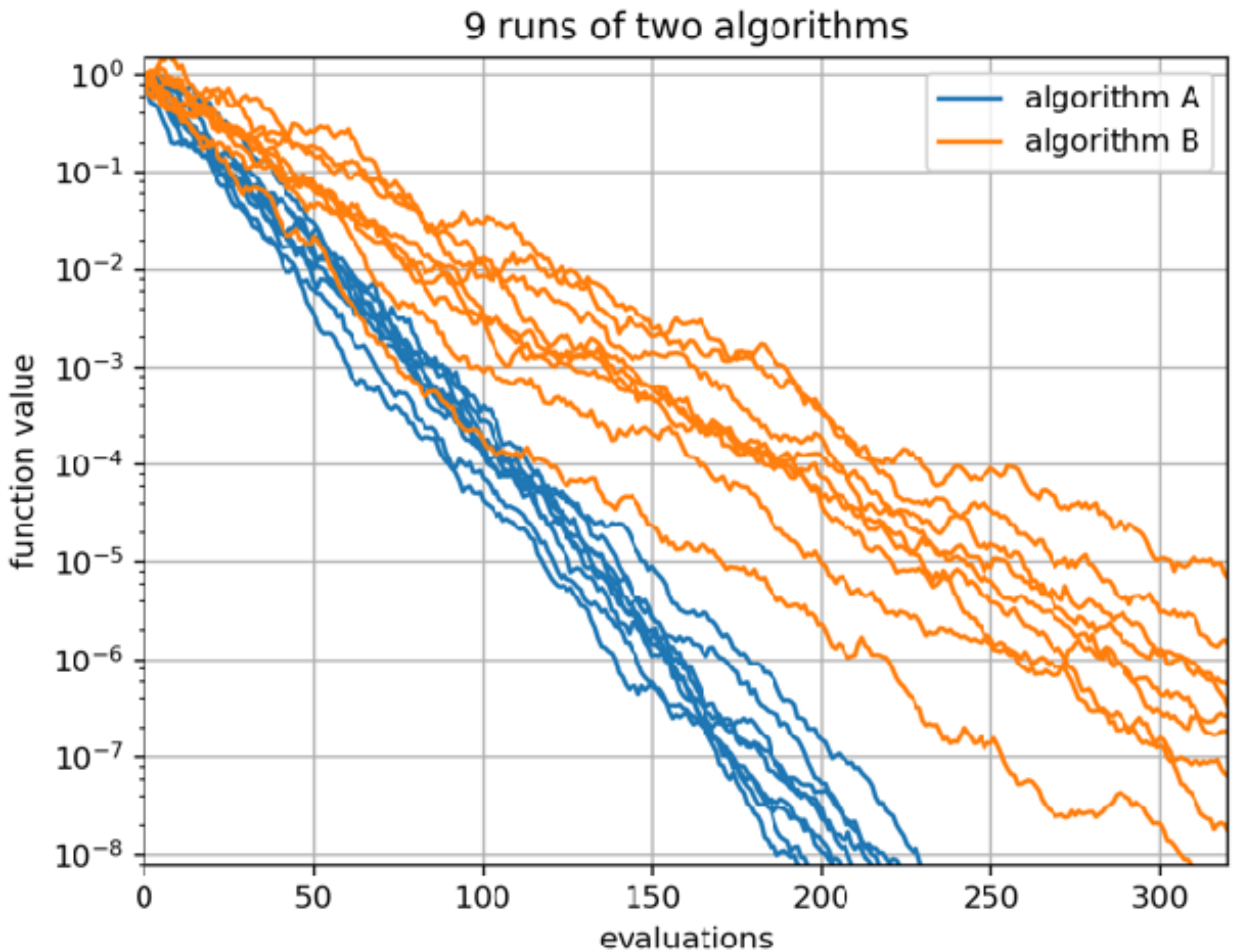
for example, invariance under search space rotation
(separable vs non-separable)

Statistical Analysis

“experimental results lacking proper statistical analysis must be considered anecdotal at best, or even wholly inaccurate”

— M. Wineberg

Agree or disagree?



Statistical Significance: General Prodecure

- first, check *the relevance* of the result, e.g., of the difference to be tested for statistical significance

  any ever so small difference can be made *statistically* significant with a simple trick,
  but *not made* significant in the sense of important or *meaningful*

- prefer “nonparametric” methods

  not based on a parametrised family of probability distributions

- p-value = significance level = probability of a false positive outcome

  smaller p-values are better
  <0.1% or <1% or <5% is usually considered significant

- for any found/observed p-value, *fewer data are better*

  to achieve the same p-value with fewer data the *between*-difference must be larger than the *within*-variation

Statistical Significance: Methods

- use the rank-sum test (aka Wilcoxon or Mann-Whitney U test)
  - Assumption: all observations (data values) are independent

    the lack of necessary preconditions is the main reason to use the rank-sum test
    yet, the test is nearly as efficient as the t-test which requires normal distributions

  - Null hypothesis: $\Pr(x < y) = \Pr(y < x)$

    the probability to be greater or smaller (better or worse) is the same

  - Procedure: compute the sum of ranks in the ranking of all (combined) data values

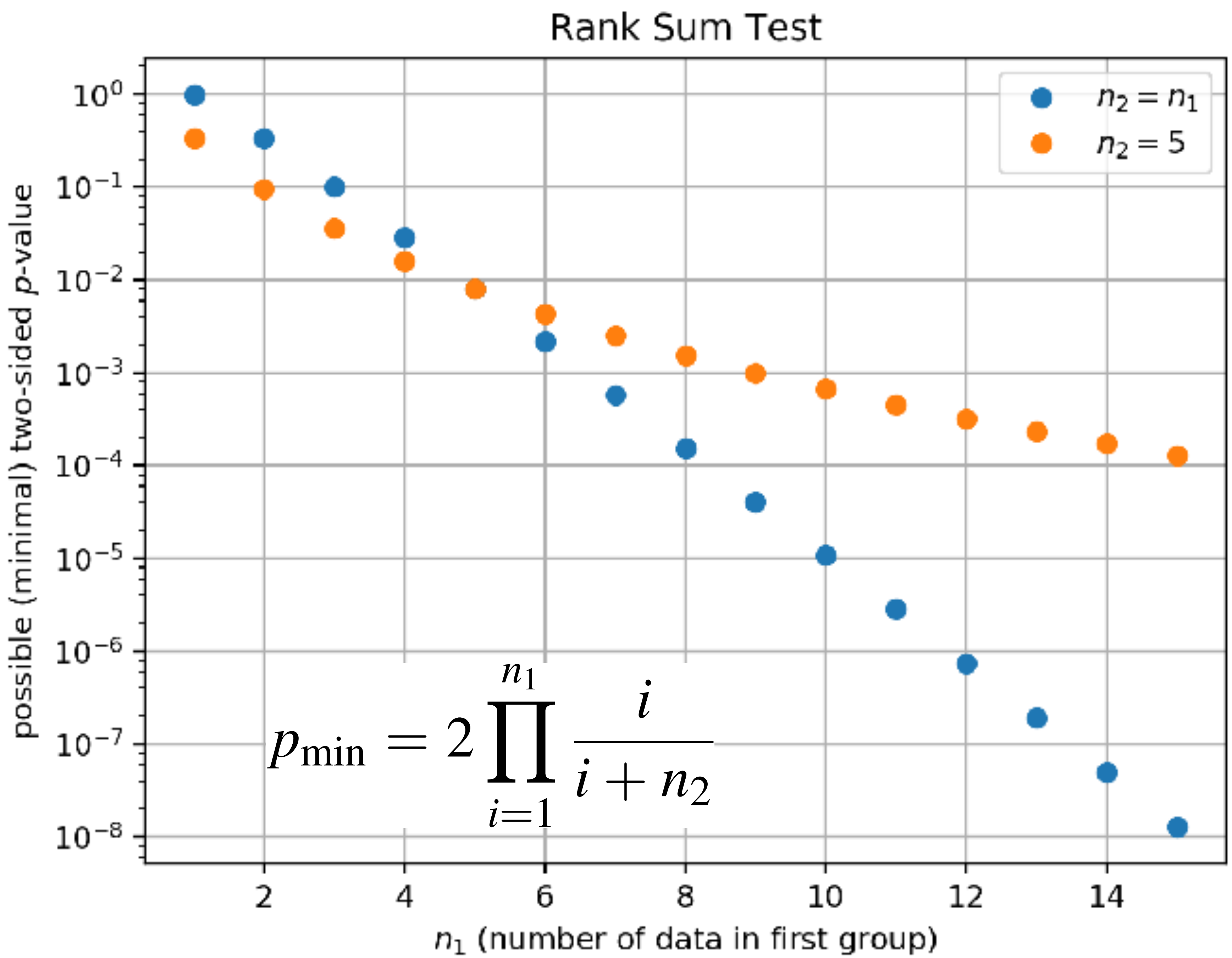
  - Outcome: a p-value

    the probability that this or a more extreme data set was generated under the null hypothesis
    the probability to *mistakenly* reject the null hypothesis

  - How many data do we need (two groups)? Five per group may suffice, *nine is plenty*.

    minimum number of data to possibly get two-sided
    $p < 1\%$: 5+5 or 4+6 or 3+9 or 2+19 or 1+200
    and $p < 5\%$: 4+4 or 3+5 or 2+8 or 1+40

Statistical Significance: How many data do we need?



$$p_{\min} = 2 \prod_{i=1}^{n_1} \frac{i}{i + n_2}$$

- observation: adding 2 data points in each group gives one additional order of magnitude

- use the Bonferroni correction for multiple tests

simple and conservative: multiply the computed p-value by the number of tests

Using Theory

“In the course of your work, you will from time to time encounter the situation where the facts and the theory do not coincide. In such circumstances, young gentlemen, it is my earnest advice to respect the facts.”

— Igor Sikorsky, airplane and helicopter designer

Agree or disagree?

Using Theory in Experimentation

- debugging / consistency checks

  theory may tell us what we expect to see

- knowing the limits (optimal bounds)

  e.g., we cannot converge faster than optimal
  trying to improve becomes a waste of time

- shape our expectations and objectives

Benchmarking

- aim: *assess performance* of algorithms

- methodology: run an algorithm on a set of test functions and extract performance measures from the generated data

  choice of measure and aggregation

- display

  subtle changes can make a big difference (in impression)

- there are surprisingly many devils in the details

Why do we want to measure performance?

- compare algorithms (the obvious)

  ideally we want standardised comparisons

- regression test after (small) changes

  as we may expect (small) changes in behaviour, conventional regression testing may not work

- algorithm selection (the obvious)

- understanding of algorithms

  very useful to improve algorithms
  non-benchmarking experimentation is often preferable

Measuring Performance

Empirically

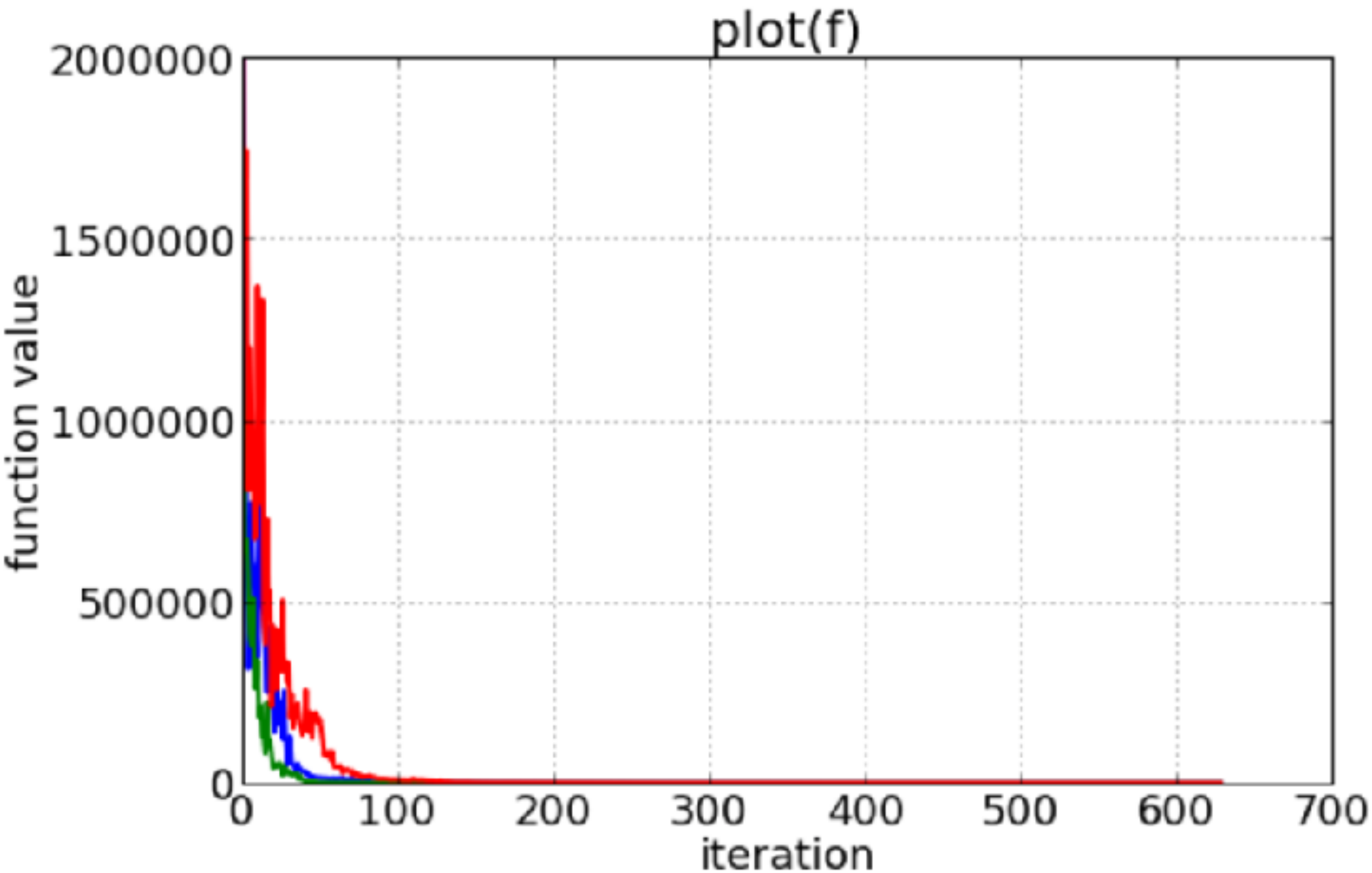
convergence graphs is all we have to start with

having the right presentation is important

too often neglected

the details are important

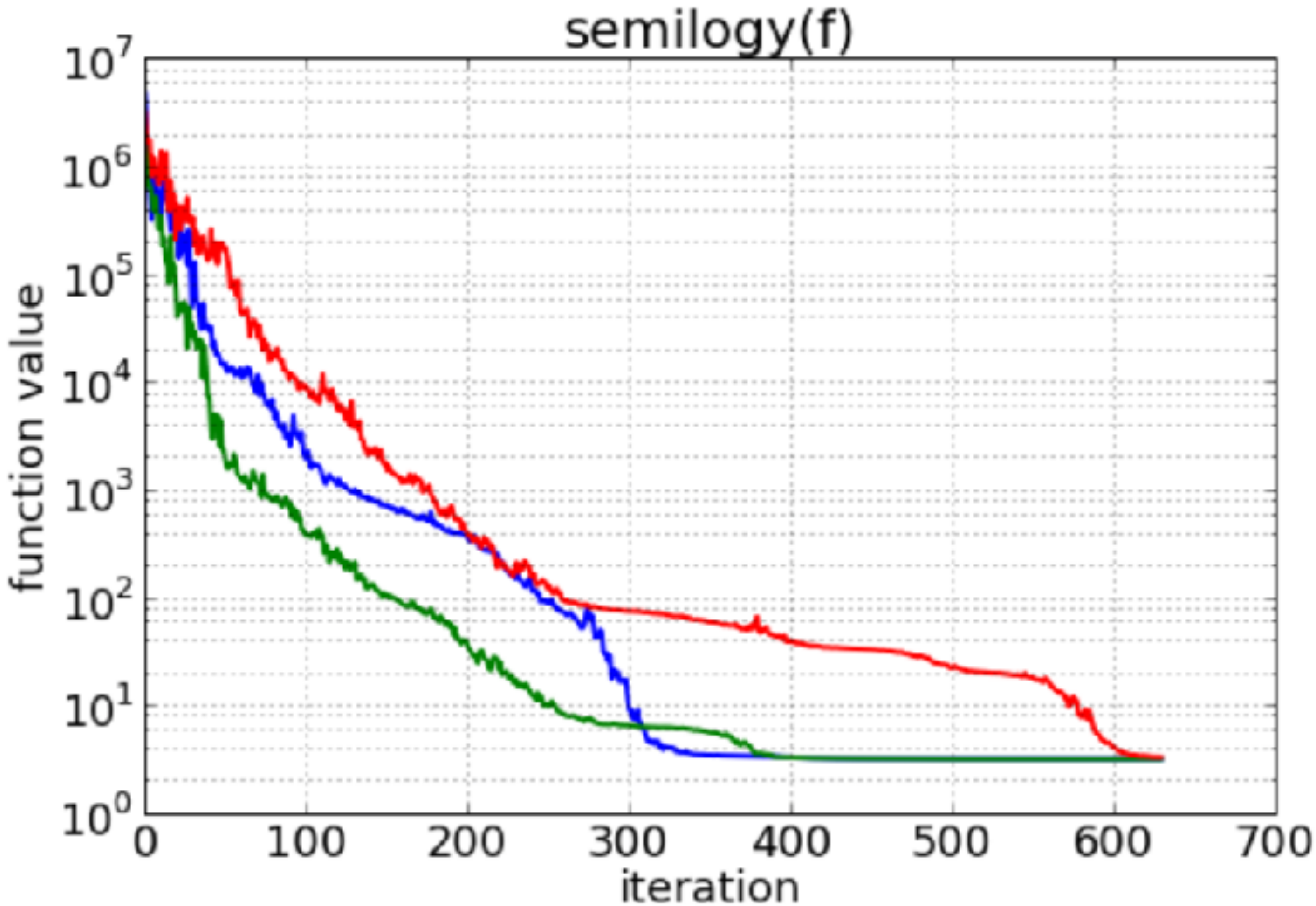
Displaying Three Runs



not like this (it's unfortunately a common picture)

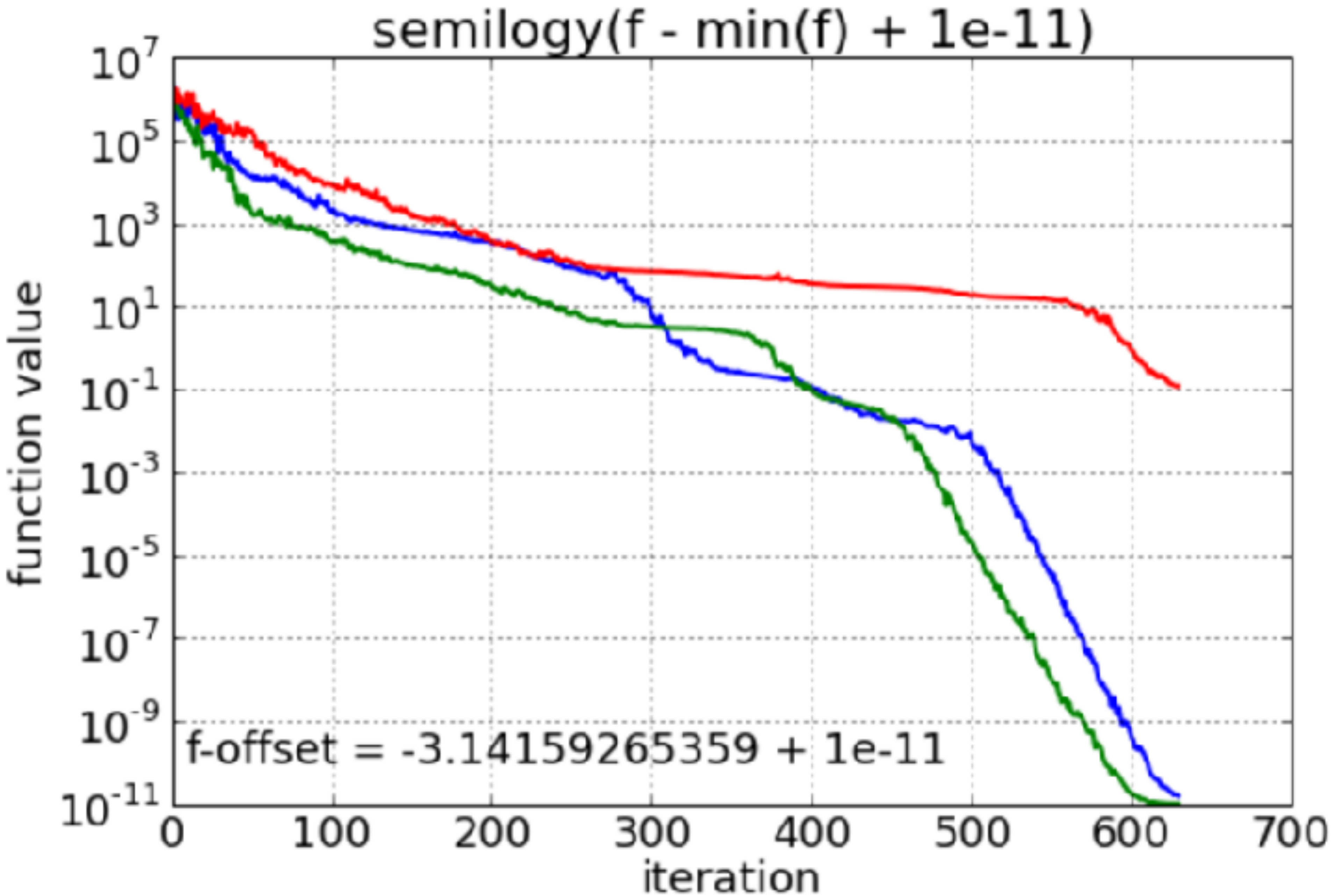
why not, what’s wrong?

Displaying Three Runs



better like this (shown are the same data), caveat: fails with negative f-values

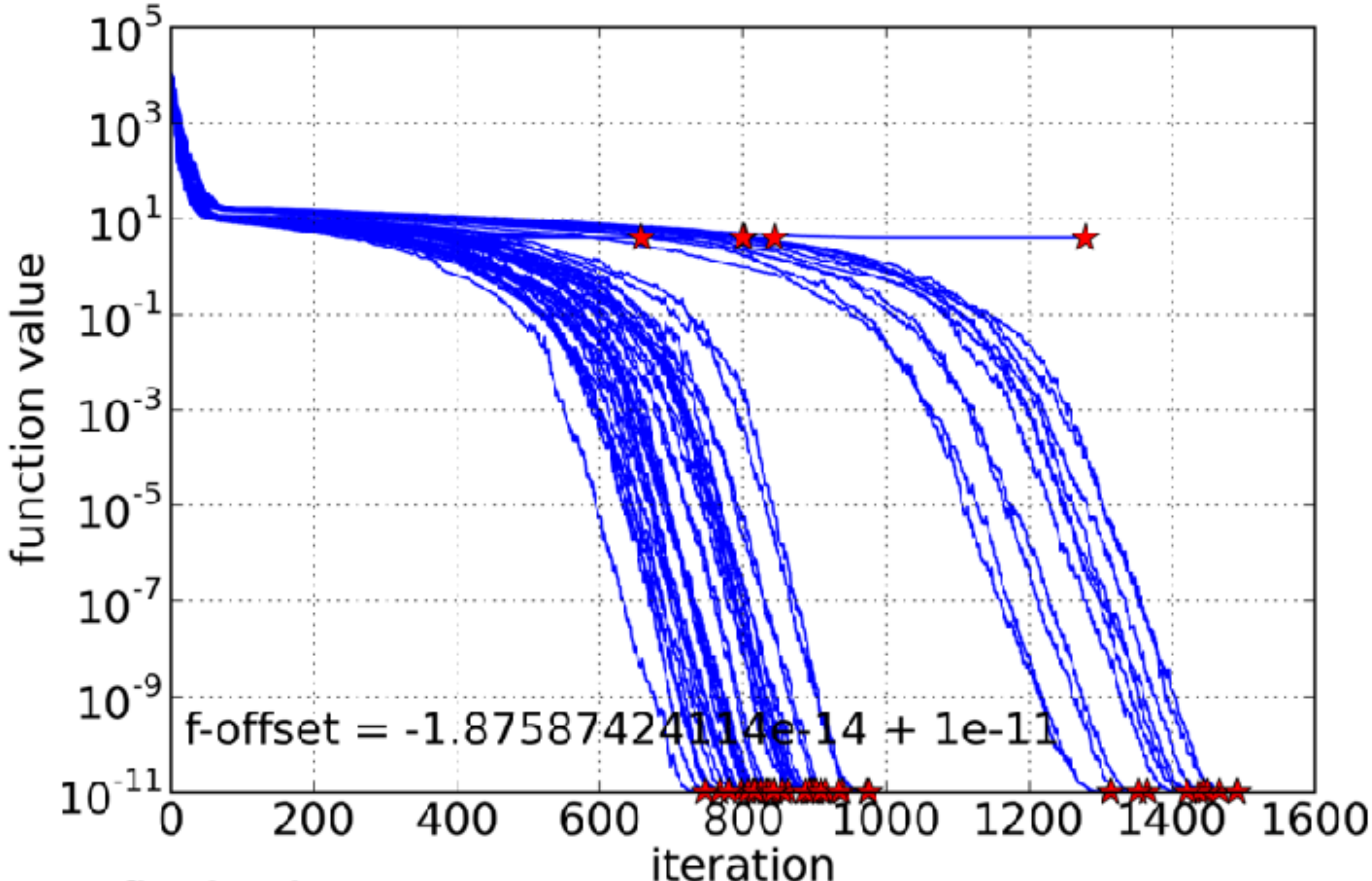
Displaying Three Runs



even better like this: subtract minimum value over all runs

Displaying 51 Runs

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



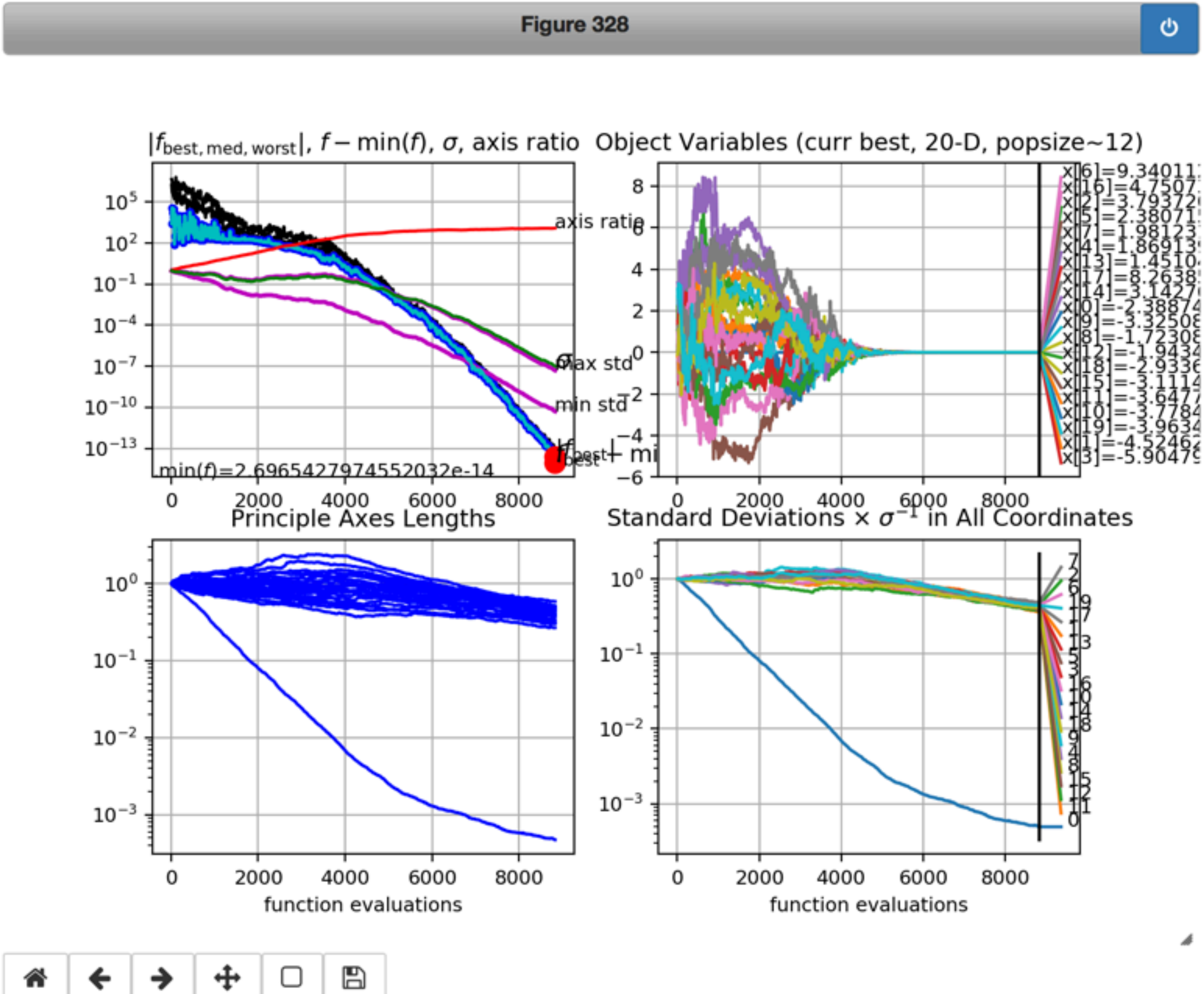
★ : final value

observation: three different "modes", which would be difficult to represent or recover in single statistics

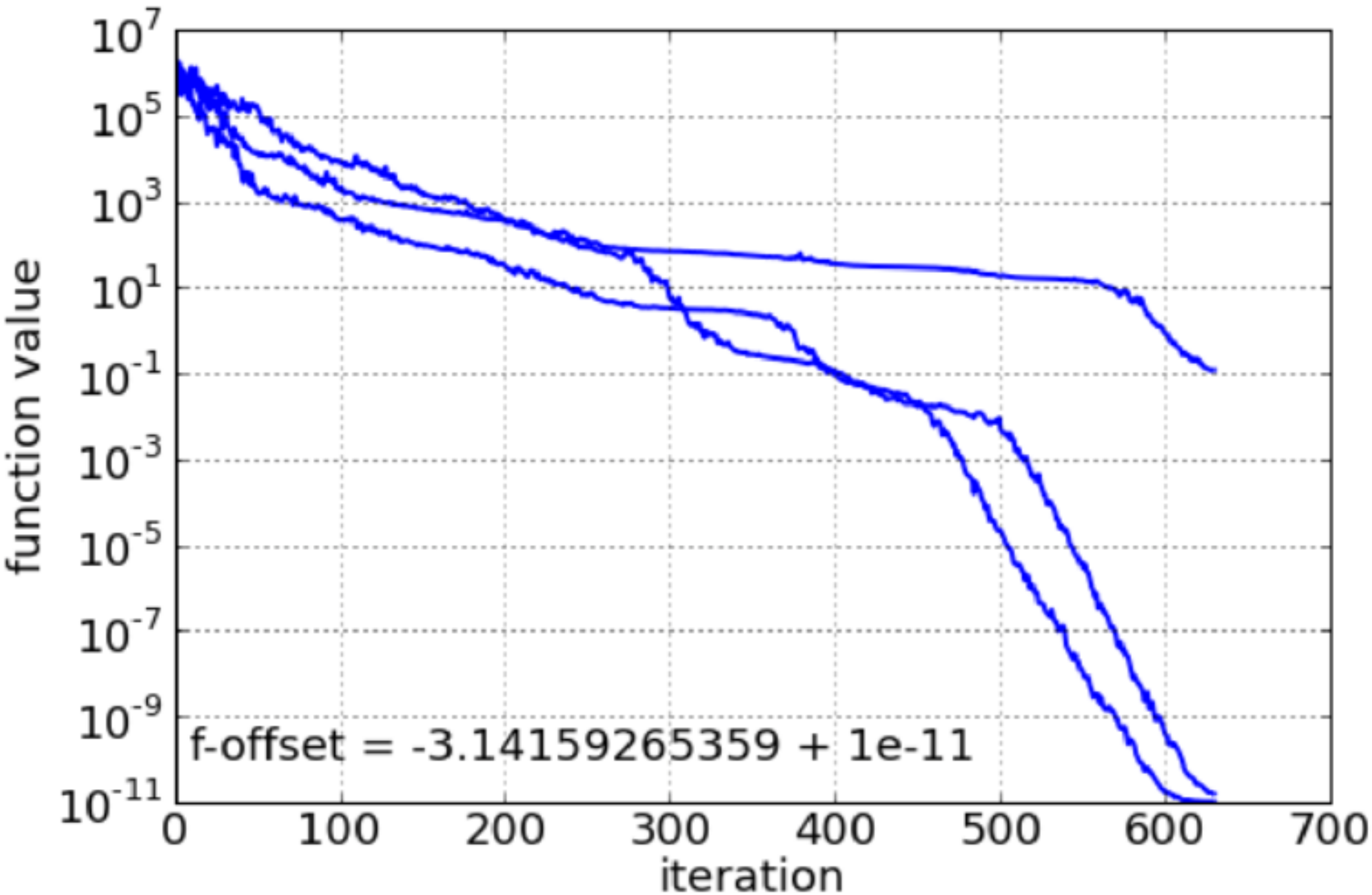
4.04686177e-08 4.38294341e-08 4.65665203e-08 5.01580767e-08 ...]

There is more to display than convergence graphs

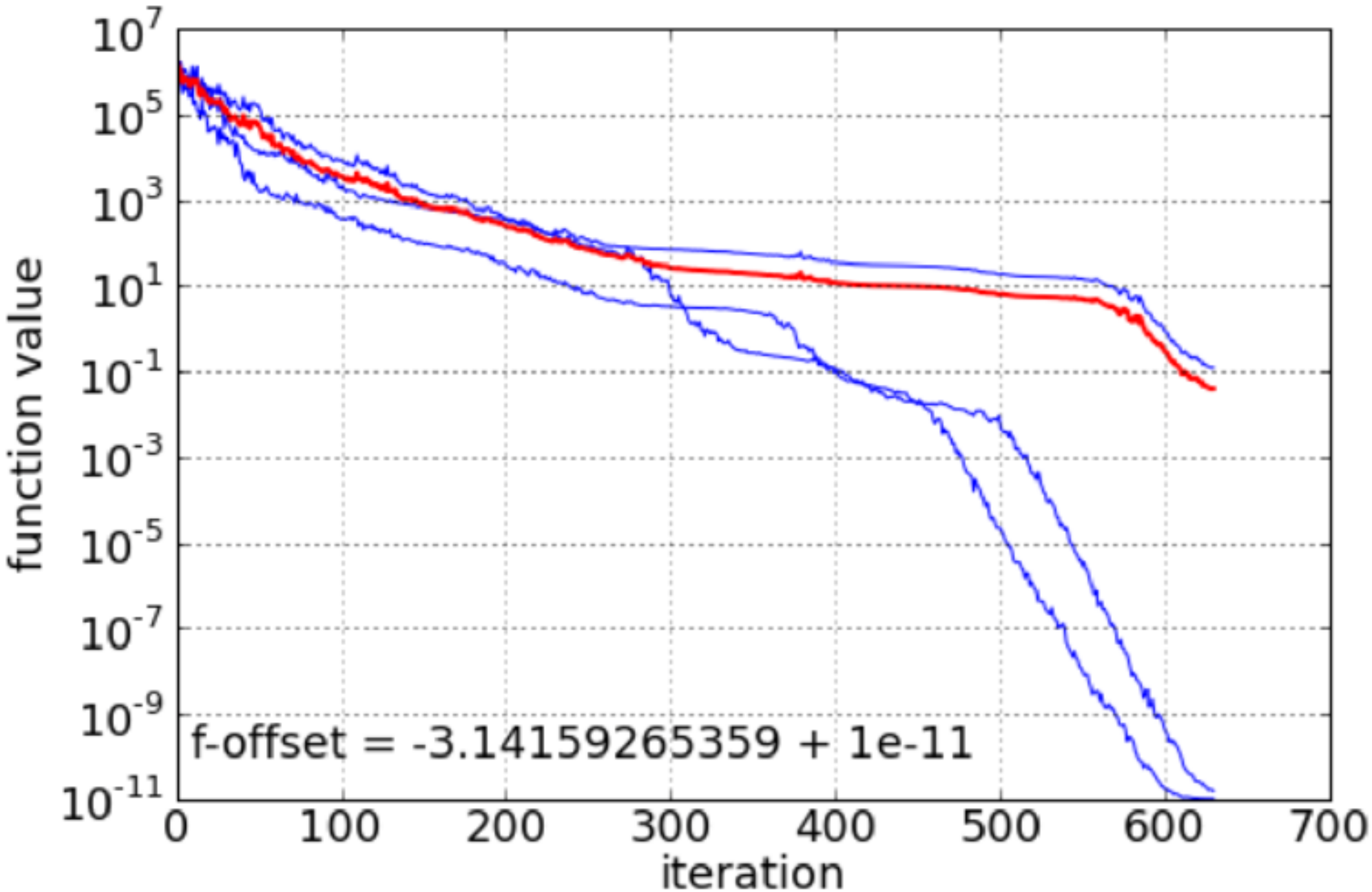
```
cma.plot()
```



Which Statistics?



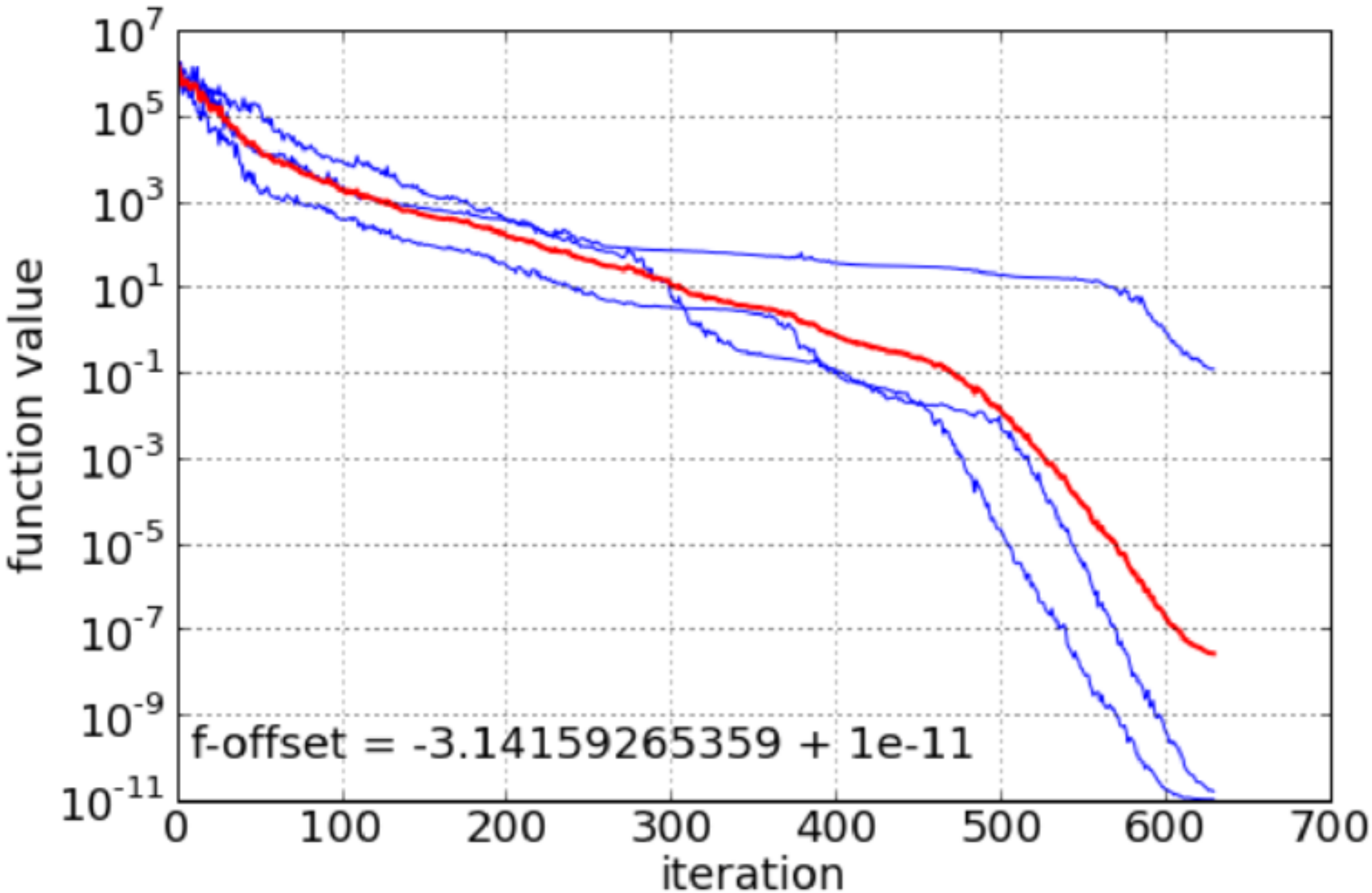
Which Statistics?



mean/average function value

- tends to emphasize large values

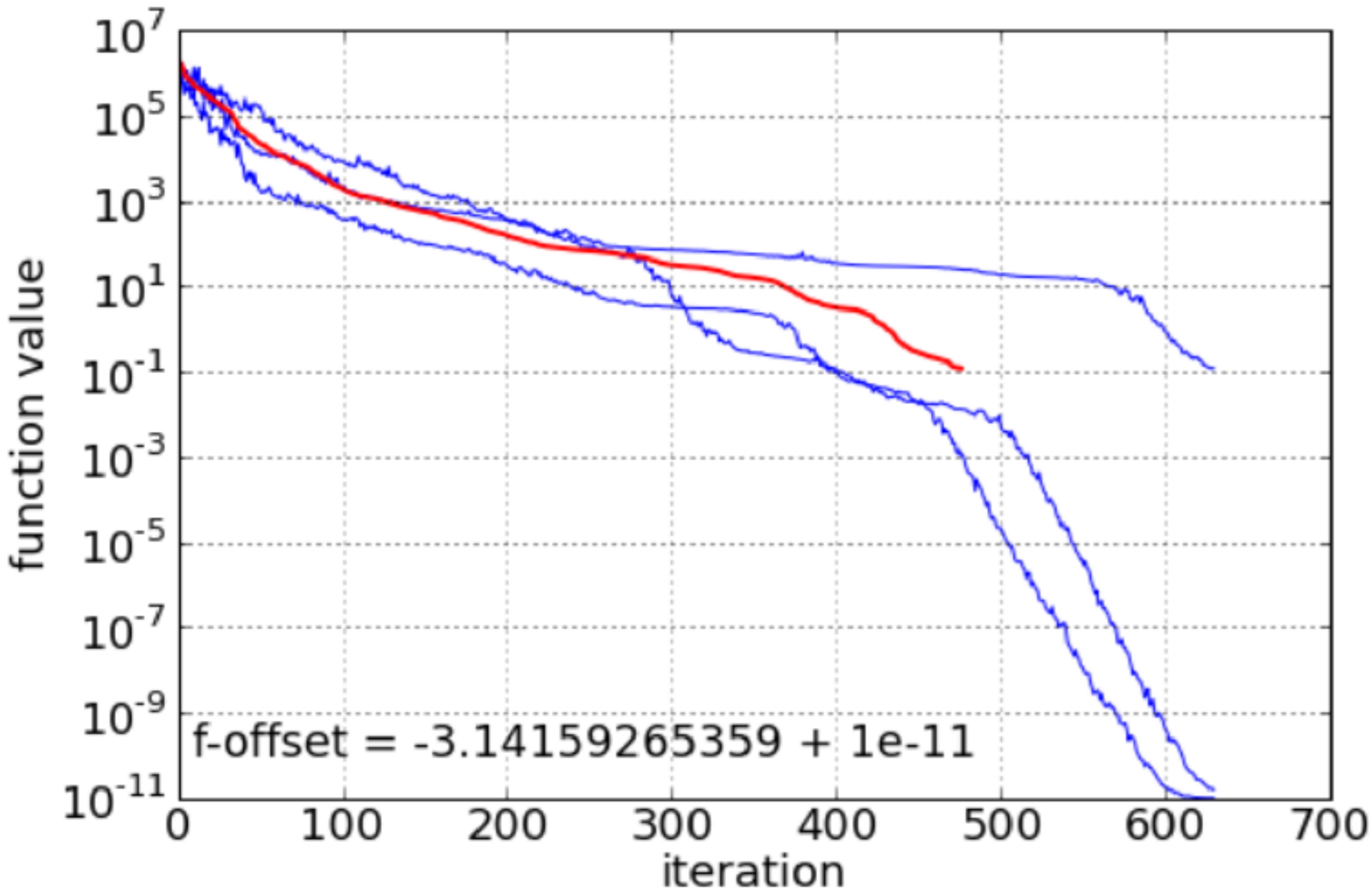
Which Statistics?



geometric average function value $\exp(\mathrm{mean_i}(\log(f_i)))$

- reflects "visual" average
- depends on offset

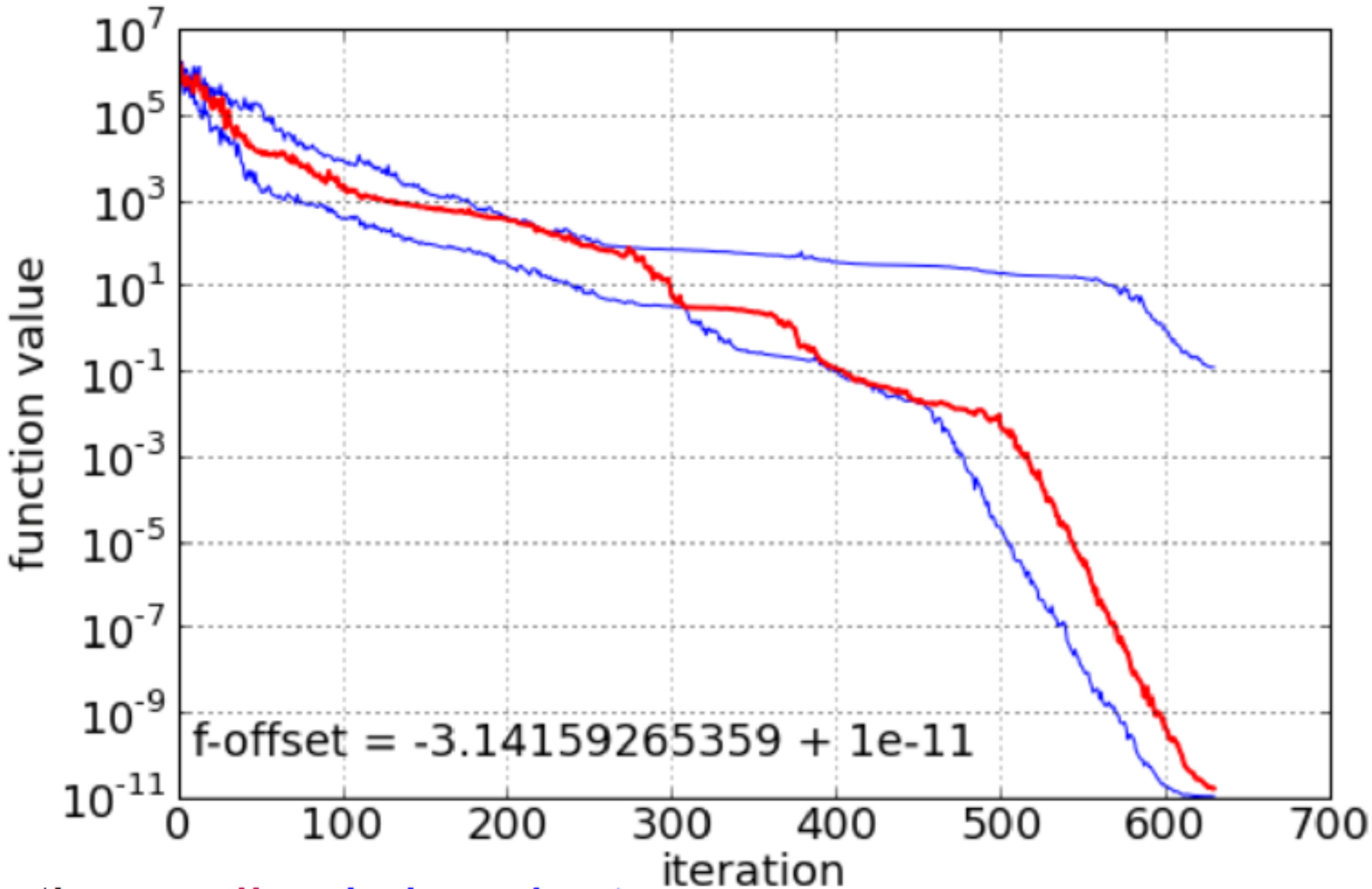
Which Statistics?



average iterations

- reflects "visual" average
- here: incomplete

Which Statistics?



the median is invariant

- 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

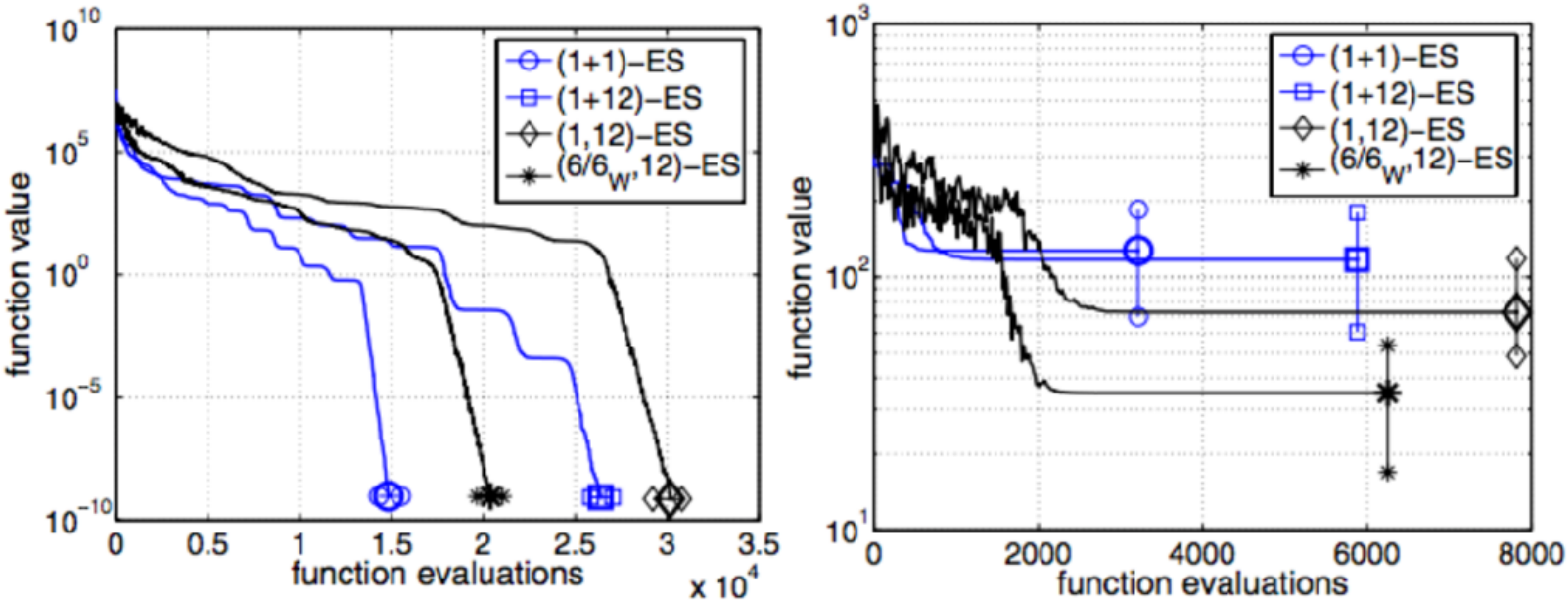
Implications

use the median as summary datum

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

unless there are good reasons for a different statistics

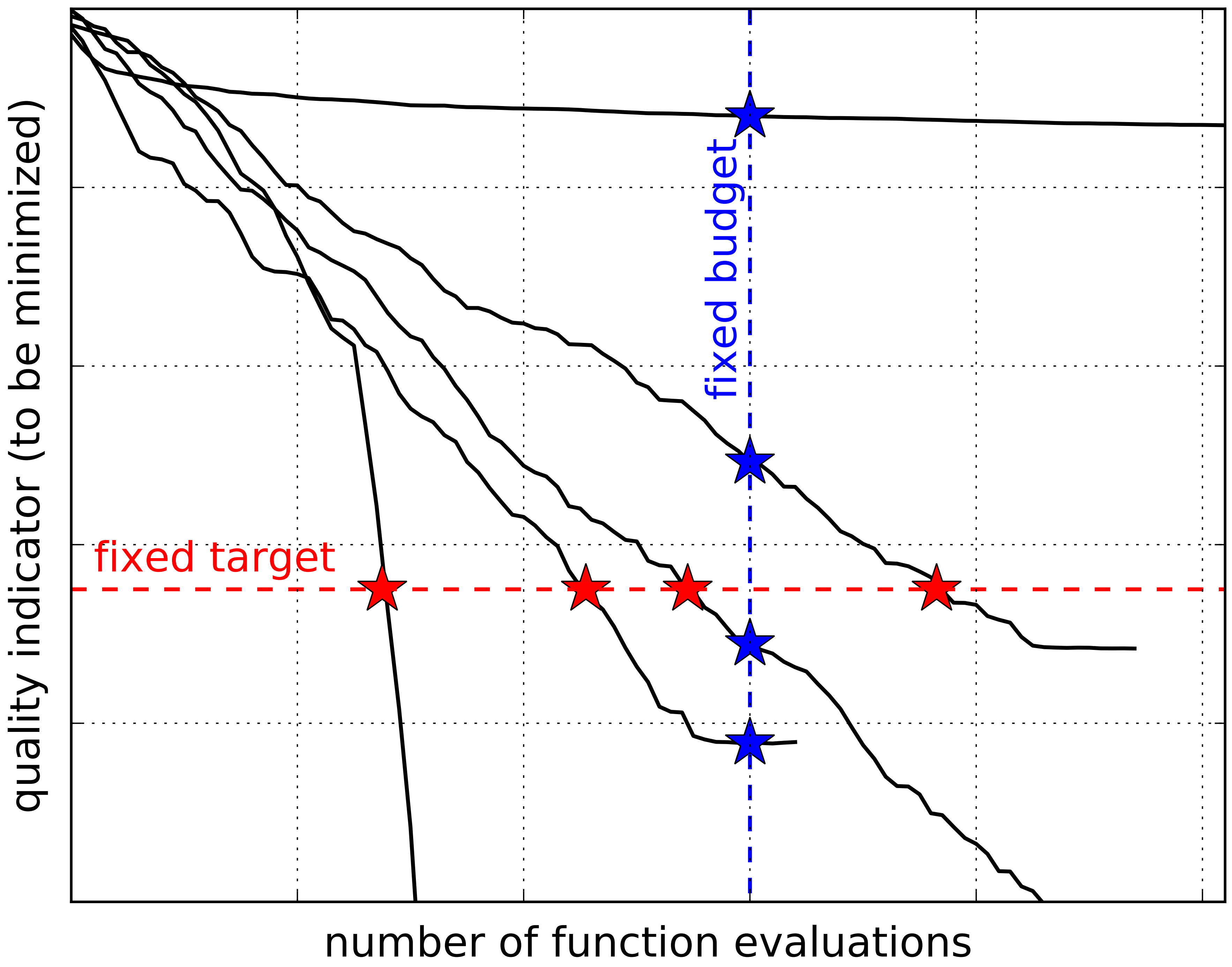
Examples



Comparison of 4 algorithms using the "median run" and the 90% central range of the final value on two different functions (Ellipsoid and Rastrigin)

caveat: this range display with simple error bars fails, if, e.g., 30% of all runs "converge"

Aggregation: Fixed Budget vs Fixed Target



- for aggregation we need comparable data
- missing data: problematic when most or all runs lead to missing data
  - fixed target approach misses out on bad results (we may correct for this)
  - fixed budget approach misses out on good results

Fixed Budget vs Fixed Target

Number of function evaluations are

- ***quantitatively*** comparable (on a ratio scale)
  ratio scale: “A is 3.5 times faster than B” (A/B = 1/3.5) is meaningful
- as measurement independent of the function
  time remains the same time

=> fixed target

Performance Measures for Evaluation

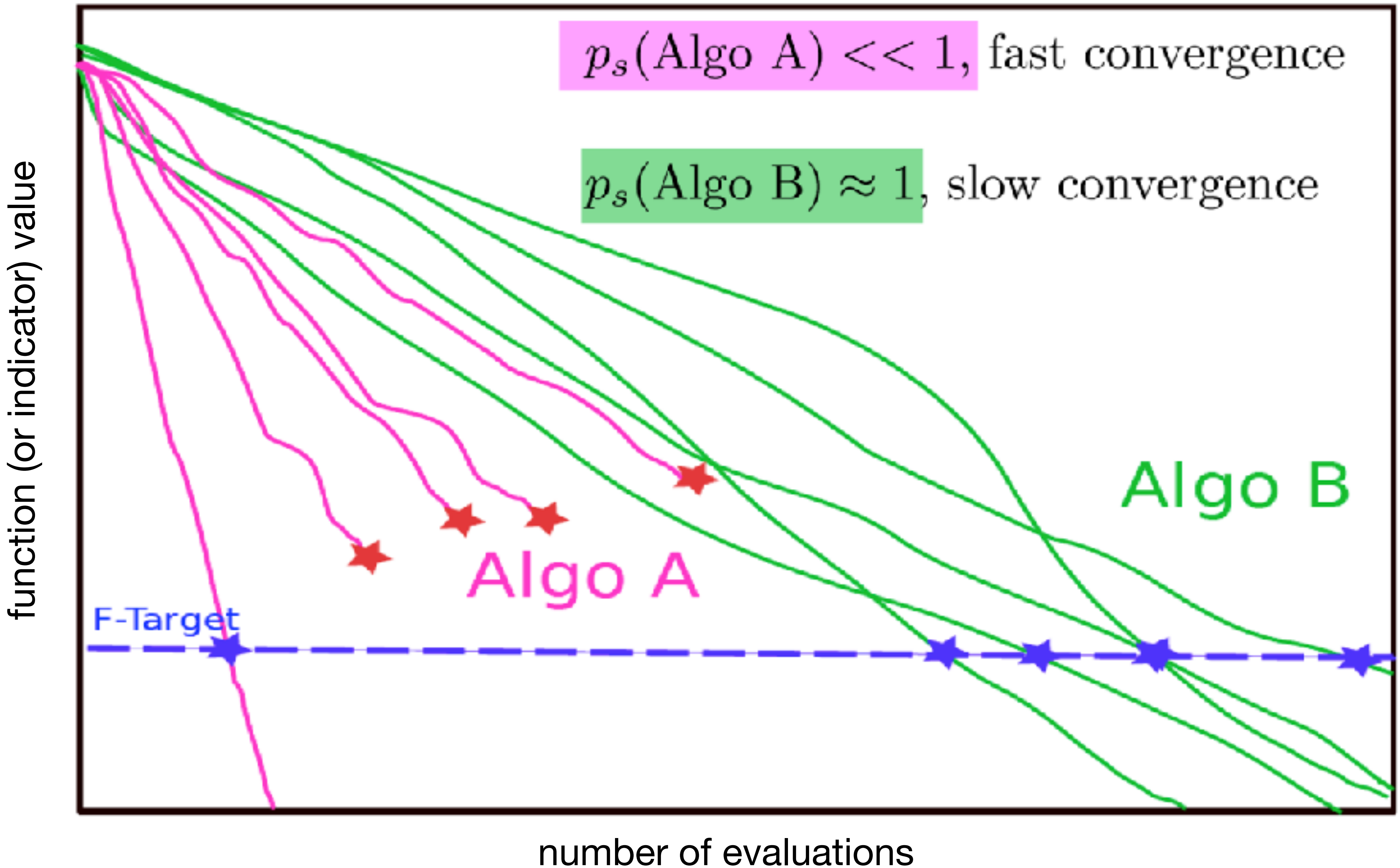
Generally, a performance measure should be

- quantitative on the ratio scale (highest possible)
  - "algorithm A is two *times* better than algorithm B" is a meaningful statement
- can 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, hence we use fixed targets

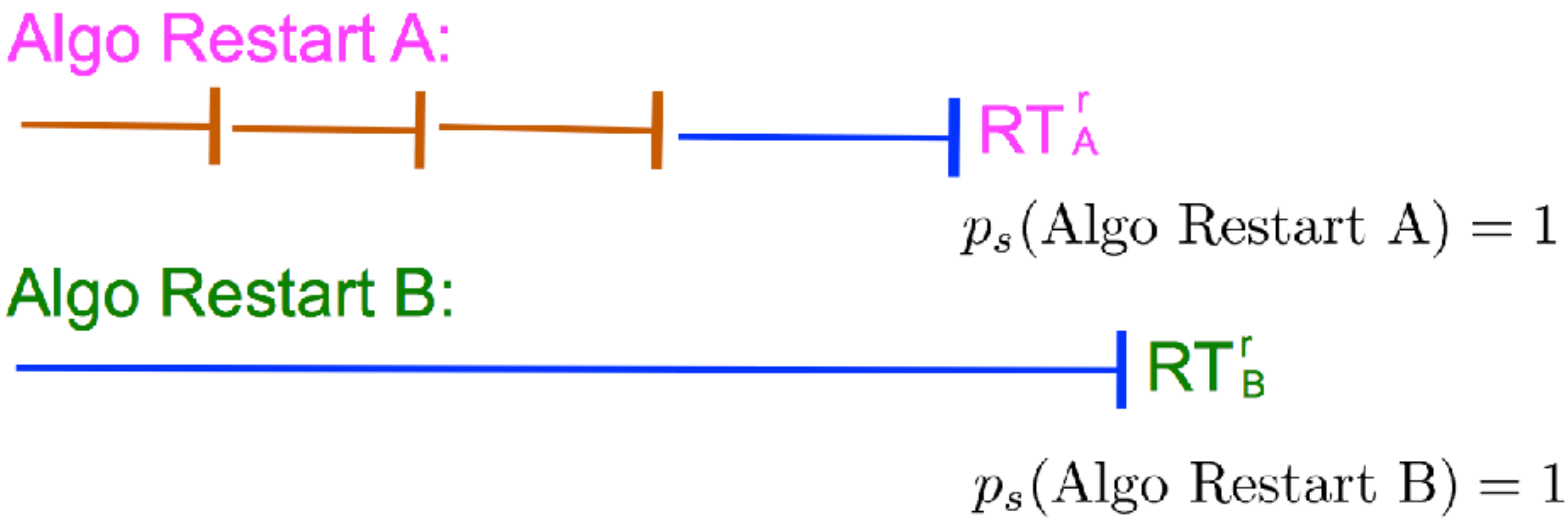
The Problem of Missing Values

how can we compare the following two algorithms?



The Problem of Missing Values

Consider simulated (artificial) restarts using the given independent runs



The Problem of Missing Values

The expected runtime (ERT, aka SP2, aRT) to hit a target value in #evaluations is computed (estimated) as:

$$\mathrm{ERT} = \frac{\#\text{evaluations(until to hit the target)}}{\#\text{successes}}$$

unsuccessful runs count (only) in the nominator

$$= \text{mean}(\text{evals}_{\text{succ}}) + \overbrace{\frac{N_{\text{unsucc}}}{N_{\text{succ}}}}^{\text{odds ratio}} \times \text{mean}(\text{evals}_{\text{unsucc}})$$

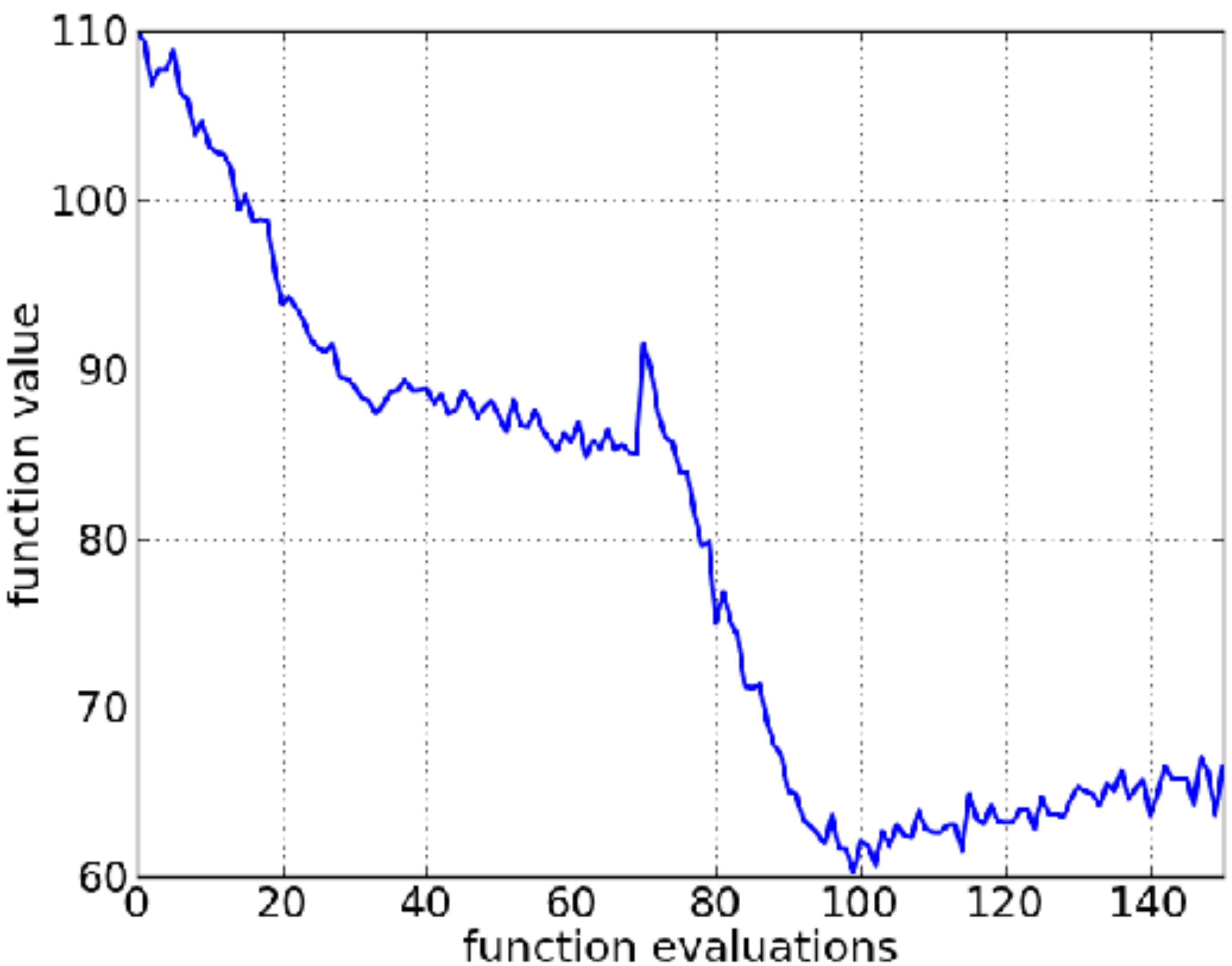
$$\approx \text{mean}(\text{evals}_{\text{succ}}) + \frac{N_{\text{unsucc}}}{N_{\text{succ}}} \times \text{mean}(\text{evals}_{\text{succ}})$$

$$= \frac{N_{\text{succ}} + N_{\text{unsucc}}}{N_{\text{succ}}} \times \text{mean}(\text{evals}_{\text{succ}})$$

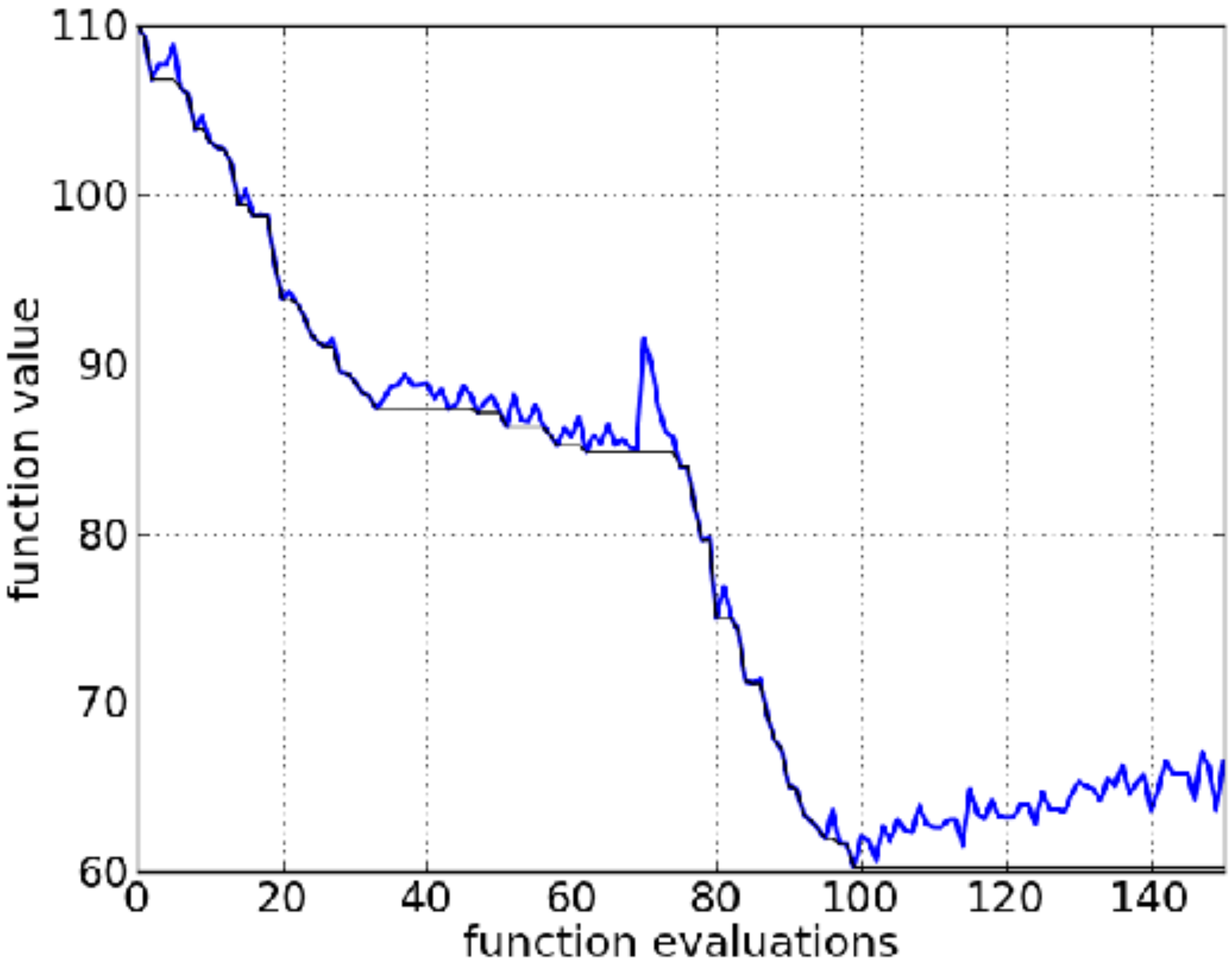
defined (only) for #successes > 0. The last two lines are aka Q-measure or SP1 (success performance).

ECDF

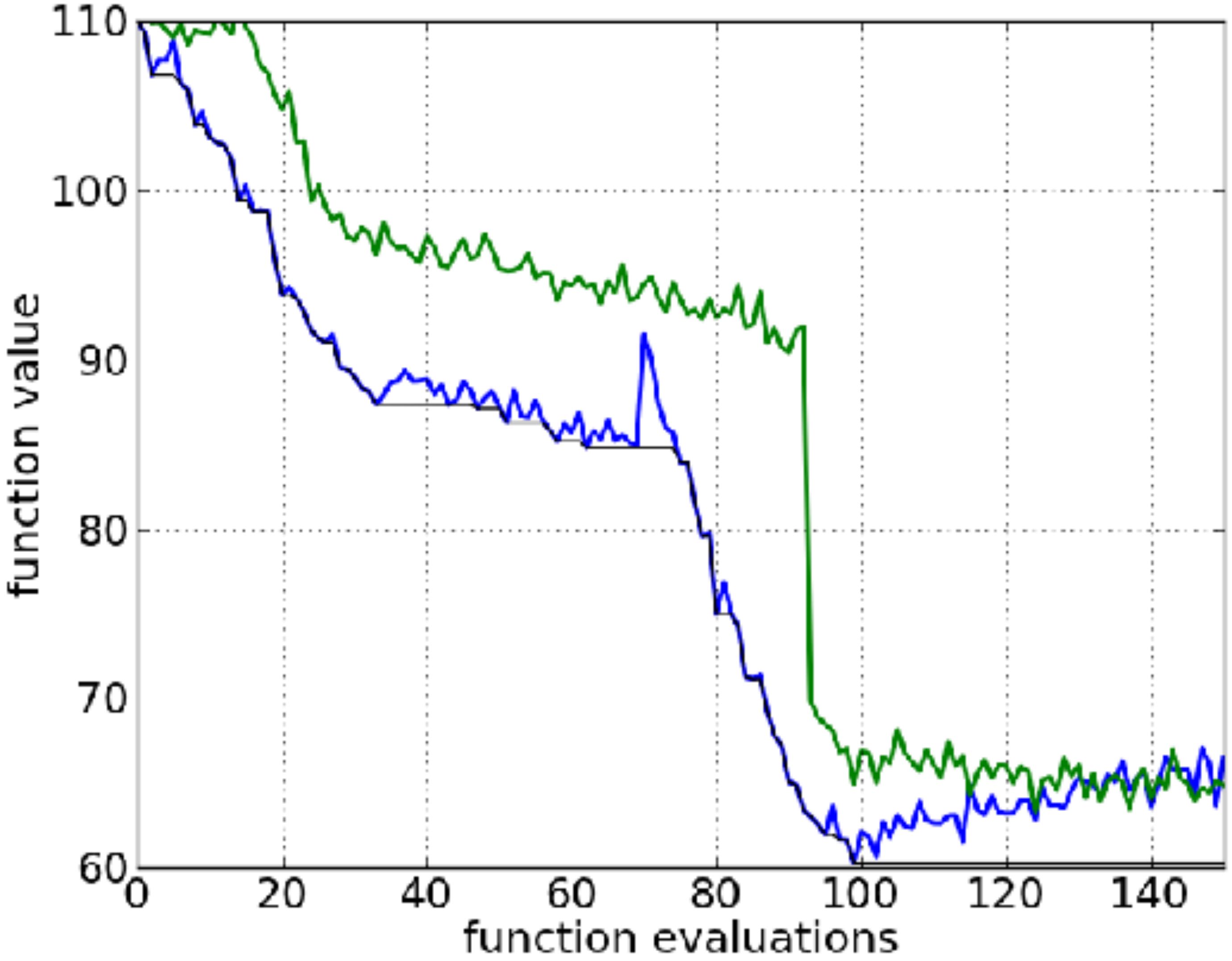
- Empirical cumulative distribution functions are arguably the single most powerful tool to display “aggregated” data.



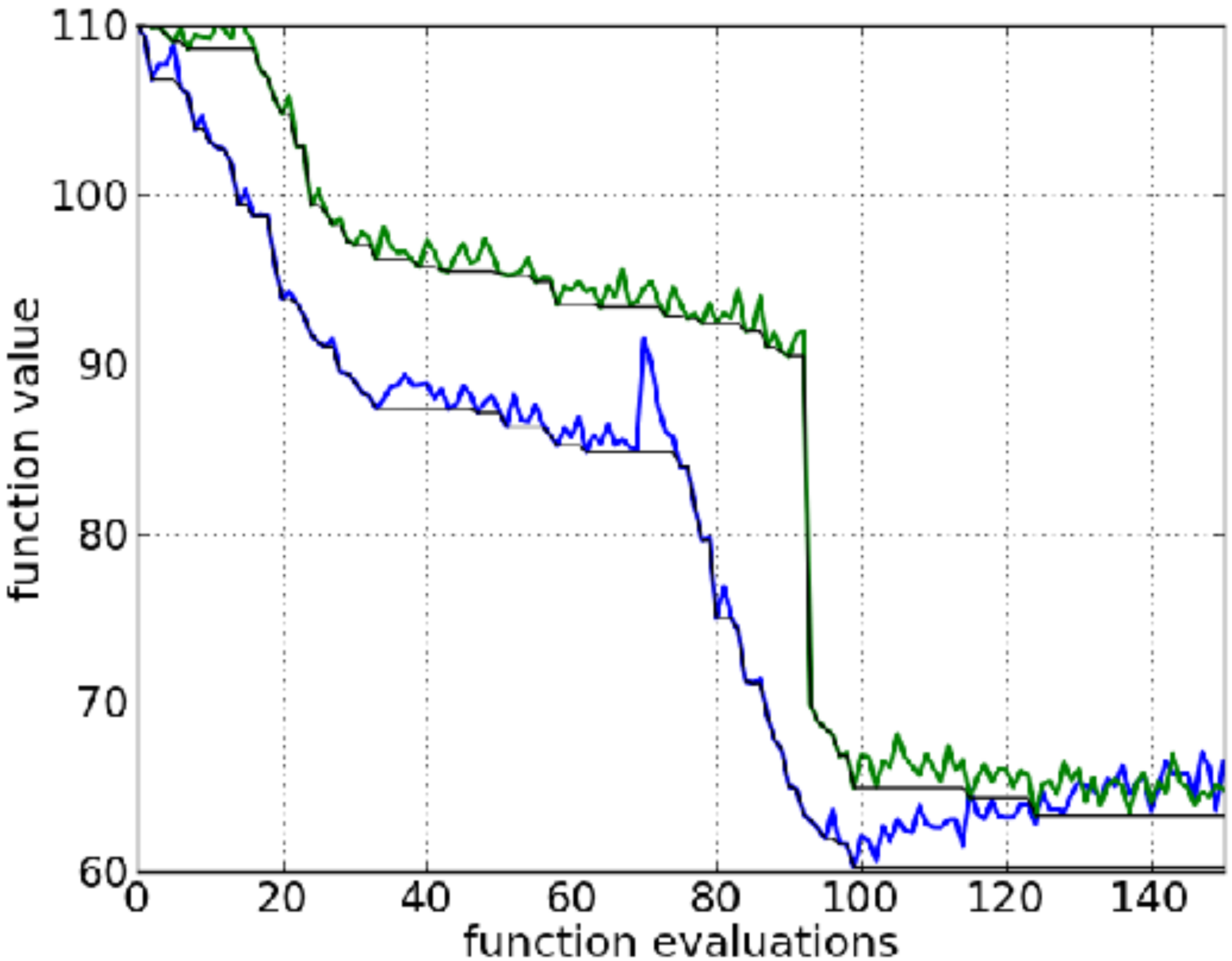
- a convergence graph



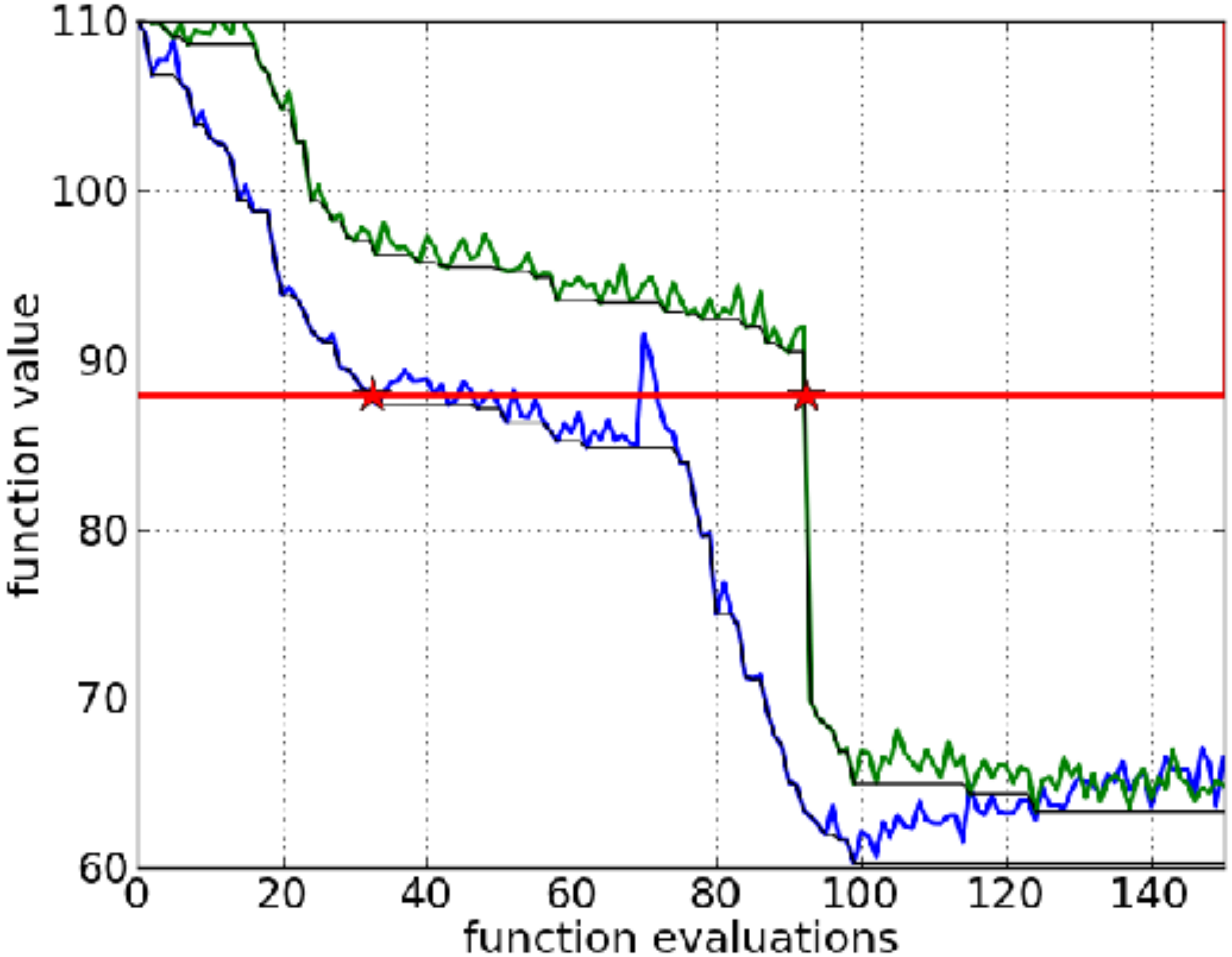
- a convergence graph
- first hitting time (black): lower envelope, a monotonous graph



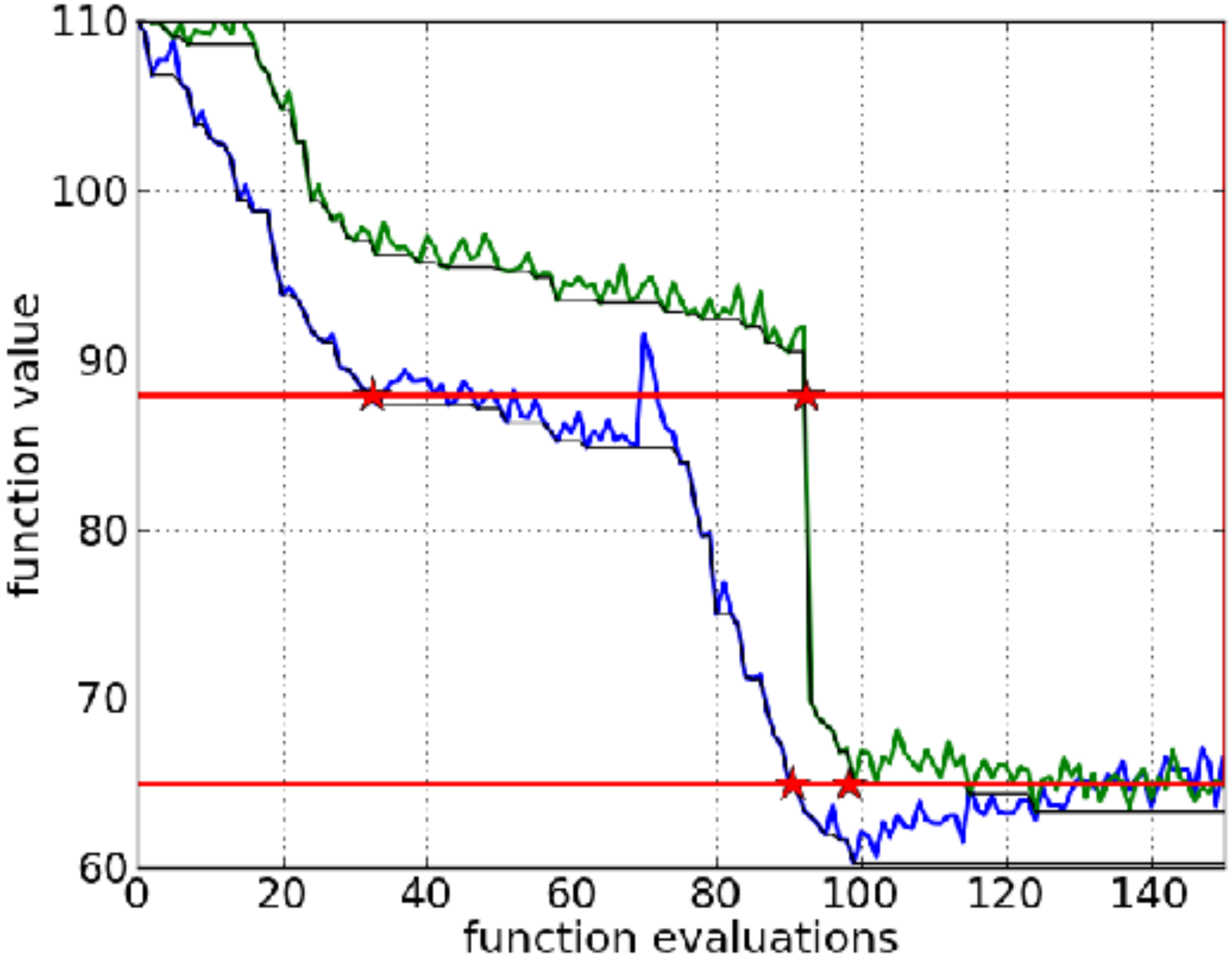
- another convergence graph



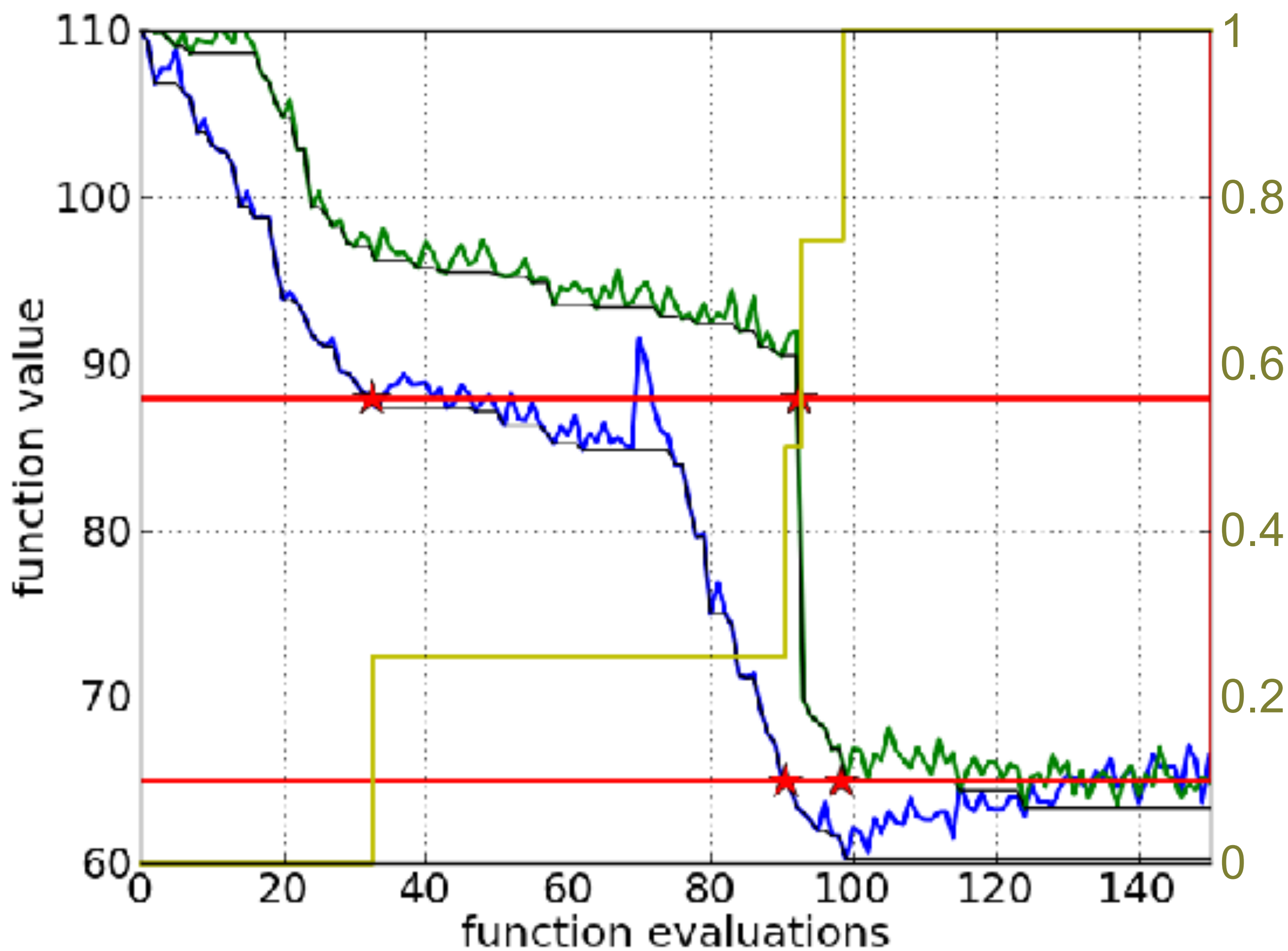
- another convergence graph with hitting time



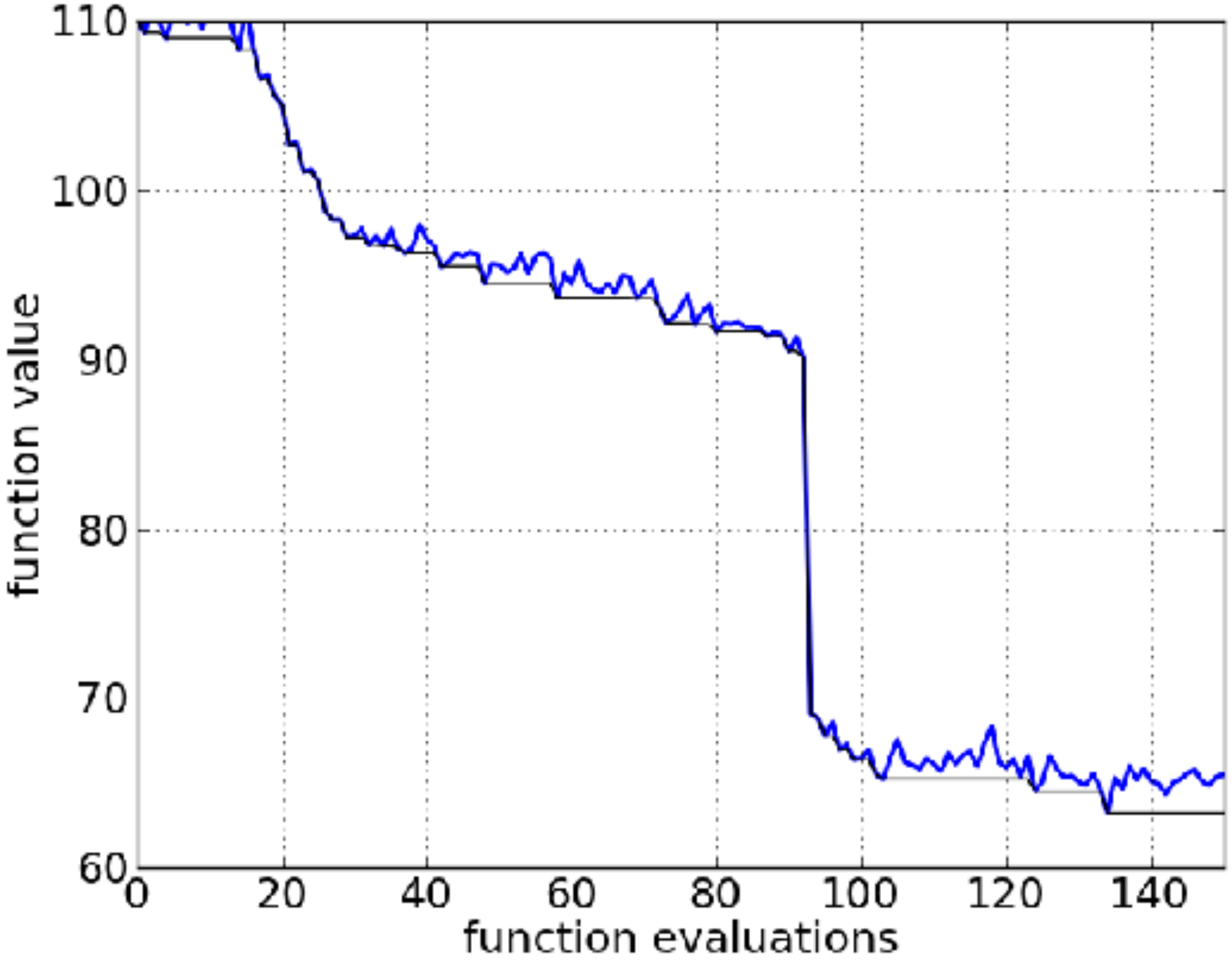
- a target value delivers two data points (possibly a missing value)



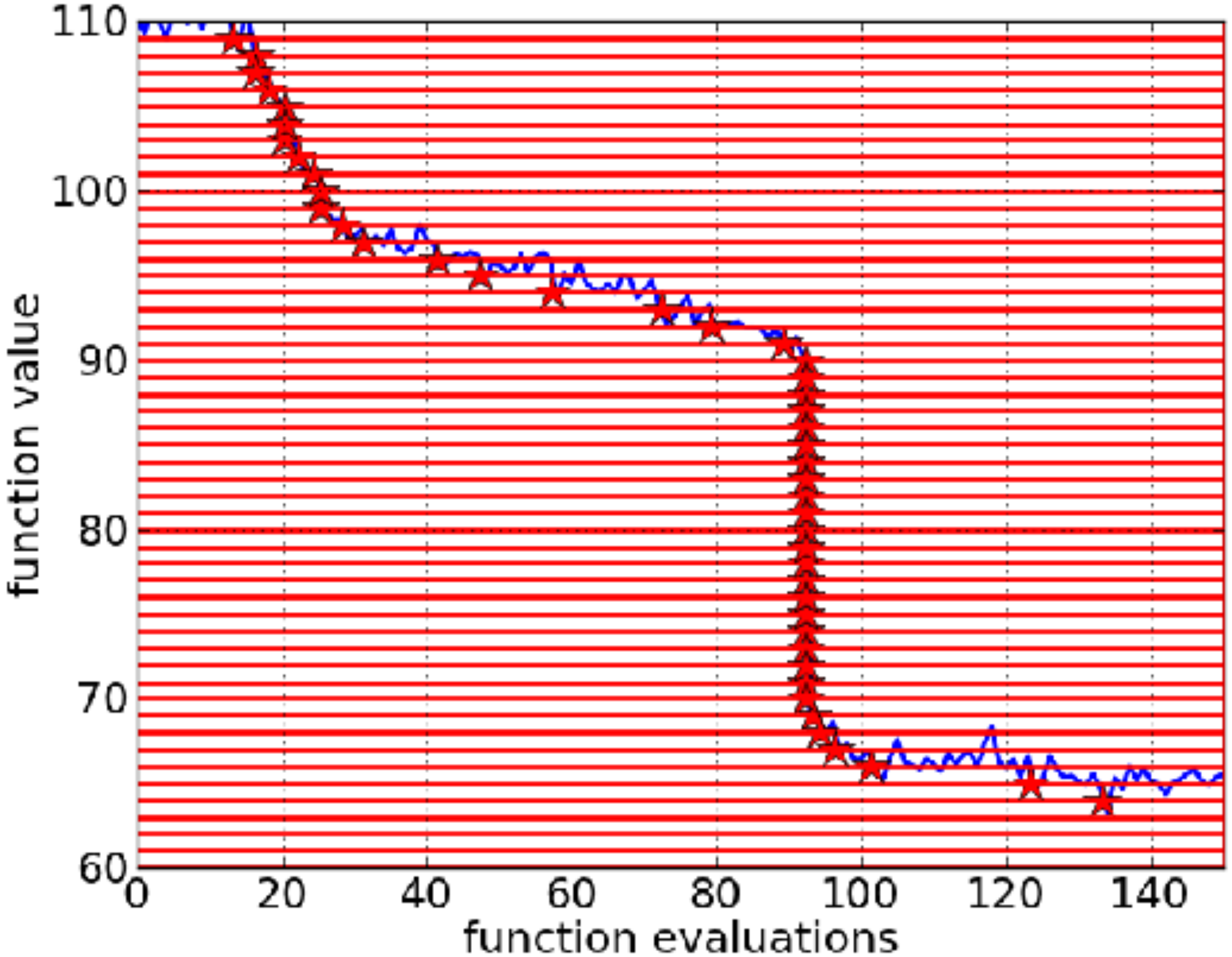
- a target value delivers two data points



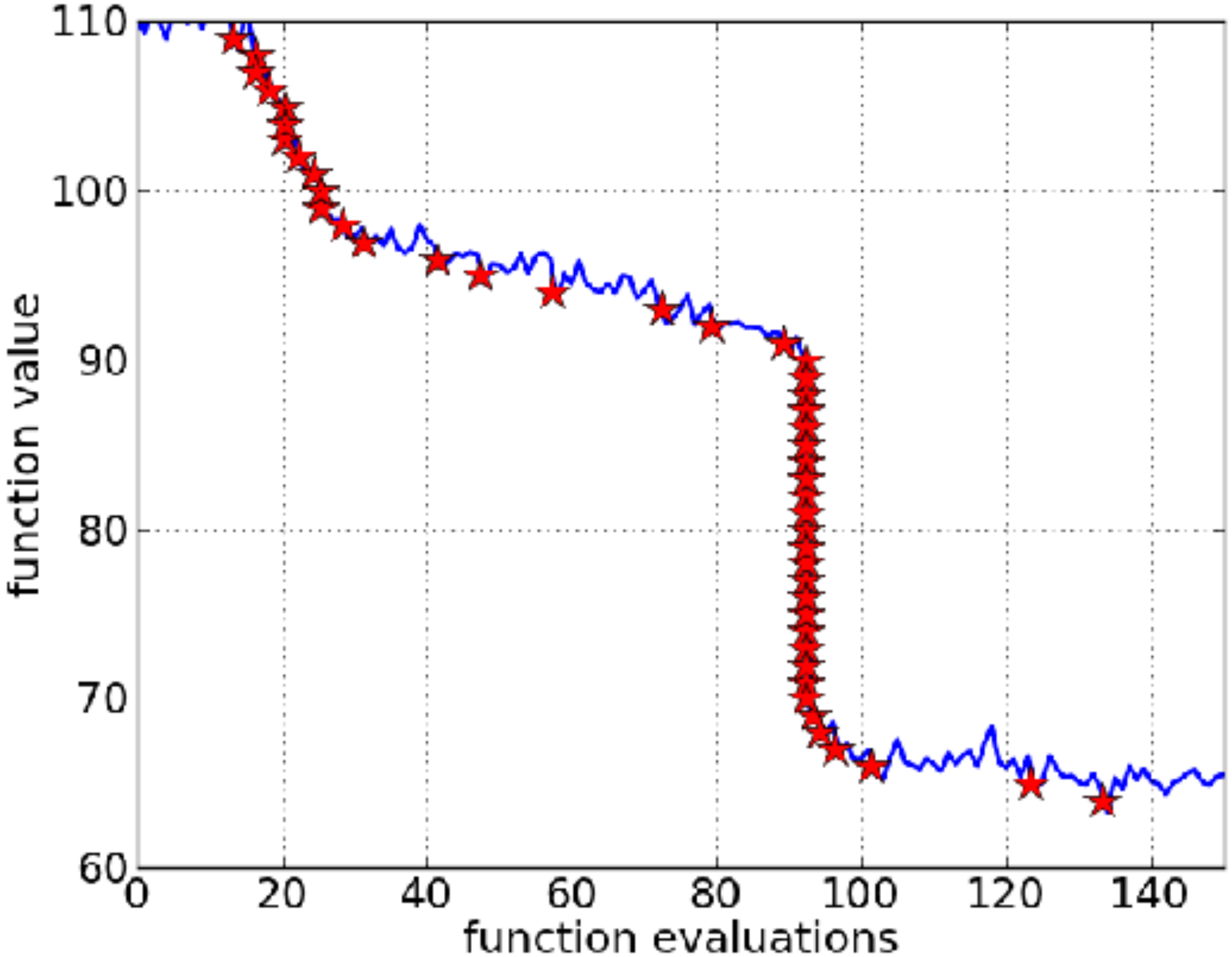
- the ECDF with four steps (between 0 and 1)

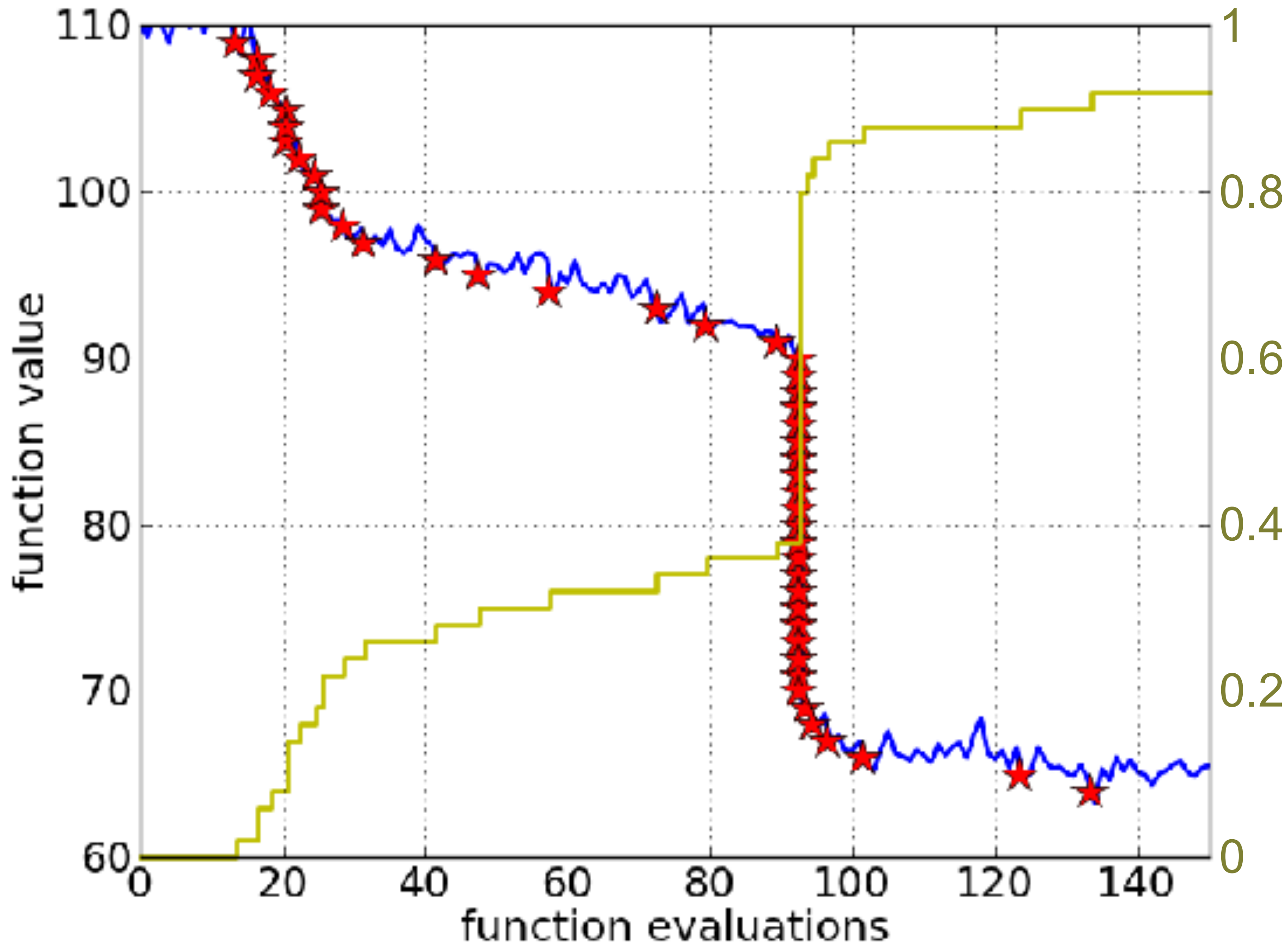


- reconstructing a single run

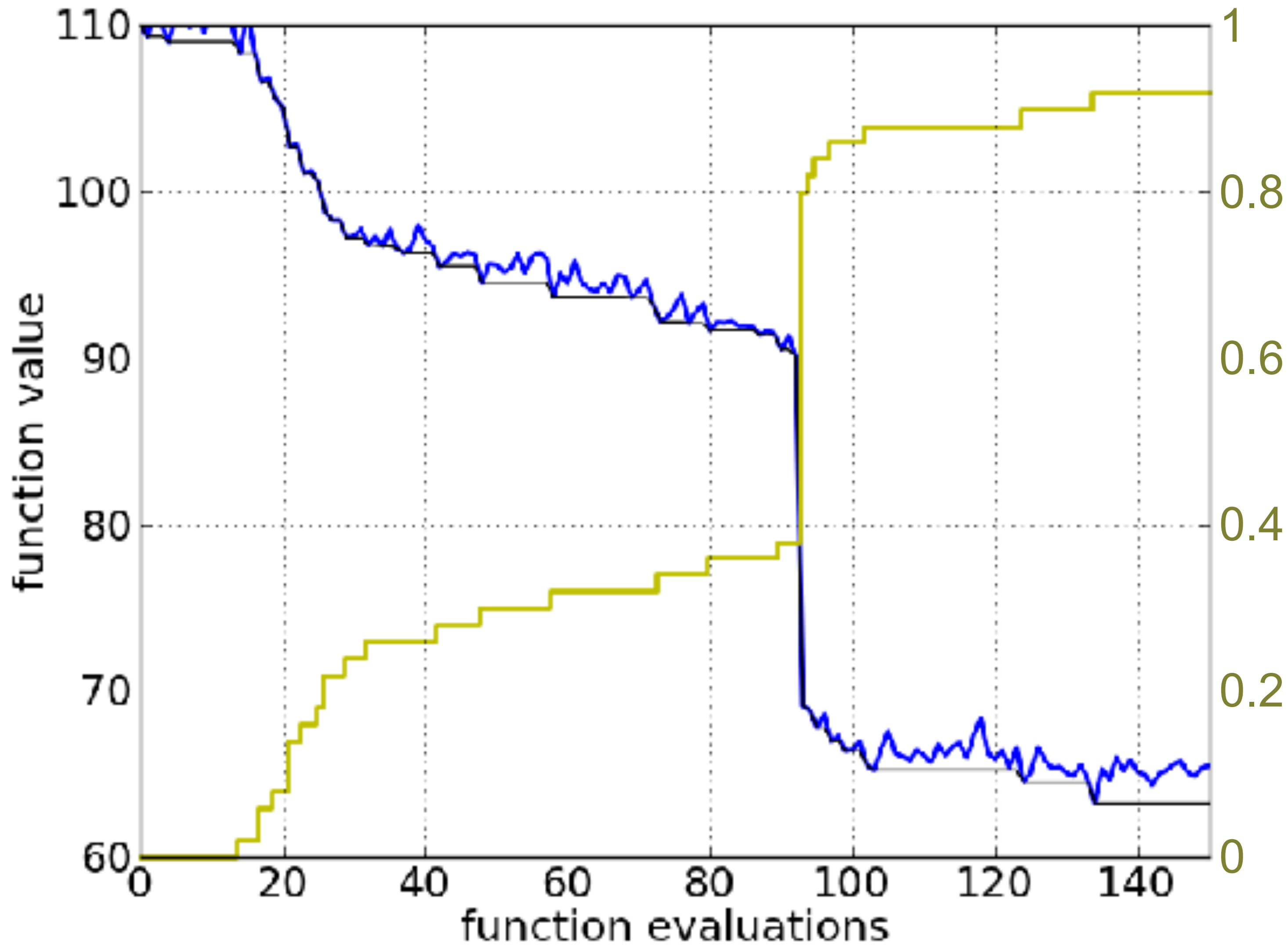


50 equally spaced targets

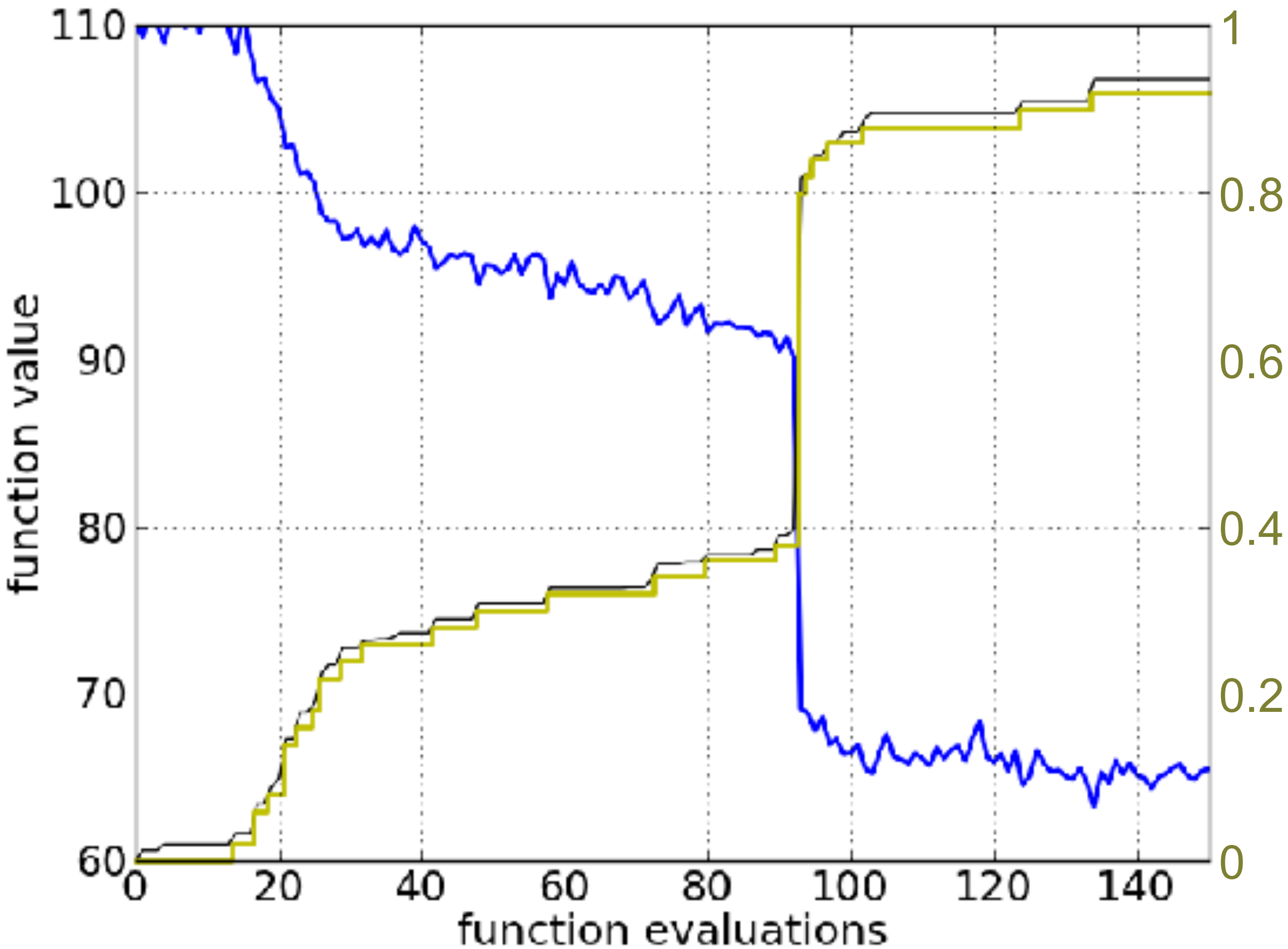

110
100
90
80
70
60
0
20
40
60
80
100
120
140
function value
function evaluations



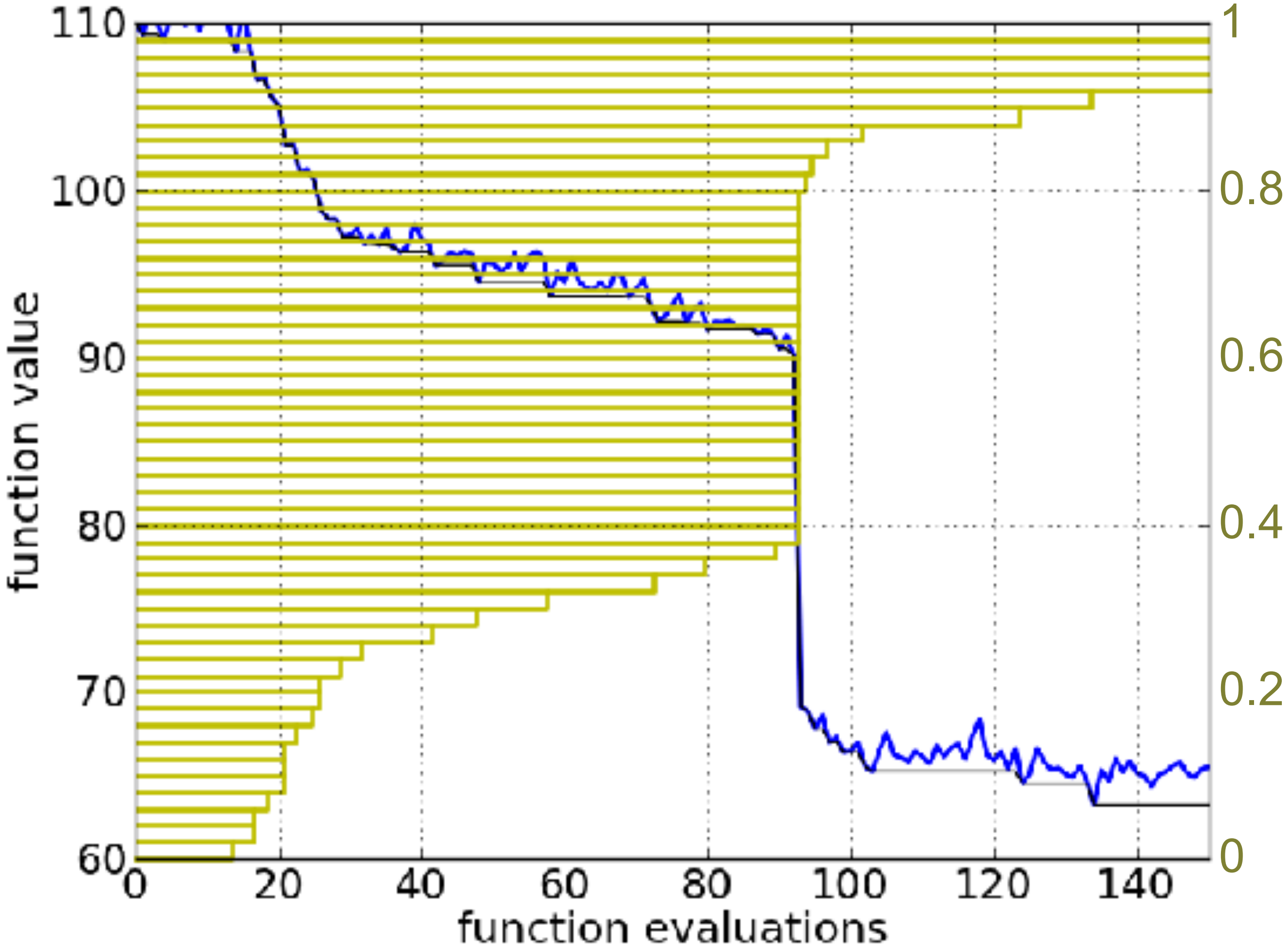
the ECDF recovers the monotonous graph



the ECDF recovers
the monotonous
graph, discretised
and flipped



the ECDF recovers the monotonous graph, discretised and flipped



the ECDF recovers the monotonous graph, discretised and flipped

the area over the ECDF curve is the average runtime (the geometric average if the x-axis is in log scale)

Benchmarking with COCO

COCO — Comparing Continuous Optimisers

- is a (software) platform for comparing continuous optimisers in a black-box scenario

  https://github.com/numbbo/coco

- *automatises* the tedious and repetitive task of *benchmarking numerical optimisation algorithms in a black-box setting*

- advantage: saves time and prevents common (and not so common) pitfalls

COCO provides

- experimental and measurement *methodology*

  main decision: what is the end point of measurement

- suites of benchmark functions

  single objective, bi-objective, noisy, constrained (in alpha stage)

- data of already benchmarked algorithms to compare with

COCO: Installation and Benchmarking in Python

```
$ ### get and install the code
$ git clone https://github.com/numbbo/coco.git  # get coco using git
$ cd coco
$ python do.py run-python  # install Python experimental module cocoex
$ python do.py install-postprocessing  # install post-processing :-)
```

```python
import os, webbrowser
from scipy.optimize import fmin
import cocoex, cocopp

# prepare
output_folder = "scipy-optimize-fmin"
suite = cocoex.Suite("bbob", "", "")
observer = cocoex.Observer("bbob", "result_folder: " + output_folder)

# run benchmarking
for problem in suite:  # this loop will take several minutes
    observer.observe(problem)  # generates the data for cocopp post-processing
    fmin(problem, problem.initial_solution)

# post-process and show data
cocopp.main(observer.result_folder)  # re-run folders look like "...-001" etc
webbrowser.open("file://" + os.getcwd() + "/ppdata/index.html")
```

Benchmark Functions

should be

- comprehensible
- difficult to defeat by “cheating”

  examples: optimum in zero, separable
- scalable with the input dimension
- reasonably quick to evaluate

  e.g. 12-36h for one full experiment
- reflect reality

  specifically, we model well-identified difficulties encountered also in real-world problems

The COCO Benchmarking Methodology

- budget-free

larger budget means more data to investigate
any budget is comparable
termination and restarts are or become relevant

- using runtime as (almost) single performance measure

measured in number of function evaluations

- runtimes are aggregated
  - in empirical (cumulative) distribution functions
  - by taking averages

geometric average when aggregating over different problems

Benchmarking Results for Algorithm ALG on the bbob Suite

Home

Runtime distributions (ECDFs) per function

Runtime distributions (ECDFs) summary and function groups

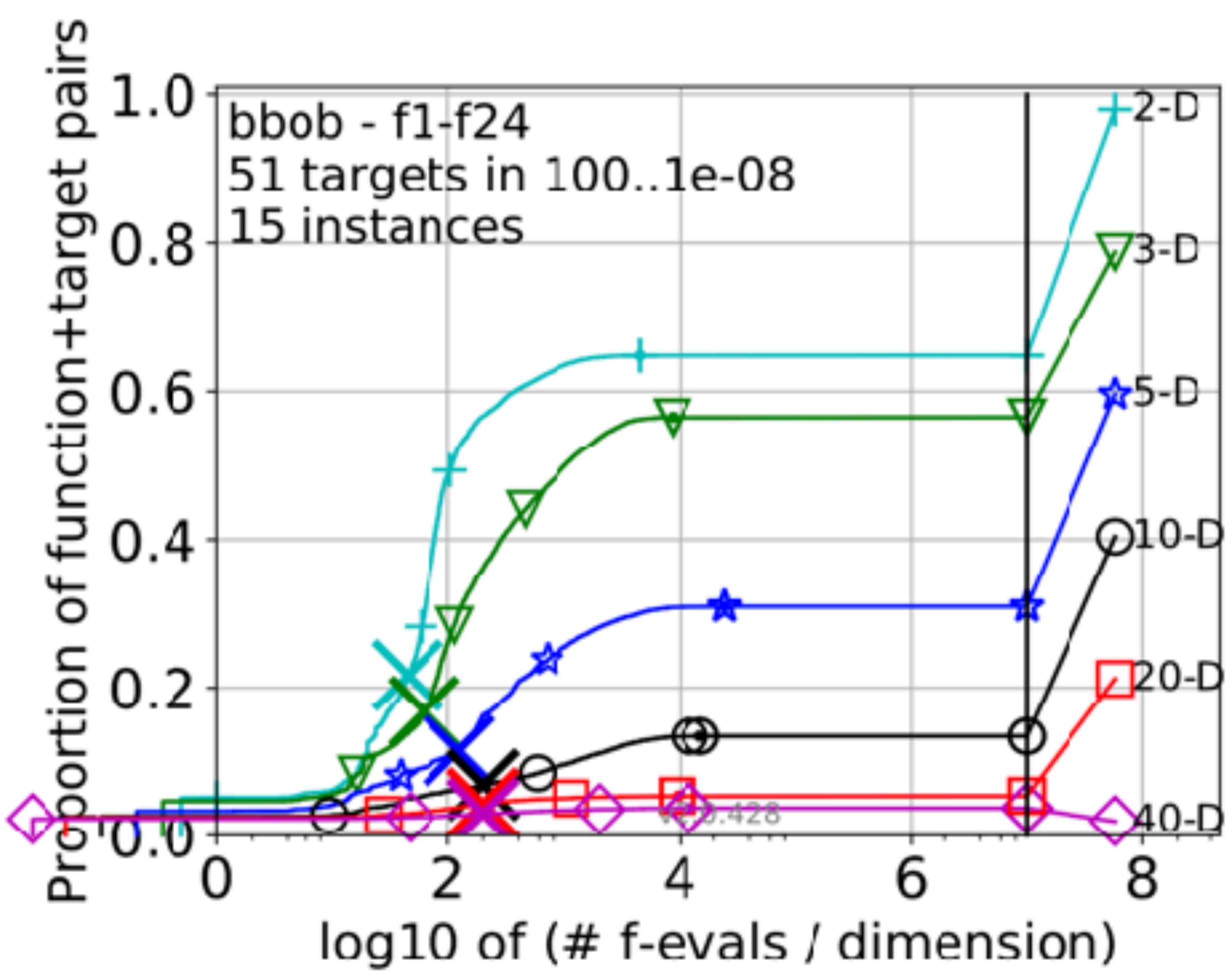
Scaling with dimension for selected targets

Tables for selected targets

Runtime distribution for selected targets and f-distributions

Runtime loss ratios

Runtime distributions (ECDFs) over all targets



FIN