

#### A Practical Guide to Experimentation (and Benchmarking)

Nikolaus Hansen

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# <u>A Practical Guide to Experimentation</u> (and Benchmarking)

Nikolaus Hansen Inria Research Centre Saclay, CMAP, Ecole polytechnique, Université Paris-Saclay

- Installing IPython is not a prerequisite to follow the tutorial
- for downloading the material, see slides: <a href="http://www.cmap.polytechnique.fr/~nikolaus.hansen/gecco2018-experimentation-guide-slides.pdf">http://www.cmap.polytechnique.fr/~nikolaus.hansen/jecco2018-experimentation-guide-notebooks</a>
   code: <a href="https://github.com/nikohansen/GECCO-2018-experimentation-guide-notebooks">https://github.com/nikohansen/GECCO-2018-experimentation-guide-notebooks</a>

#### Overview

- Scientific experimentation
- Invariance
- Statistical Analysis
- A practical experimentation session
- Approaching an unknown problem
- Performance Assessment
  - What to measure
  - How to display
  - Aggregation
  - Empirical distributions

Do not hesitate to ask questions!

### 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 If it disagrees with experiment, it's wrong. And that simple statement is the key to science. — R. Feynman

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 and (by definition) not well-understood

 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

What are the dos and don'ts?

- what is most helpful to do?
- what is better to avoid?

 What is the aim? Answer a question, ideally quickly (minutes, seconds) and comprehensively

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

do not (blindly) trust in what one needs to rely upon (code, claims, ...)
 without good reasons

check/test "everything" yourself, practice stress testing (e.g. weird parameter setting) which also boosts understanding one key element for success interpreted/scripted languages have an advantage Why Most Published Research Findings Are False [loannidis 2005]

- practice to make predictions of the (possible) outcome(s)
  - to develop a mental model of the object of interest to practice being proven wrong, to overcome *confirmation bias*
- run rather many than few experiments iteratively, practice online experimentation (see demonstration)

to run many experiments they must be quick to implement and run, ideally seconds rather than minutes (start with small dimension/budget) develops a feeling for the effect of setup changes

 run rather many than few experiments iteratively, practice online experimentation (see demonstration)

to run many experiments they must be quick to implement and run, ideally seconds rather than minutes (start with small dimension/budget) 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/dispersion/variance

· 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, study them carefully!

don't make minimising CPU-time a primary objective

avoid spending time in implementation details to tweak performance prioritize code clarity (minimize time to *change* code, to debug code, to maintain code) yet code optimization may be necessary to run experiments efficiently

don't make minimising CPU-time a primary objective

avoid spending time in implementation details to tweak performance yet code optimization may be necessary to run experiments efficiently

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

mainly because an algorithm is applied to unknown functions, not to f, and the "why" allows to predict the effect of design changes

 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

- 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

# Invariance: binary variables

Assigning 0/1 (for example minimize  $\sum_{i} x_{i} \text{ vs } \sum_{i} 1 - x_{i}$  )

- is an "arbitrary" and "trivial" encoding choice and
- amounts to the affine linear transformation  $x_i \mapsto -x_i + 1$  this transformation or the identity are the coding choice in each variable in continuous domain: norm-preserving (isotropic, "rigid") transformation
- does not change the function "structure"
  - all level sets  $\{x \mid f(x) = \text{const}\}$  have the same size (number of elements, same volume)
  - the same neighbourhood
  - no variable dependencies are introduced (or removed)

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

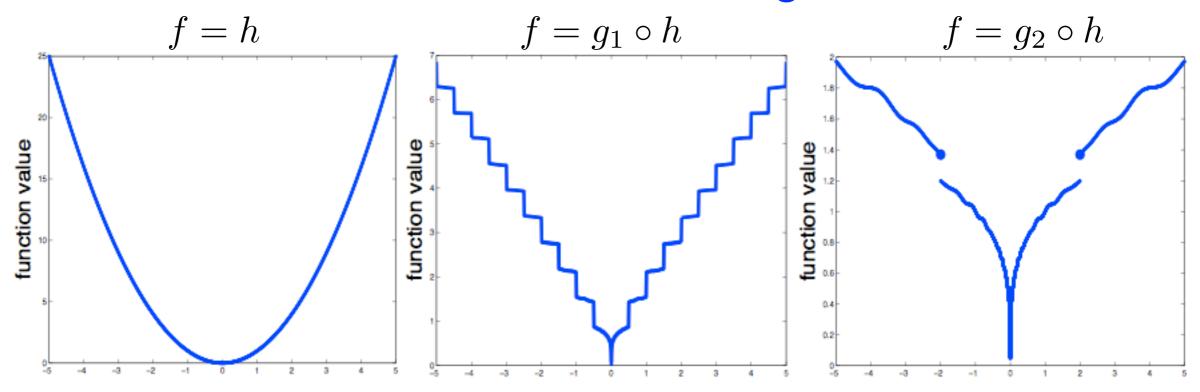
# Invariance: binary variables

#### Permutation of variables

- is another "arbitrary" and "trivial" encoding choice and
- is another norm-preserving transformation
- does not change the function "structure" (as above)
- consider one-point vs two-point crossover: which is better choice?
   only two-point crossover is invariant to variable permutation

Instead of 1 function, we now consider n! different but equivalent functions  $n! \gg 2^n$  is much larger than the size of the search space

#### Invariance Under Order Preserving Transformations



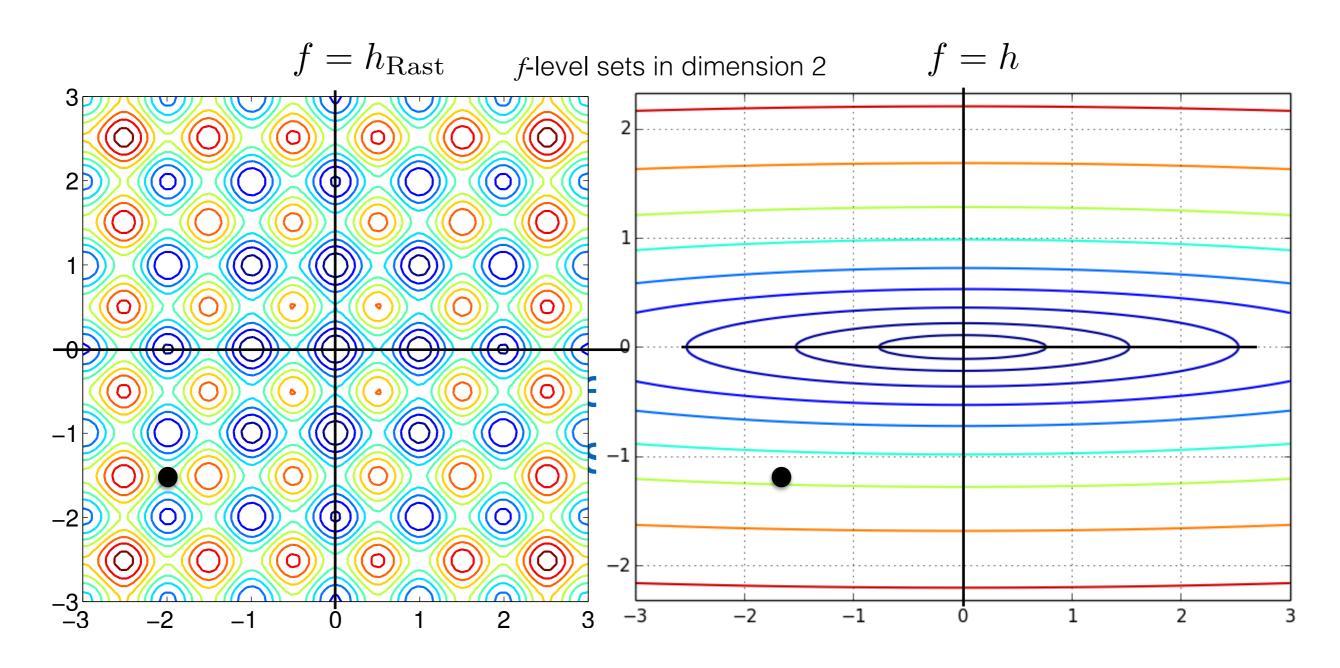
Three functions belonging to the same equivalence class

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

#### Invariances make

- observations meaningful
- as a rigorous notion of generalization
- algorithms predictable and/or "robust"

#### Invariance Under Rigid Search Space Transformations

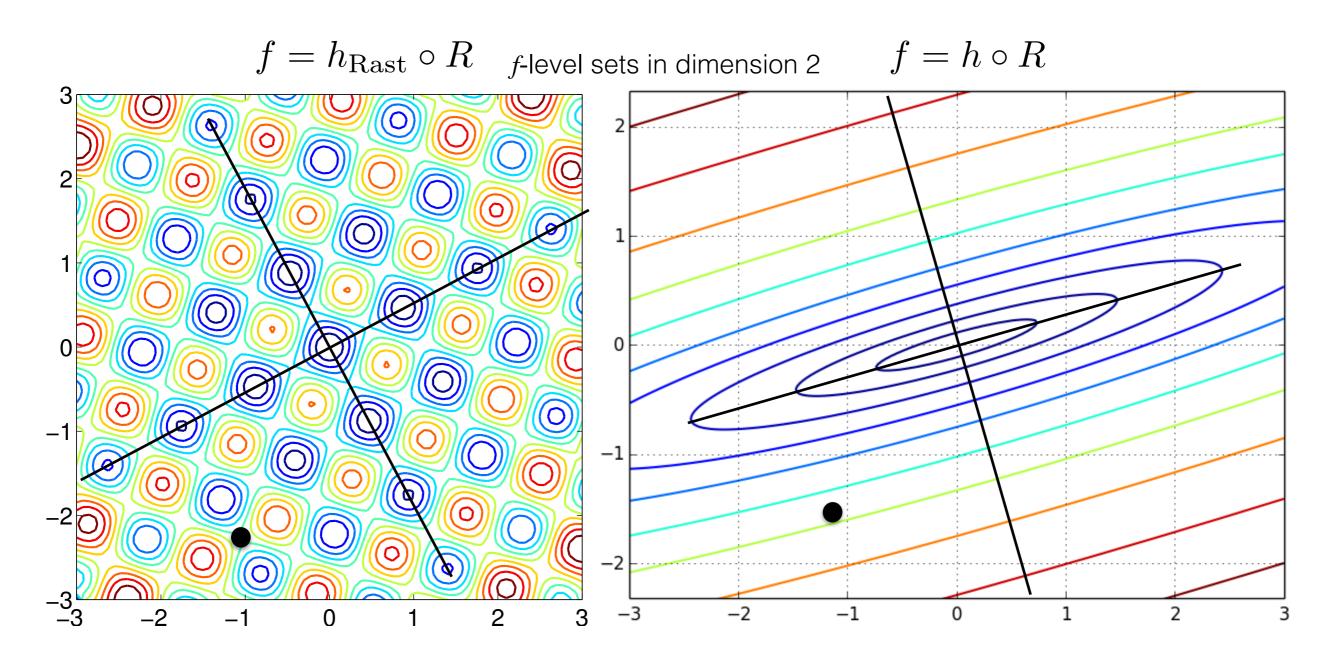


for example, invariance under search space rotation (separable vs non-separable)

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#### Invariance Under Rigid Search Space Transformations



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

#### 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.

#### Statistical Analysis

"The first principle is that you must not fool yourself, and you are the easiest person to fool. So you have to be very careful about that. After you've not fooled yourself, it's easy not to fool other[scientist]s. You just have to be honest in a conventional way after that."

- Richard P. Feynman

# Statistical Analysis

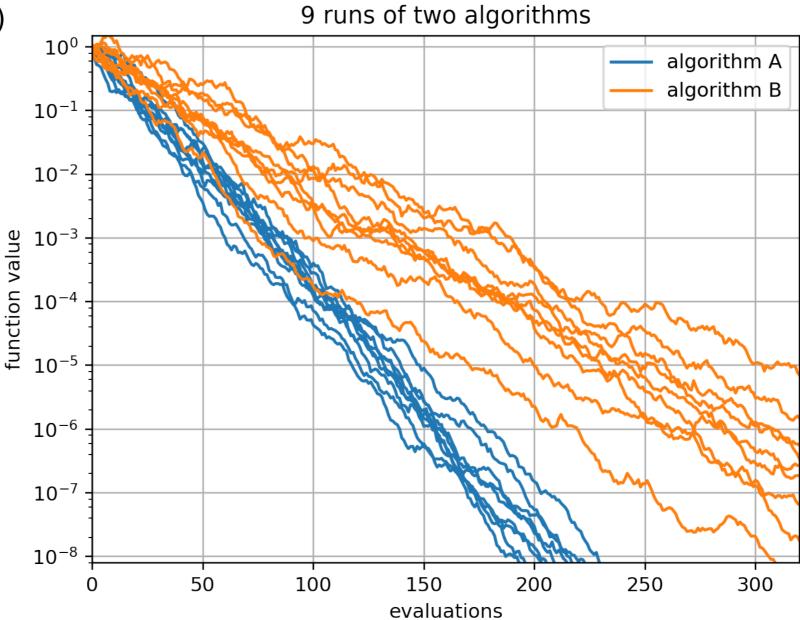
"experimental results lacking proper statistical analysis must be considered anecdotal at best, or even wholly inaccurate"

M. Wineberg

Do you agree (sounds about right) or disagree (is taken a little over the top) with the quote?

an experimental result (shown are *all data obtained*):

Do we (even) need a statistical analysis?



### Statistical Significance: General Prodecure

 first, check the relevance of the result, for example of the difference which is to be tested for statistical significance

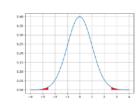
this also means: do not *explorative testing* (e.g. test *all* pairwise combinations) any ever so small difference can be made *statistically* significant with a simple trick,

but not made significant in the sense of important or meaningful

prefer "nonparametric" methods

not assuming that the data come from a parametrised family of probability distributions

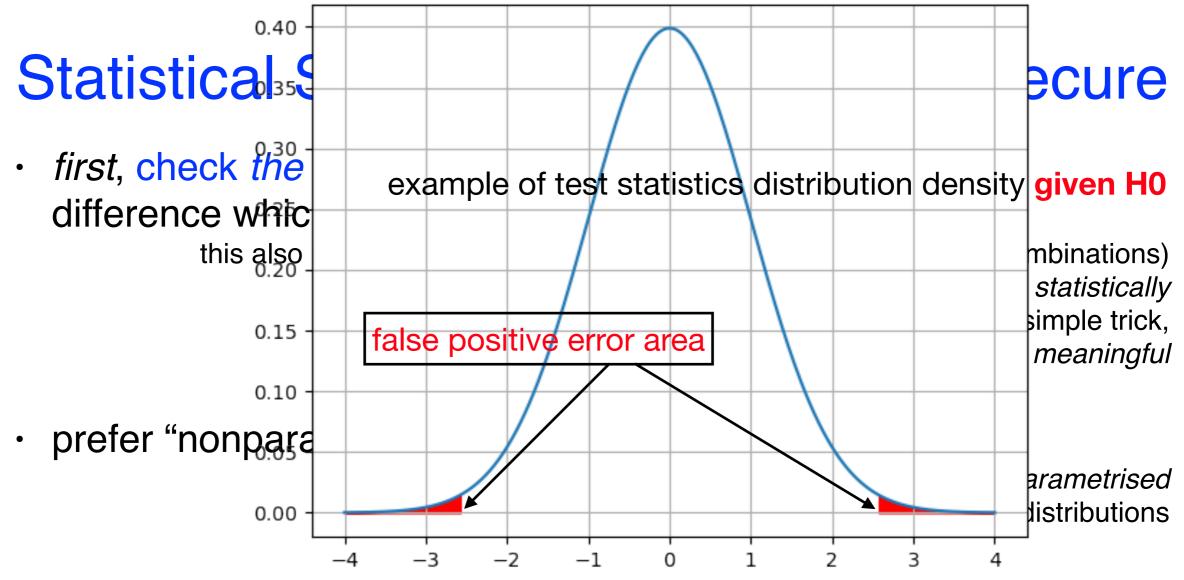
 p-value = significance level = probability of a false positive outcome, given H0 is true



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

given a found/observed p-value, fewer data are better

more data (almost inevitably) lead to smaller p-values, hence to achieve the same p-value with fewer data, the *between*-difference must be larger compared to the *within*-variation



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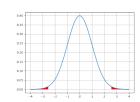
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### Statistical Significance: Methods

- use the rank-sum test (aka Wilcoxon or Mann-Whitney U test)
  - Assumption: all observations (data values) are obtained independently and no equal values are observed

The "lack" of necessary preconditions is the main reason to use the rank-sum test.

even a few equal values are not detrimental the rank-sum test is nearly as efficient as the t-test which requires normal distributions

• Null hypothesis (nothing relevant is observed if): Pr(x < y) = Pr(y < x)

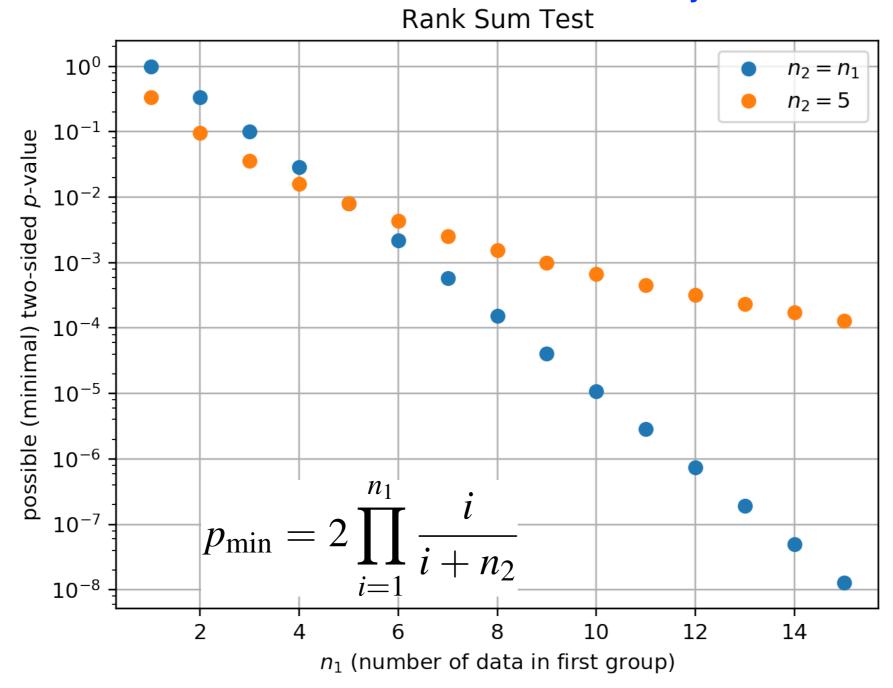
H0: the probability to be greater or smaller (better or worse) is the same the aim is to be able to reject the null hypothesis

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

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

#### Statistical Significance: How many data do we need?

#### AKA as test efficiency



- assumption: data are fully "separated", that is,  $\forall i, j : x_i < y_j$  or  $\forall i, j : x_i > y_j$  (two-sided)
- observation: adding 2 data points in each group gives about one additional order of magnitude
- use the Bonferroni correction for multiple tests

#### Statistical Significance: How many data do we need?

 In the best case: at least ten (two times five) and two times nine is plenty

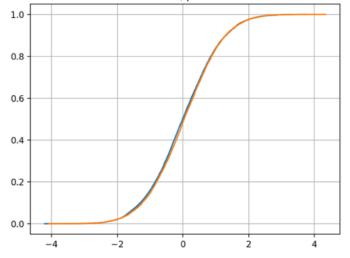
minimum number of data to possibly get two-sided p < 1%: 5+5 or 4+6 or 3+9 or 2+19 or 1+200 and p < 5%: 4+4 or 3+5 or 2+8 or 1+40

I often take two times 11 or 31 or 51

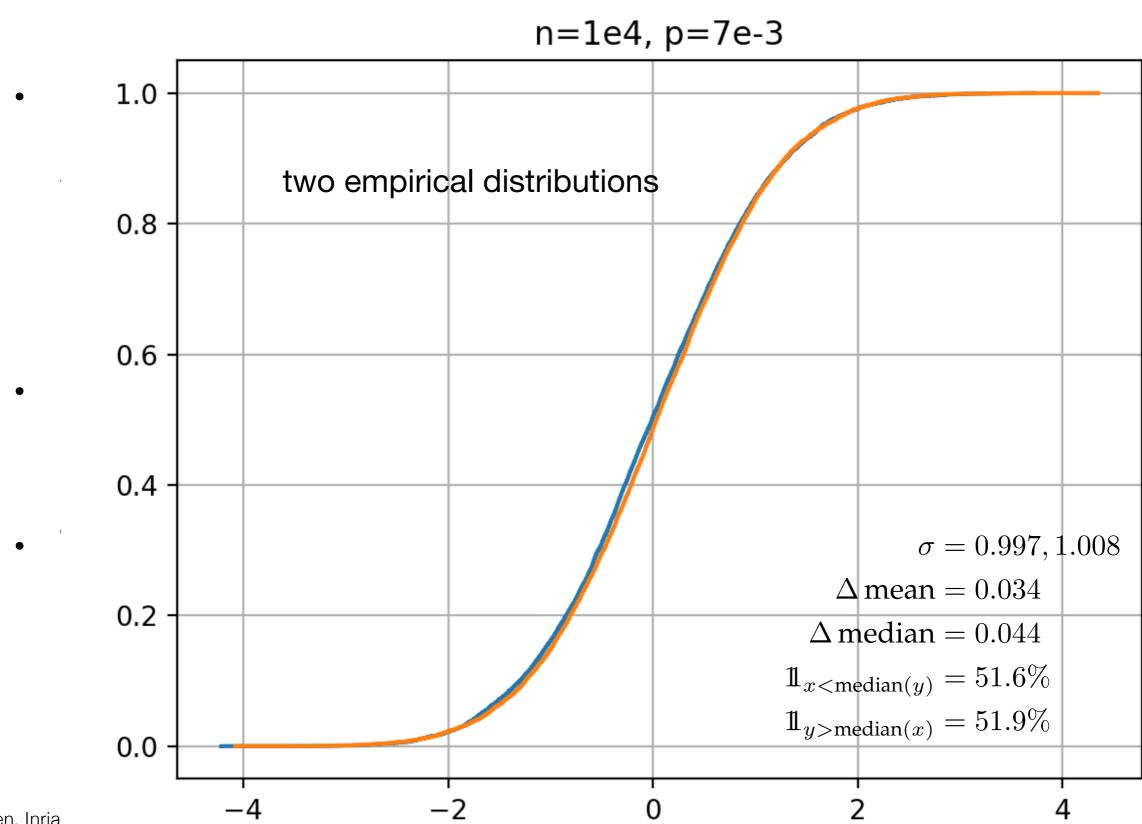
median, 5%-tile and 95%-tile are easily accessible with 11 or 31 or 51... data

Too many data make statistical significance

meaningless



#### Statistical Significance: How many data do we need?



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# Statistical Analysis

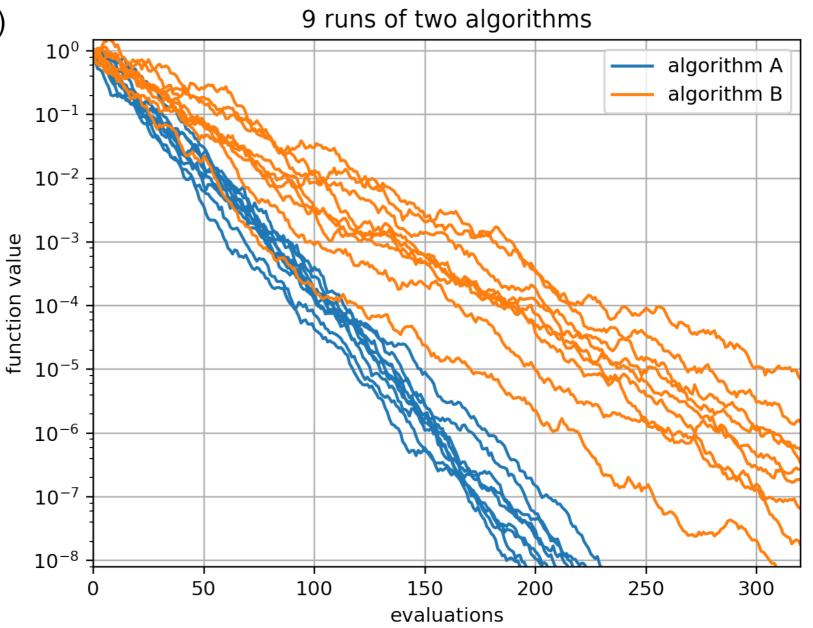
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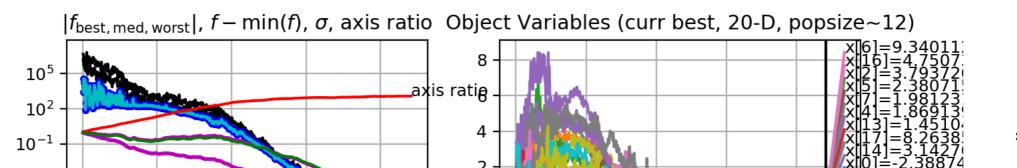
an experimental result (shown are *all data obtained*):

Do we (even) need a statistical analysis?



### 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)
              function value axis ratio sigma min&max std t[m:s]
Iterat #Fevals
         12 2.637846492377813e+03 1.0e+00 9.49e-01 9e-01 1e+00 0:00.0
         24 3.858353384747645e+04 1.1e+00 9.13e-01 9e-01 9e-01 0:00.0
         36 1.589934793439056e+04 1.2e+00 8.94e-01 9e-01 9e-01 0:00.0
       1200 1.805167565570186e+02 6.6e+00 2.52e-01 6e-02 3e-01 0:00.1
  100
  200
       2400 9.260486860109009e+01 4.2e+01 2.79e-01 1e-02 4e-01 0:00.3
       3600 8.460045942108286e+00 2.0e+02 3.20e-01 4e-03 4e-01 0:00.4
  300
  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
       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
                                                    6.92049899e-09 ...1
                                  4.23137381e-08
                                                                    4.36659472e-08
std deviations: [ 5.07976963e-11 4.52415829e-08
                                                   4.67529085e-08
   4.04686177e-08 4.38294341e-08 4.65665203e-08 5.01580767e-08 ...]
 cma.plot()
                                      Figure 328
                                                                                      心
```

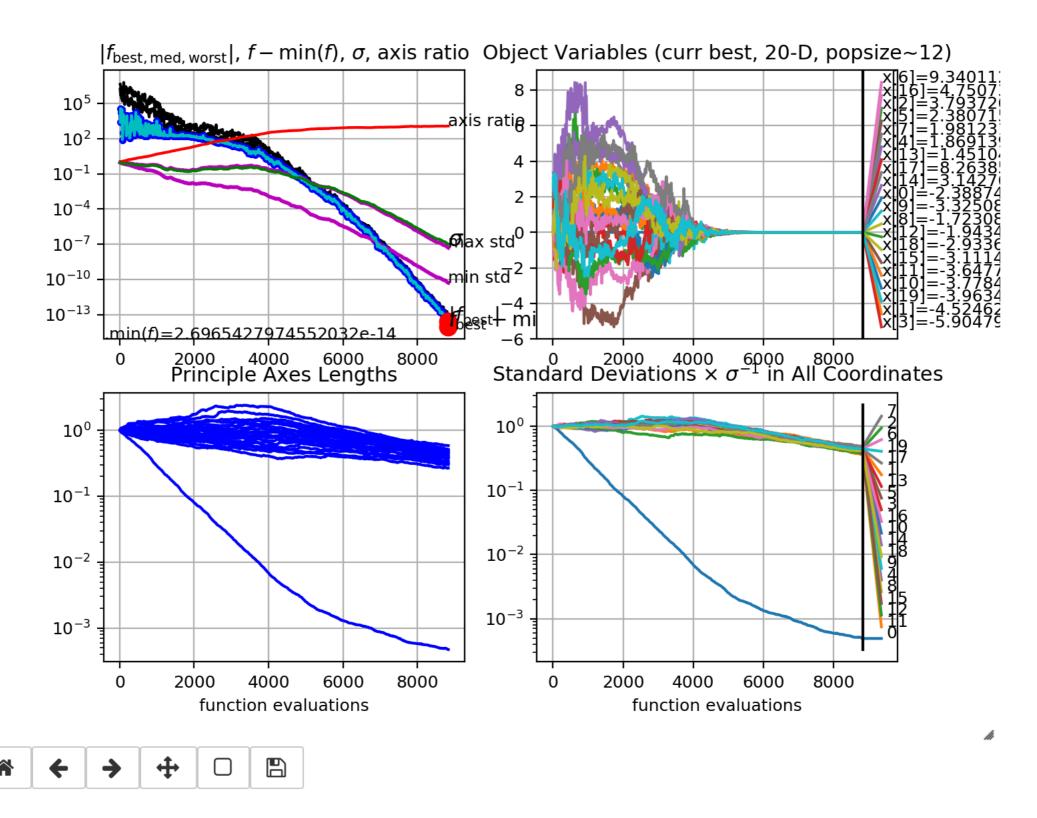


4.04686177e-08 4.38294341e-08 4.65665203e-08 5.01580767e-08 ...]

cma.plot()

Figure 328

Ф



Questions?

# 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

- See <a href="https://github.com/nikohansen/GECC0-2018-experimentation-guide-notebooks">https://github.com/nikohansen/GECC0-2018-experimentation-guide-notebooks</a>
- Demonstrations
  - A somewhat typical working mode
  - A parameter investigation

# Approaching an unknown problem

Problem/variable encoding

for example log scale vs linear scale vs quadratic transformation

Fitness formulation

for example  $\sum_{i} |x_{i}|$  and  $\sum_{i} x_{i}^{2}$  have the same optimal (minimal) solution but may be very differently "optimizable".

- Try to locally improve a given (good) solution
- Start local search from different initial solutions.
   Ending up always in different solutions? Or always in the same?
- Apply "global search" setting
- SEE also <a href="http://cma.gforge.inria.fr/cmaes\_sourcecode\_page.html#practical">http://cma.gforge.inria.fr/cmaes\_sourcecode\_page.html#practical</a>

Questions?

#### Performance Assessment

 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 display changes can make a huge difference

there are surprisingly many devils in the details

#### Why do we want to measure performance?

compare algorithms and algorithm selection (the obvious)

ideally we want standardized comparisons

- regression testing after (small) changes
   as we may expect (small) changes in behaviour,
   conventional regression testing may not work
- understanding of algorithms

to improve algorithms non-standard experimentation is often preferable or necessary

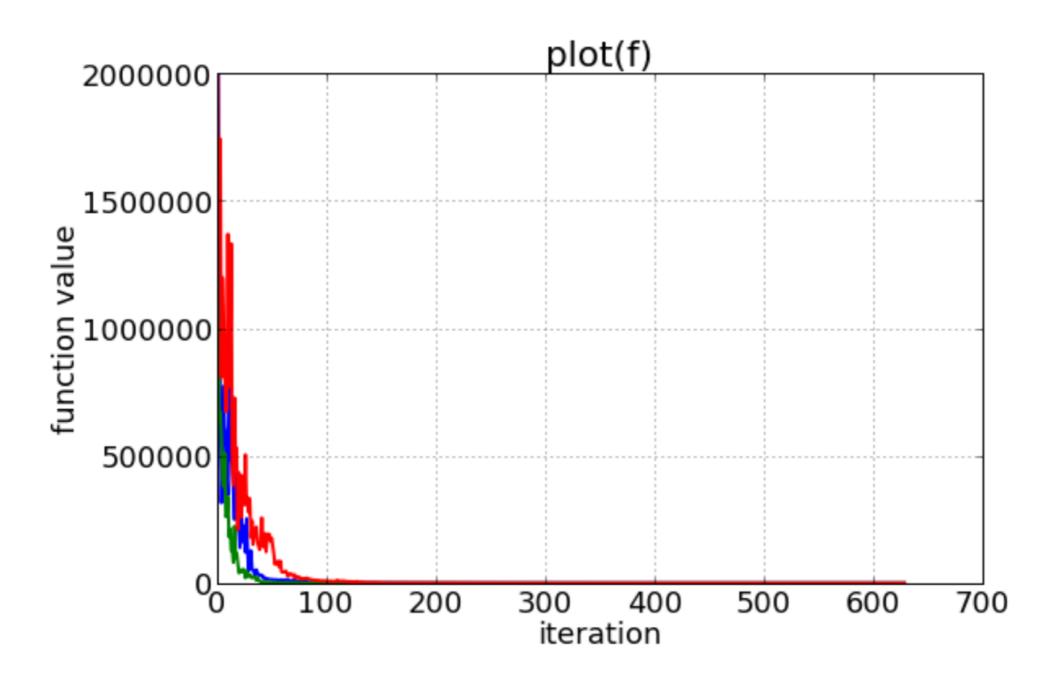
### Measuring Performance

**Empirically** 

convergence graphs is all we have to start with

the right presentation is important!

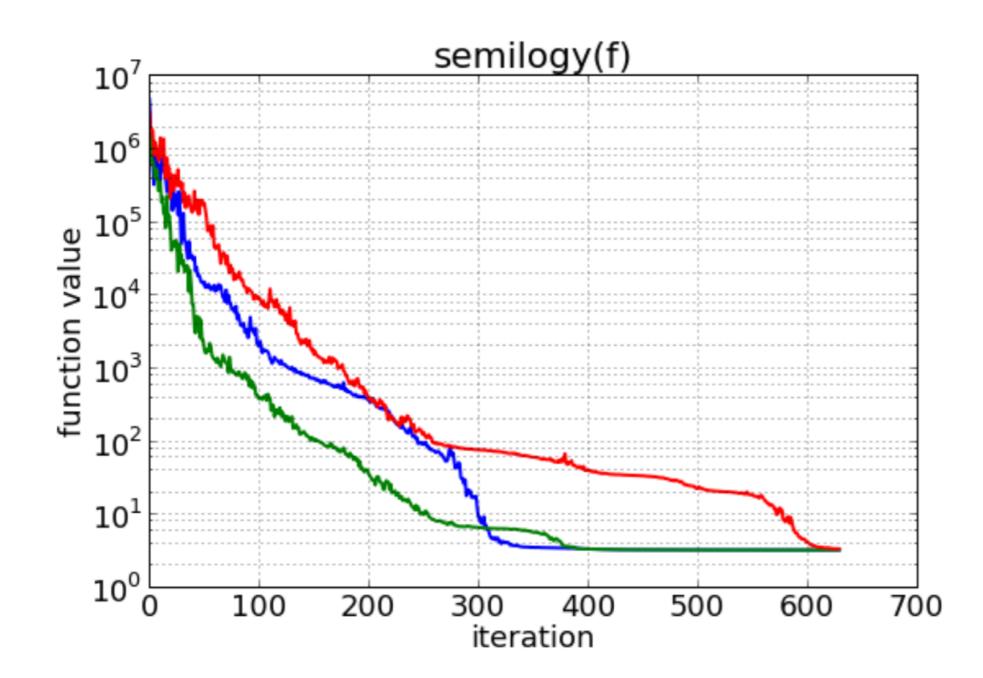
# Displaying Three Runs



not like this (it's unfortunately not an uncommon picture)

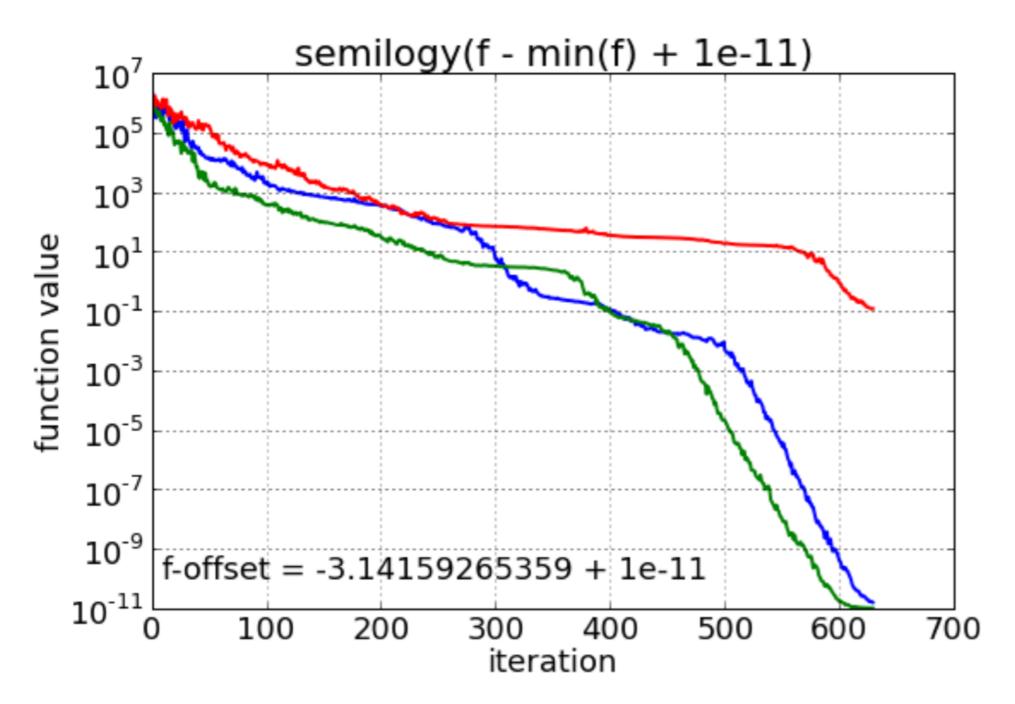
why not, what's wrong with it?

# Displaying Three Runs



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

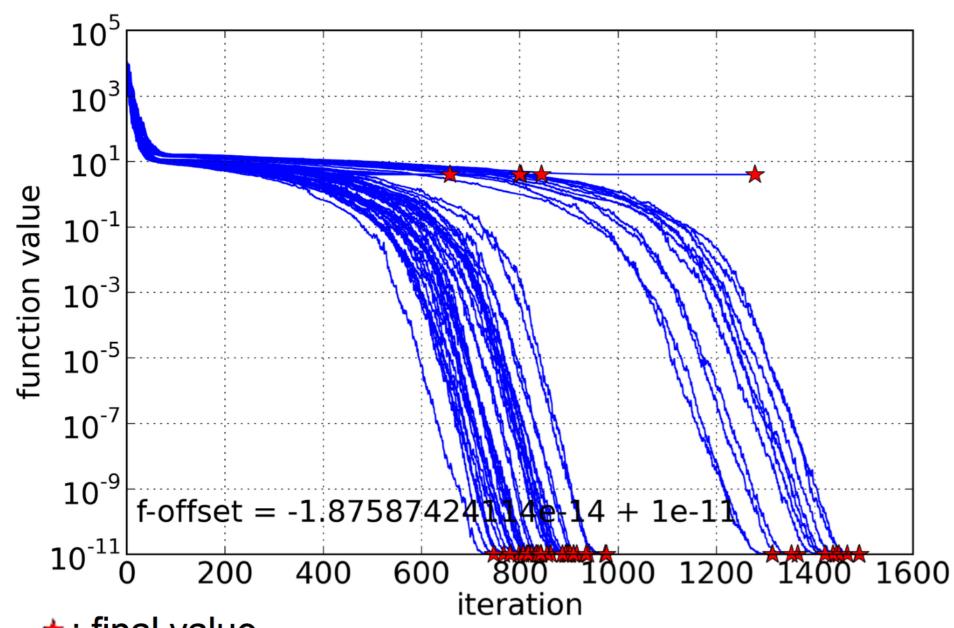
#### Displaying Three Runs



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

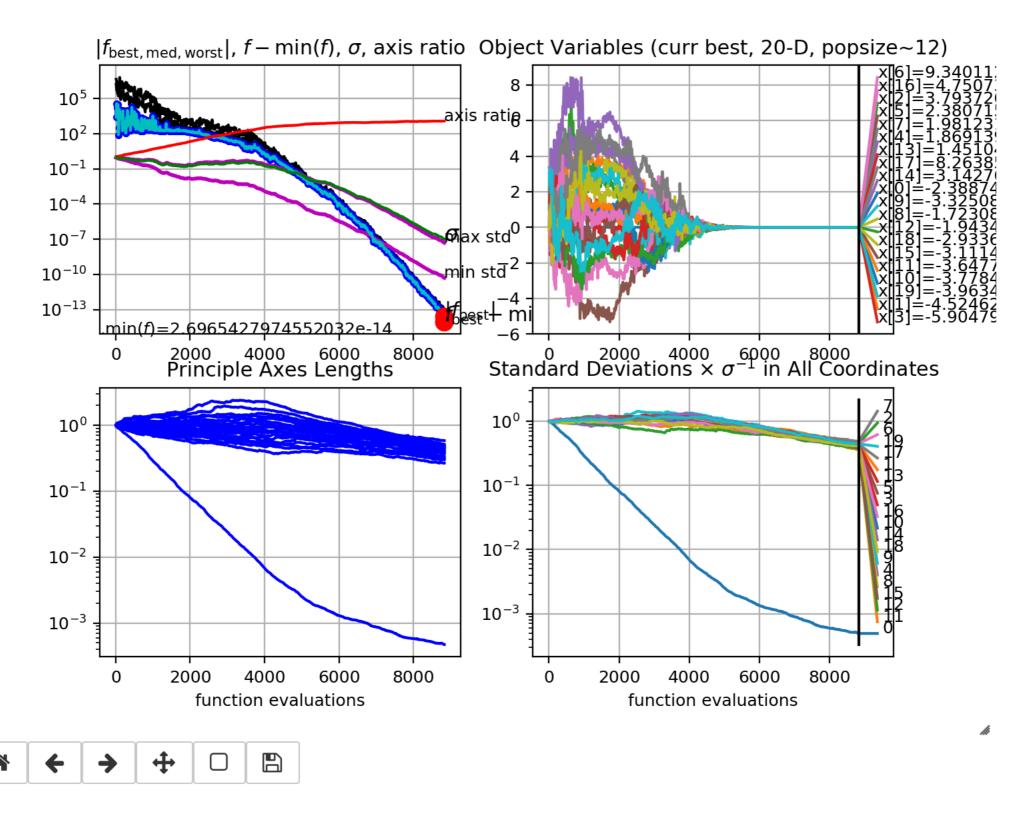
observation: three different "modes", which would be difficult to represent or recover in single statistics

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

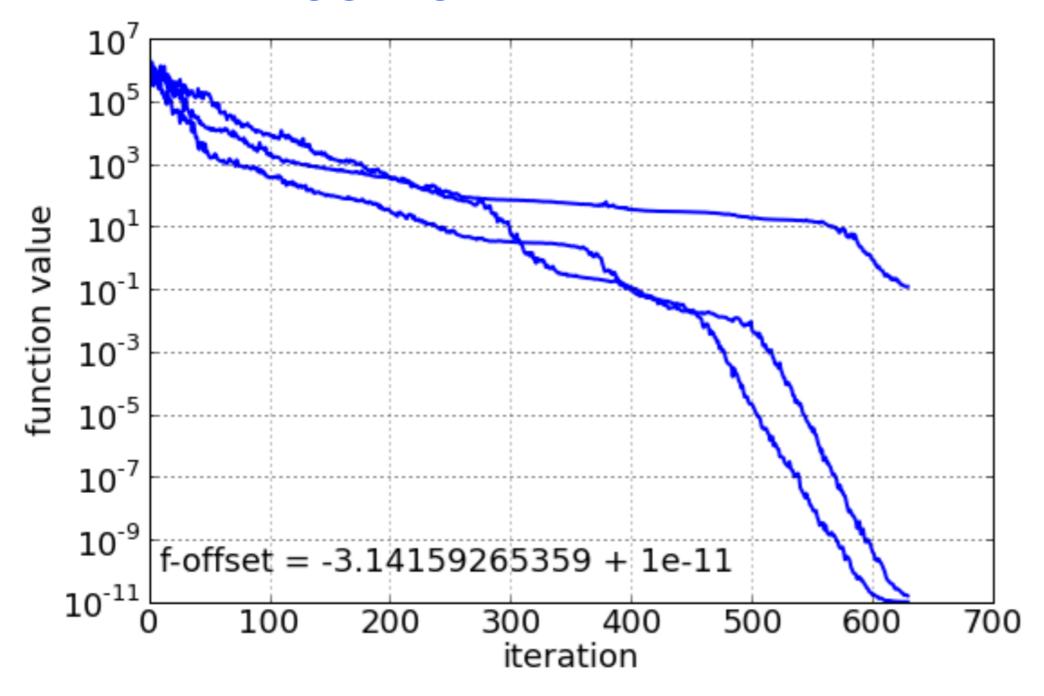
#### There is more to display than convergence graphs

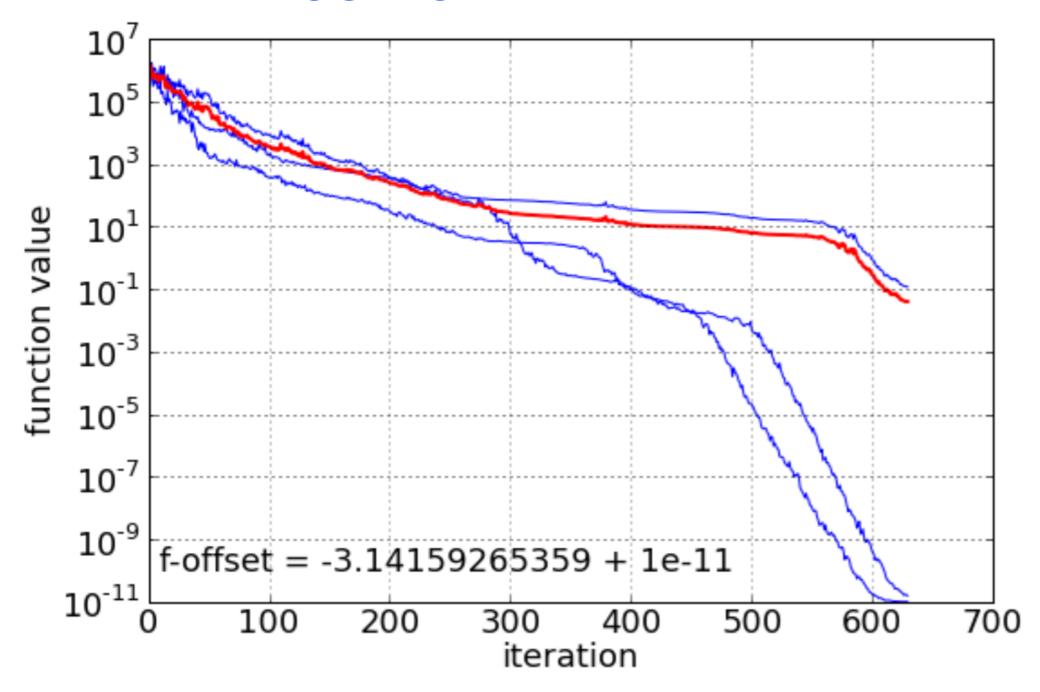
Figure 328

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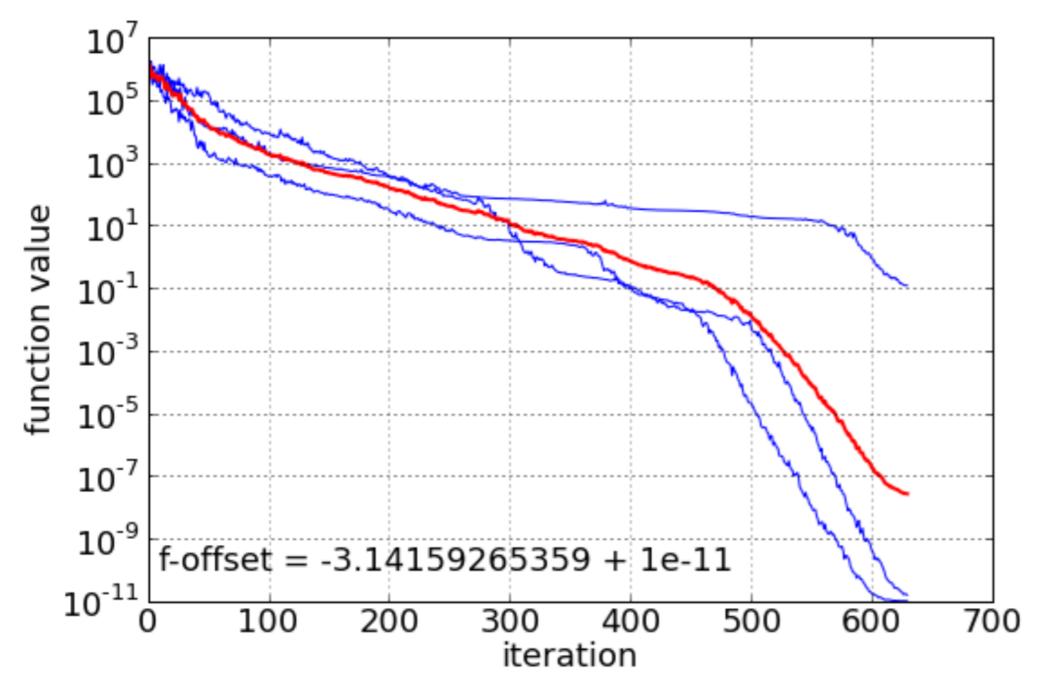
cma.plot()





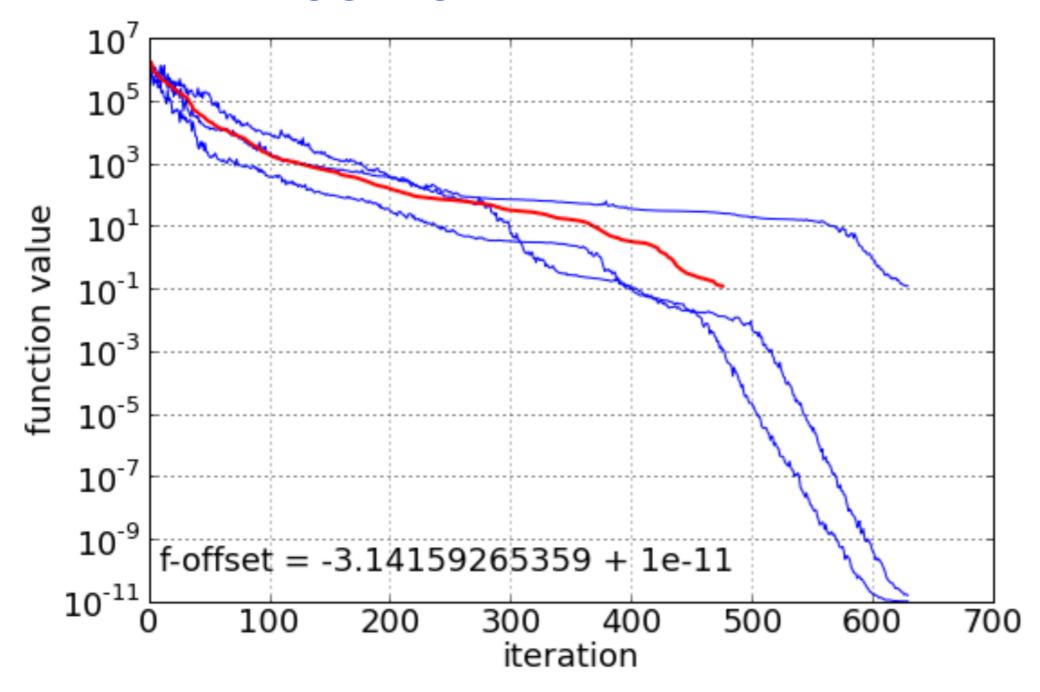
#### mean/average function value

tends to emphasize large values



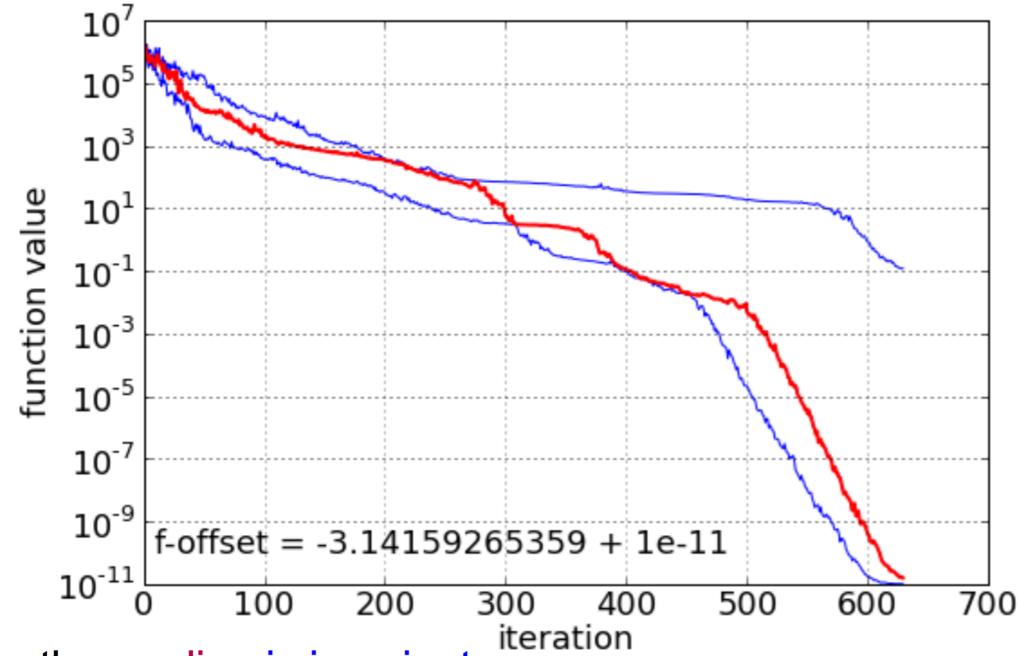
geometric average function value  $\exp(\mathrm{mean_i}(\log(f_i)))$  :

- reflects "visual" average
- depends on offset



#### average iterations

- reflects "visual" average
- here: incomplete



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**

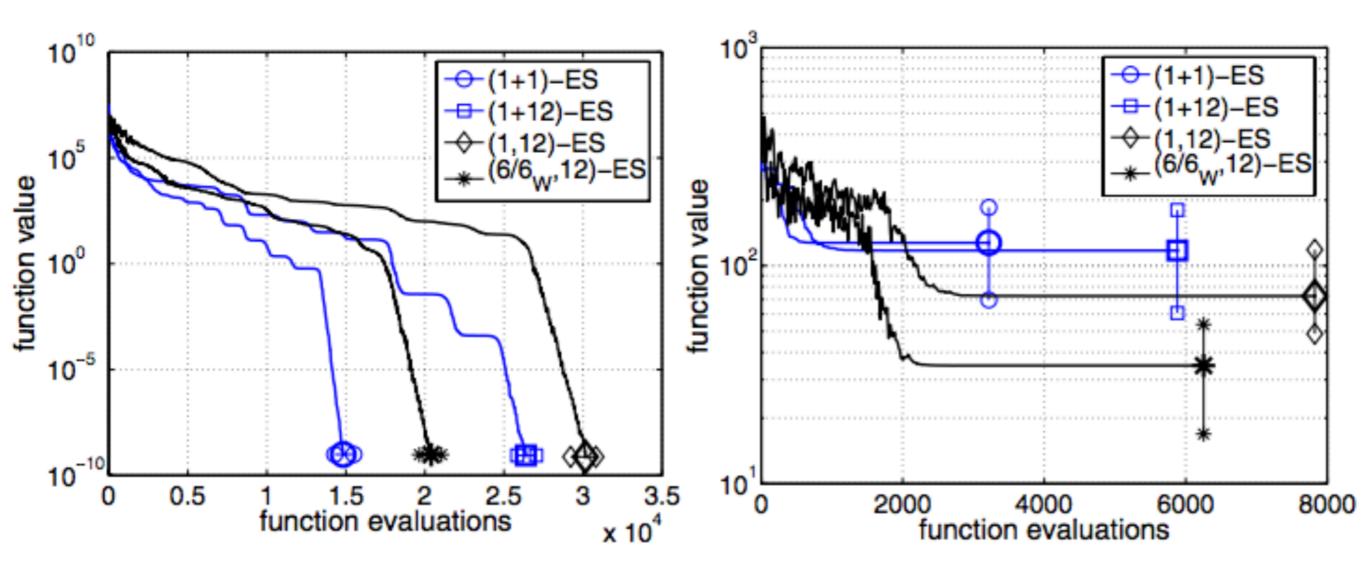
use the median as summary datum

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

more general: use quantiles as summary data

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

#### Examples

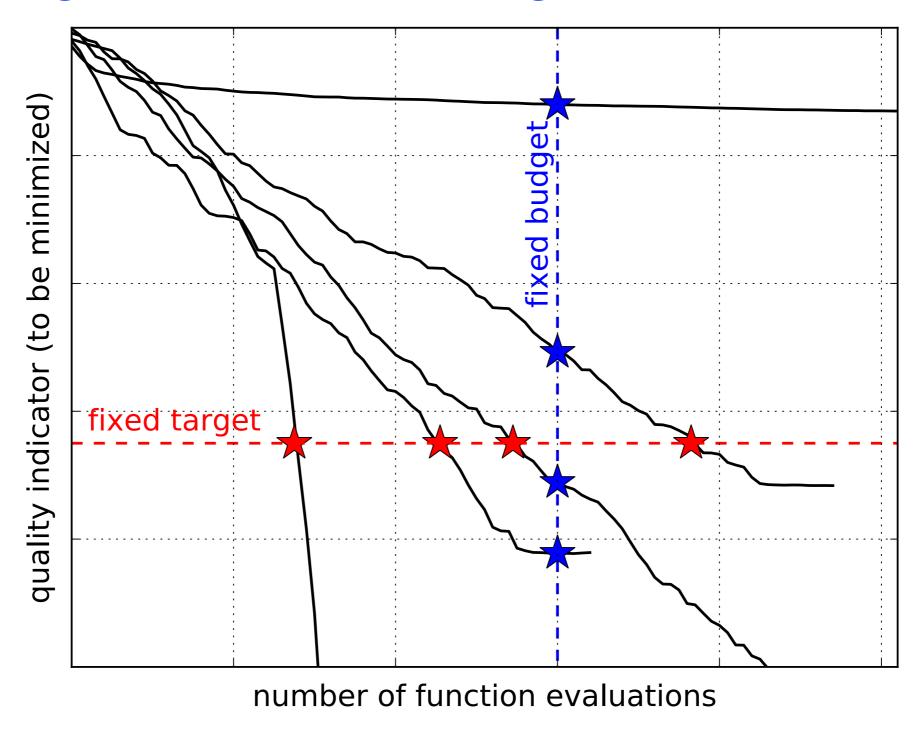


Comparison of 4 algorithms using the "median run" and the 90% central range of the final value on two different functions (Ellipsoid and Rastrigin)

caveat: the range display with error bars fails, if, for example, only 30% of all runs "converge"

How can we deal with large variations?

#### Aggregation: Fixed Budget vs Fixed Target



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

#### Performance Measures for Evaluation

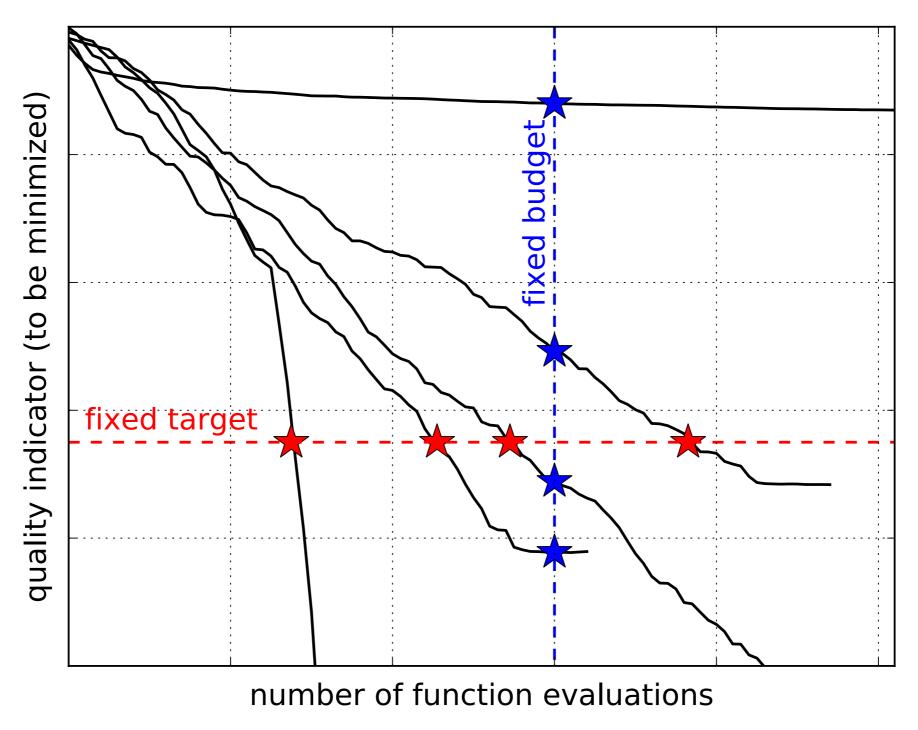
#### Generally, a performance measure should be

- quantitative on the ratio scale (highest possible)
   "algorithm A is two times better than algorithm B" as "performance(B) / performance(A) = 1/2 = 0.5"
   should be meaningful statements
- assuming a wide range of values
- meaningful (interpretable) with regard to the real world

transfer the measure from benchmarking to real world

runtime or first hitting time is the prime candidate

#### Aggregation: Fixed Budget vs Fixed Target



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## Fixed Budget vs Fixed Target

Fixed budget => measuring/display final/best f-values

Fixed target => measuring/display needed budgets (#evaluations)

Number of function evaluations:

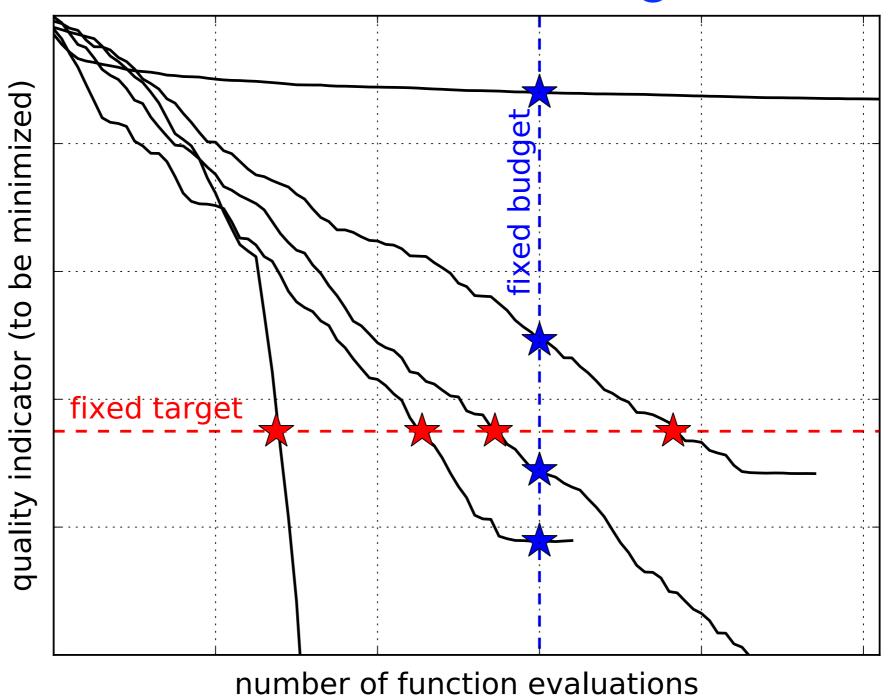
are quantitatively comparable (on a ratio scale)

ratio scale: "A is 3.5 times faster than B", A/B = 1/3.5 is a meaningful notion

- the measurement itself is interpretable independently of the function time remains the same time regardless of the underlying problem 3 times faster is 3 times faster is 3 times faster on every problem
- there is a clever way to account for missing data

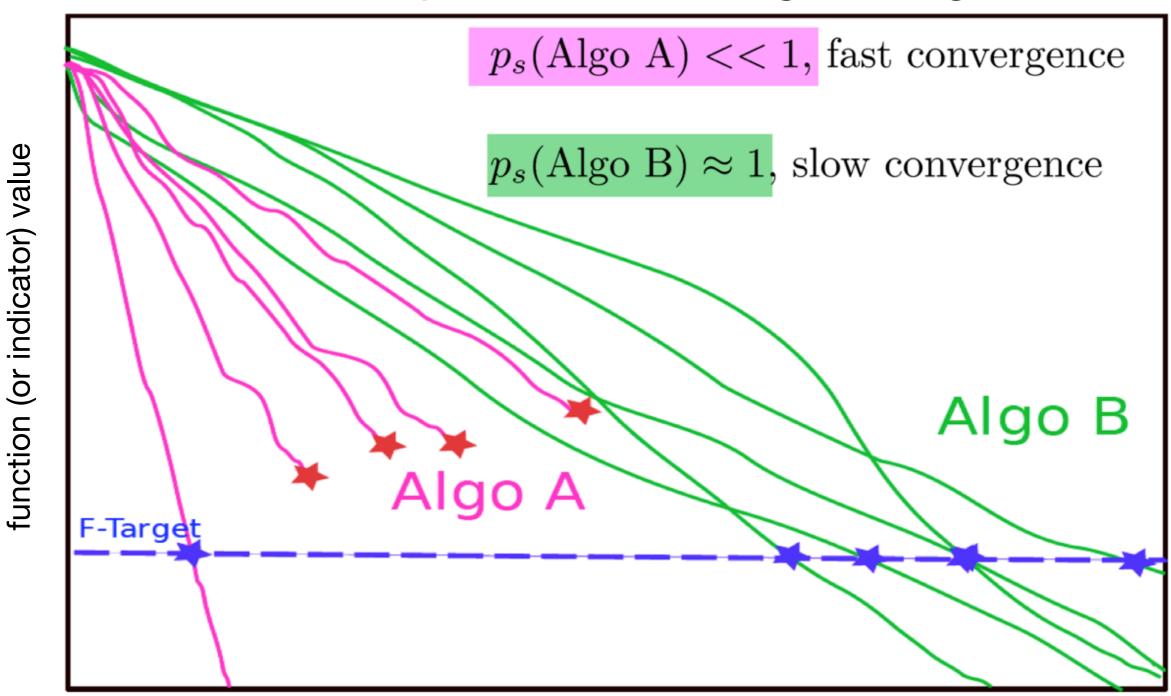
via restarts

=> fixed target is (much) preferable



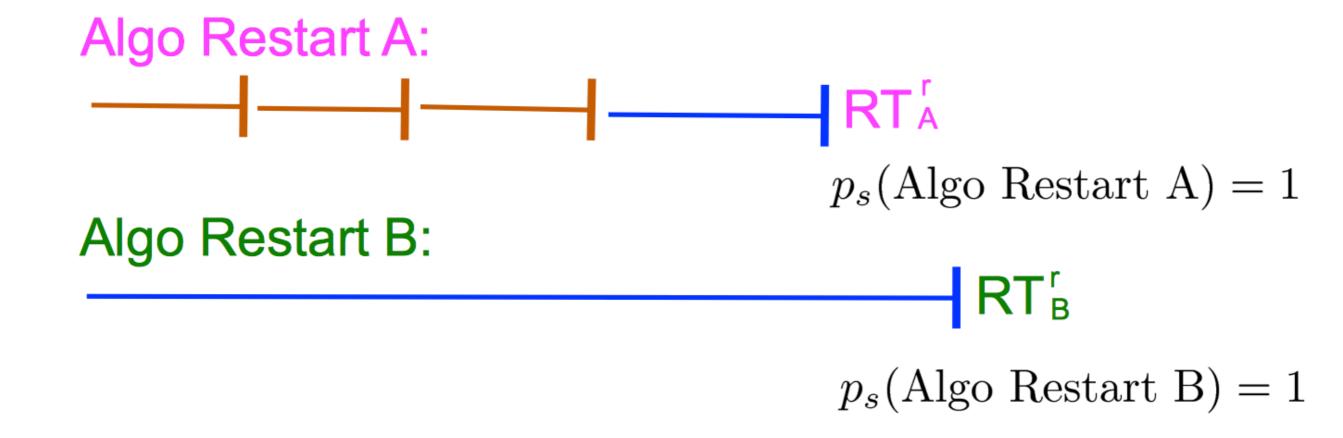
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how can we compare the following two algorithms?



number of evaluations

Consider simulated (artificial) restarts using the given independent runs



Caveat: the performance of algorithm A critically depends on termination methods (before to hit the target)

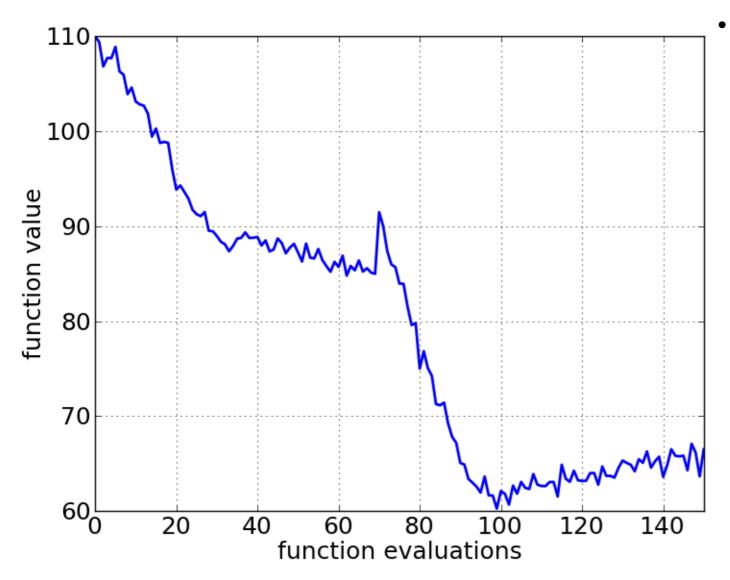
The expected runtime (ERT, aka SP2, aRT) to hit a target value in #evaluations is computed (estimated) as:

$$\begin{split} \text{ERT} &= \frac{\# \text{evaluations}(\text{until to hit the target})}{\# \text{successes}} & \text{unsuccessful runs count (only) in the nominator} \\ &= \text{avg}(\text{evals}_{\text{succ}}) + \frac{\overbrace{N_{\text{unsucc}}}^{\text{odds ratio}}}{N_{\text{succ}}} \times \text{avg}(\text{evals}_{\text{unsucc}}) \\ &\approx \text{avg}(\text{evals}_{\text{succ}}) + \frac{N_{\text{unsucc}}}{N_{\text{succ}}} \times \text{avg}(\text{evals}_{\text{succ}}) \\ &= \frac{N_{\text{succ}} + N_{\text{unsucc}}}{N_{\text{succ}}} \times \text{avg}(\text{evals}_{\text{succ}}) \\ &= \frac{1}{\text{success rate}} \times \text{avg}(\text{evals}_{\text{succ}}) \end{split}$$

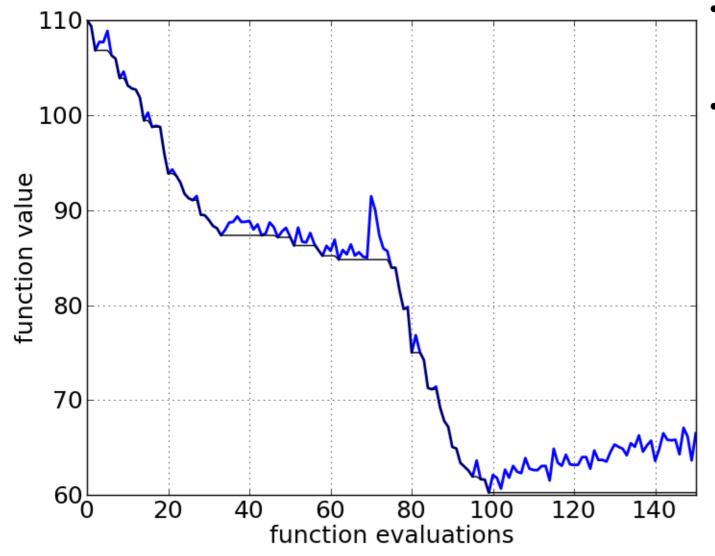
defined (only) for #successes > 0. The last three lines are aka Q-measure or SP1 (success performance).

#### **Empirical Distribution Functions**

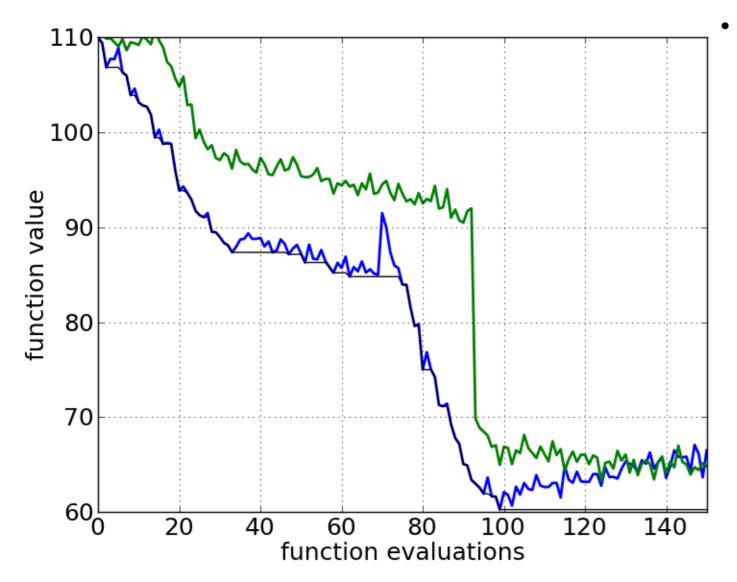
 Empirical cumulative distribution functions (ECDF, or in short, *empirical distributions*) are arguably the single most powerful tool to "aggregate" data in a display.



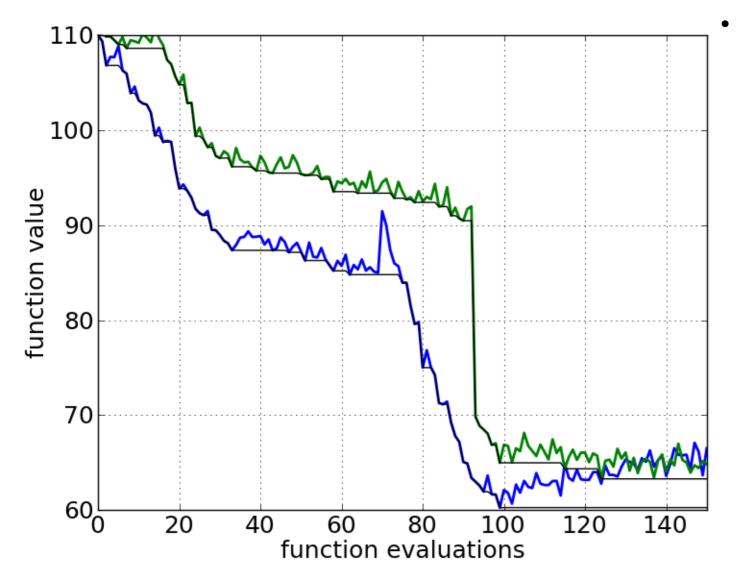
a convergence graph



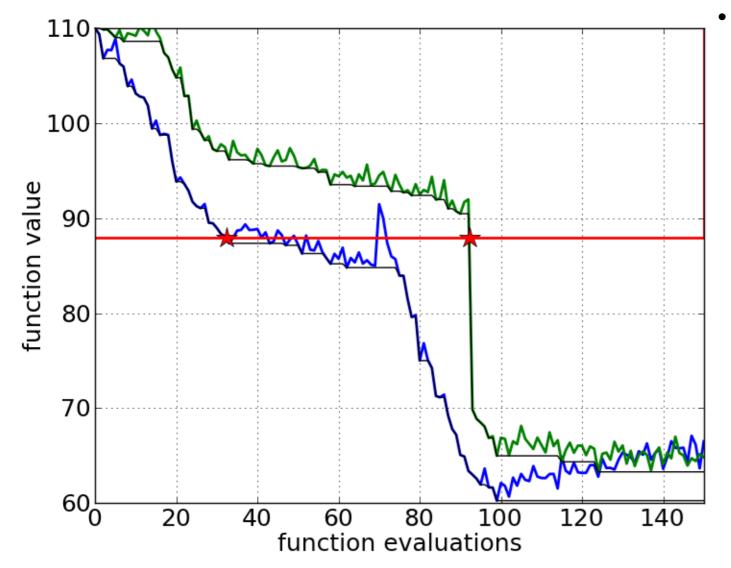
- a convergence graph
- first hitting time (black): lower envelope, a monotonous graph



another convergence graph

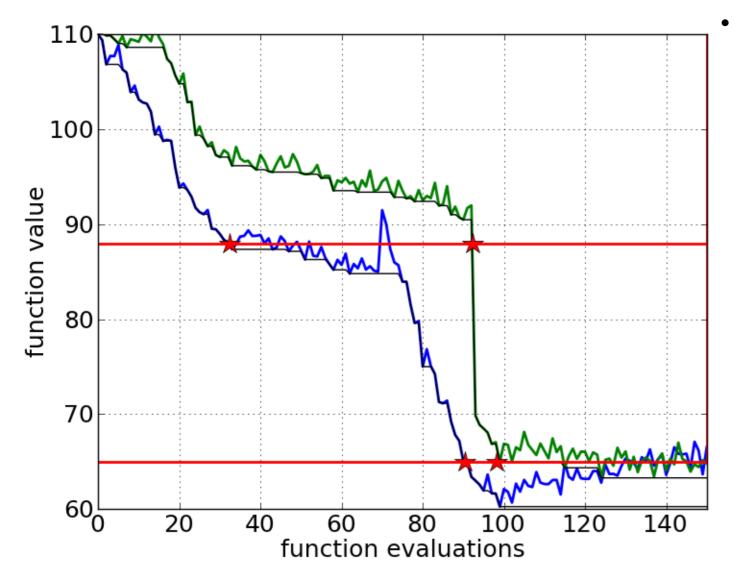


another convergence graph with hitting time

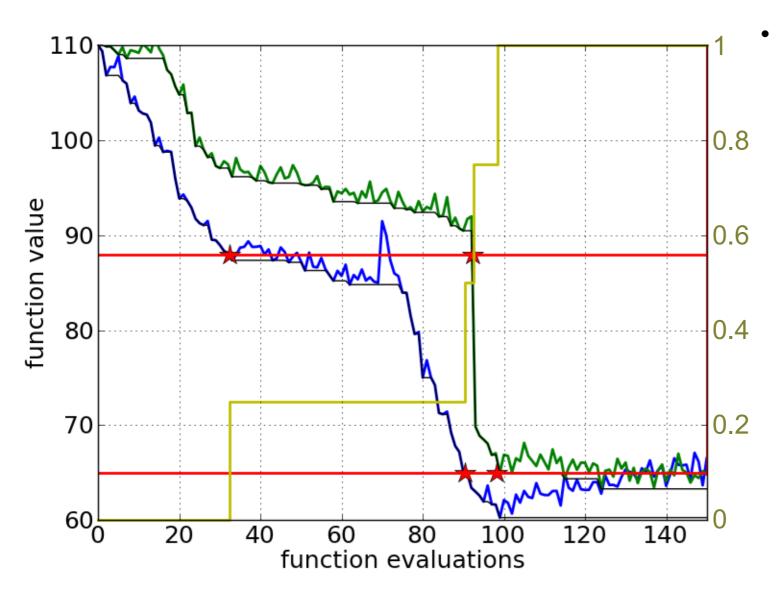


a target value delivers two data points (or possibly missing values)

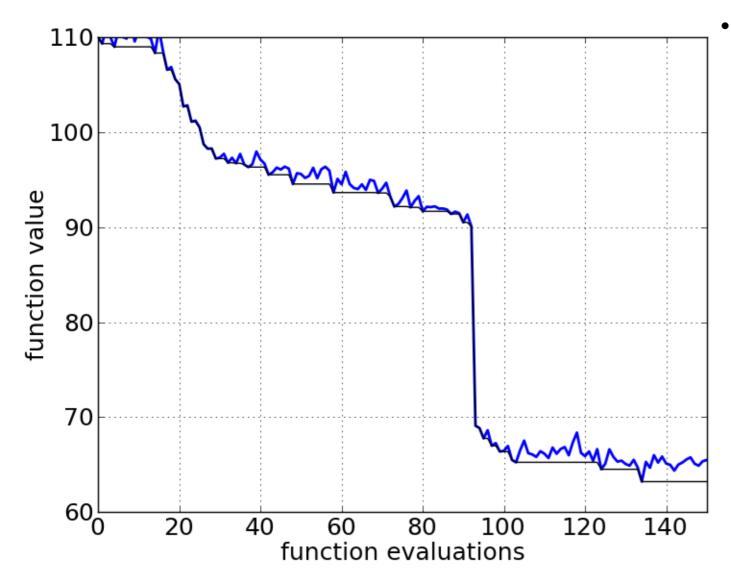
59



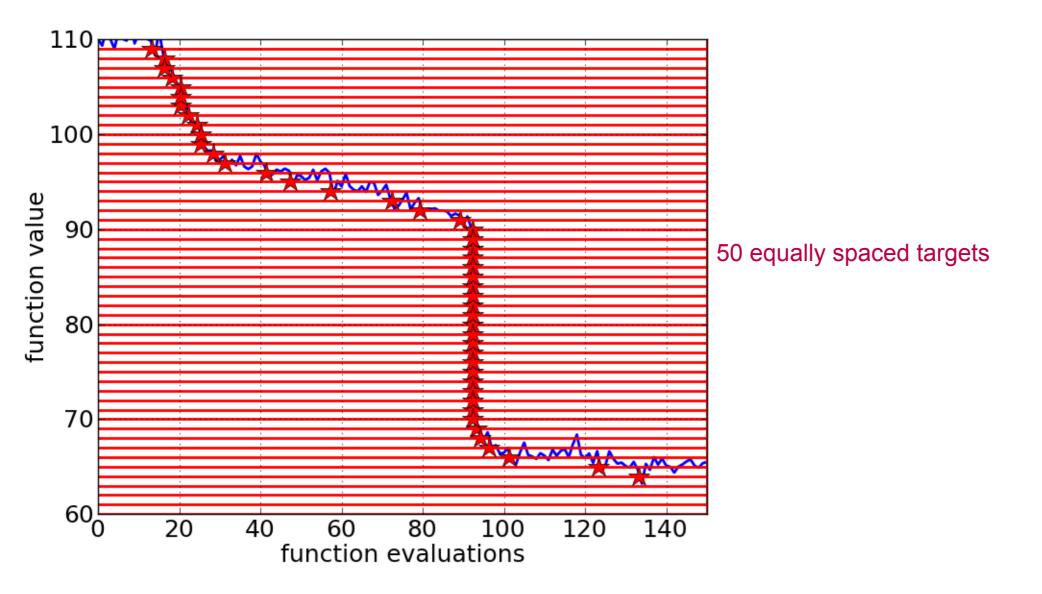
another target value delivers two more data points

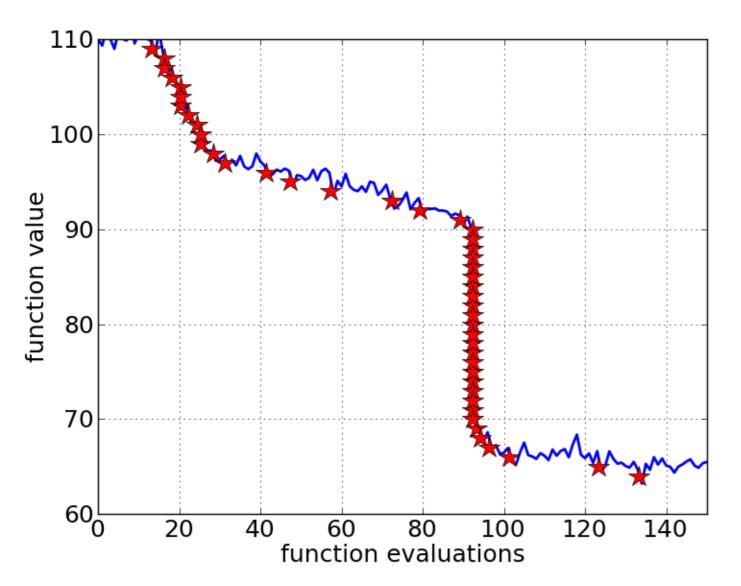


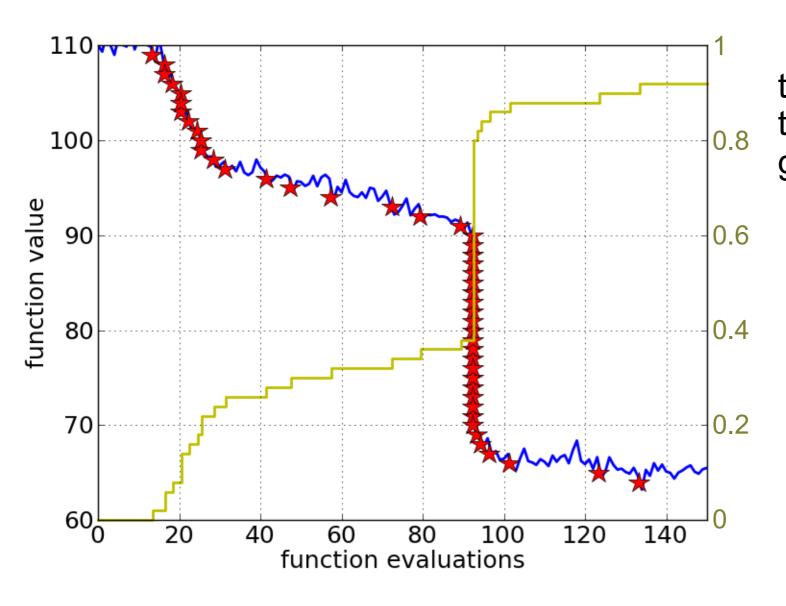
 the ECDF with four steps (between 0 and 1)



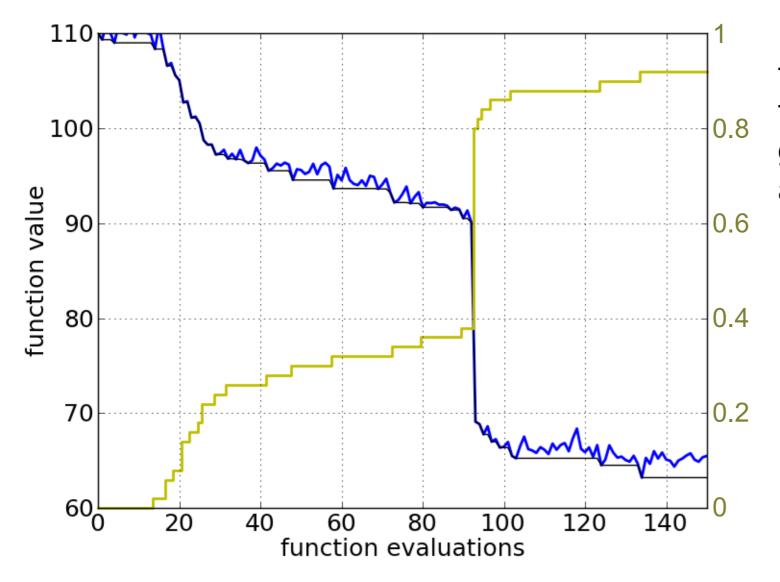
reconstructing a single run



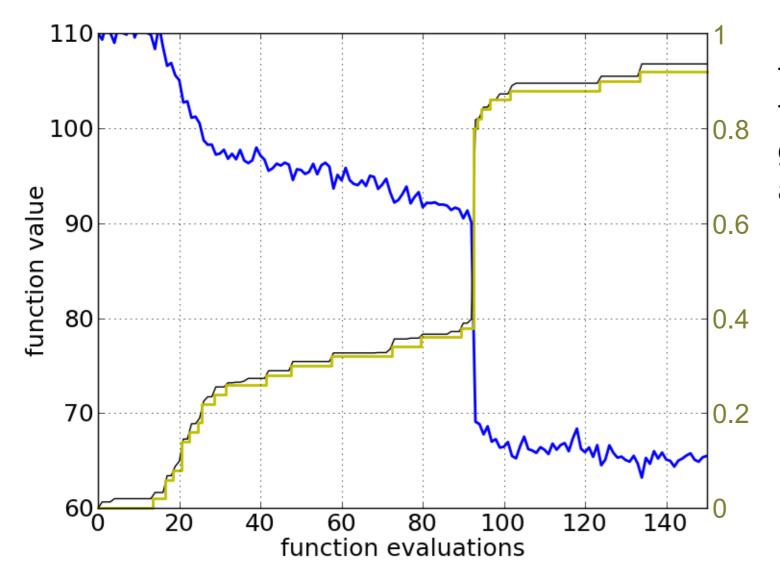




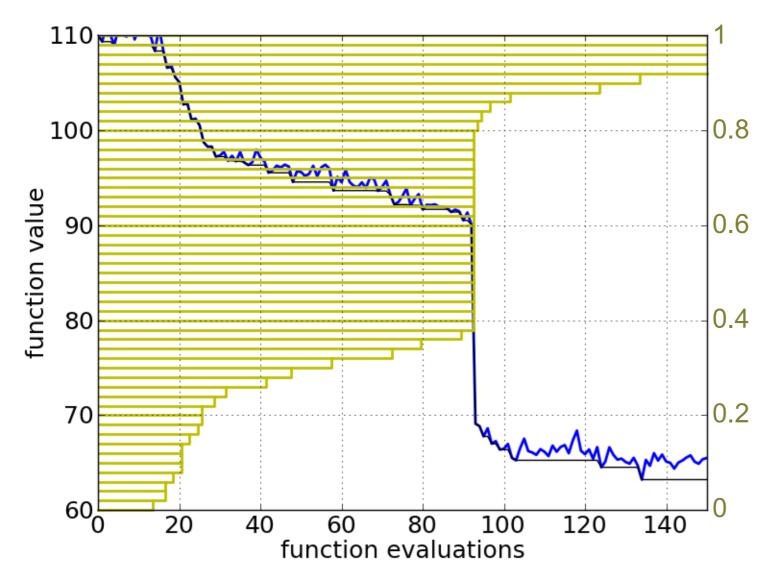
the ECDF recovers the monotonous graph



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)

#### Data and Performance Profiles

 so-called Data Profiles (Moré and Wild 2009) are empirical distributions of runtimes [# evaluations] to achieve a given single target

usually divided by dimension + 1

 so-called *Performance profiles* (Dolan and Moré 2002) are empirical distributions of *relative* runtimes [# evaluations] to achieve a given single target

normalized by the runtime of the fastest algorithm on the respective problem

# 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 beta 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 :-)
```

```
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

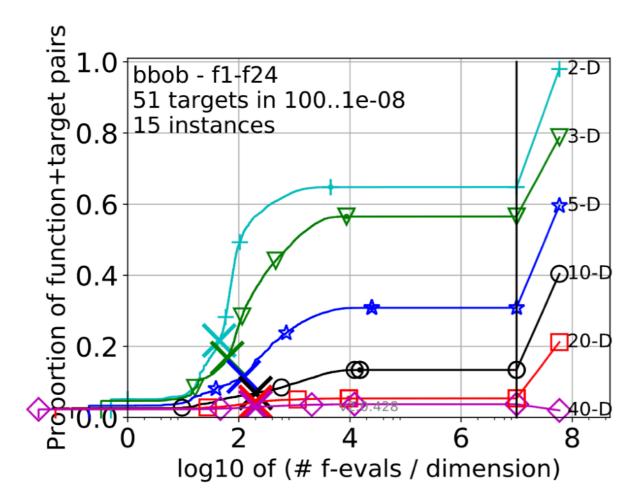
**Scaling with dimension for selected targets** 

**Tables for selected targets** 

Runtime distribution for selected targets and f-distributions

**Runtime loss ratios** 

#### Runtime distributions (ECDFs) over all targets



#### **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

## Using Theory in Experimentation

- shape our expectations and objectives
  - debugging / consistency checks
     theory may tell us what we expect to see
  - knowing the limits (optimal bounds)
     for example, we cannot converge faster than optimal trying to improve is a waste of time
- utilize invariance

it may be possible to design a much simpler experiment and get to the same or stronger conclusion by invariance considerations change of coordinate system is a powerful tool

FIN