A Practical Guide to Experimentation (and Benchmarking)

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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

Scientific Experimentation (dos and don'ts)

- 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?

Scientific Experimentation (dos and don’ts)

- 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 [Ioannidis 2005]

- practice to make predictions of the (possible/expected) 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

Scientific Experimentation (dos and don’ts)

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  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

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- *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

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- Invariance is a very powerful, almost indispensable tool

Invariance: binary variables

Assigning 0/1 (for example minimize $\sum_i x_i$ 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

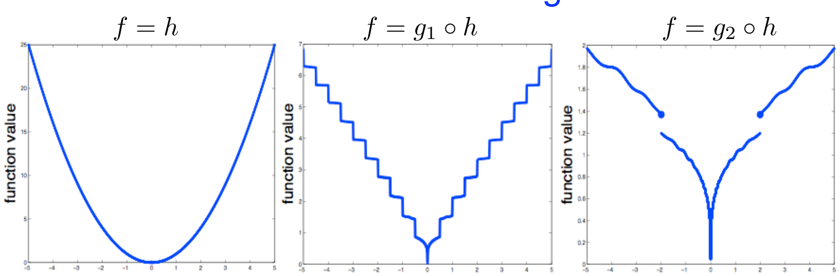
Invariance: binary variables

Permutation of variables

- is another "arbitrary" and "trivial" encoding choice and
- is another norm-preserving transformation
- does not change the function "structure" (as above)
- may affect the neighbourhood depending on the operators (recombination, mutation)

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

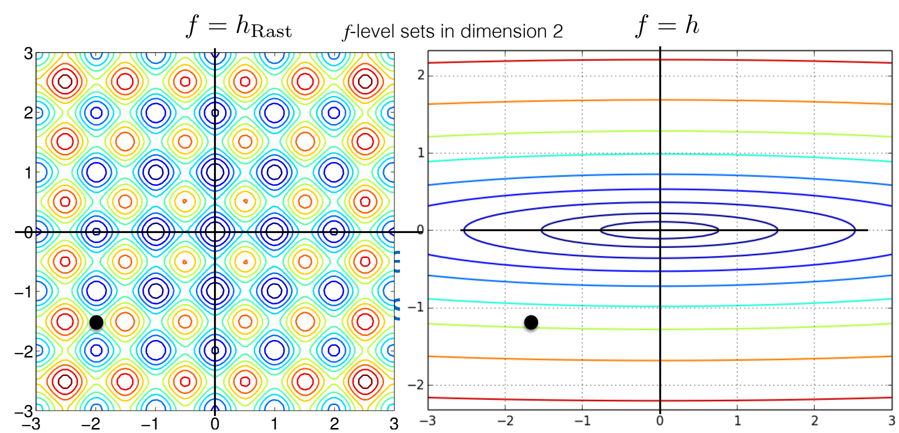
A *function-value free search algorithm* is invariant under the transformation with any order preserving (strictly increasing) g.

Invariances make

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

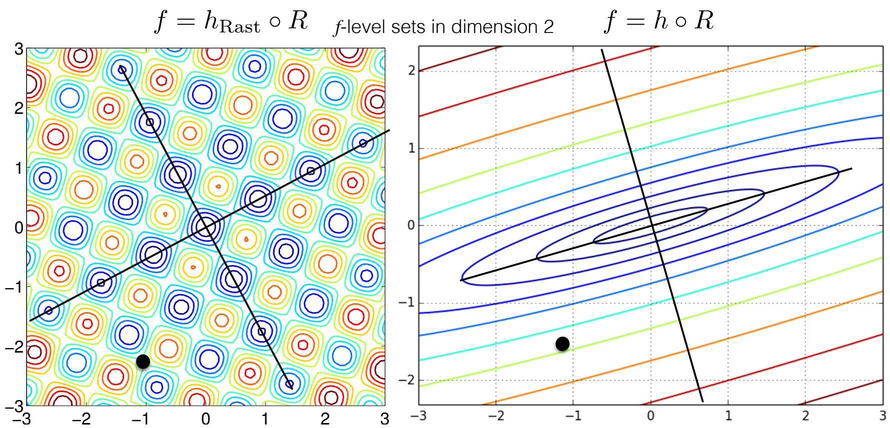
as a rigorous notion of generalization

Invariance Under Rigid Search Space Transformations



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

Invariance Under Rigid Search Space Transformations



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.

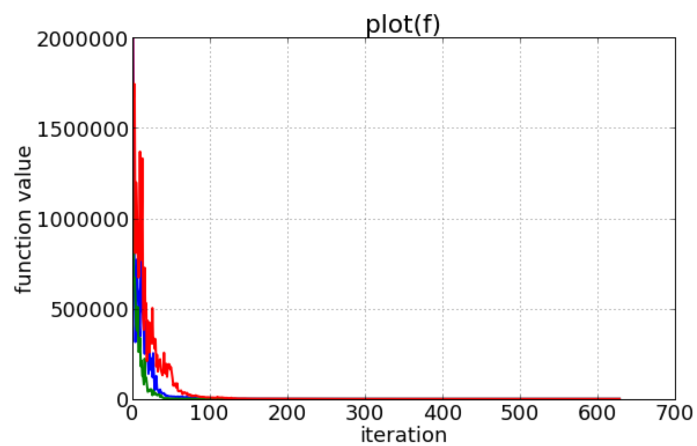
Measuring Performance

Empirically

convergence graphs is all we have to start with

the right presentation is important!

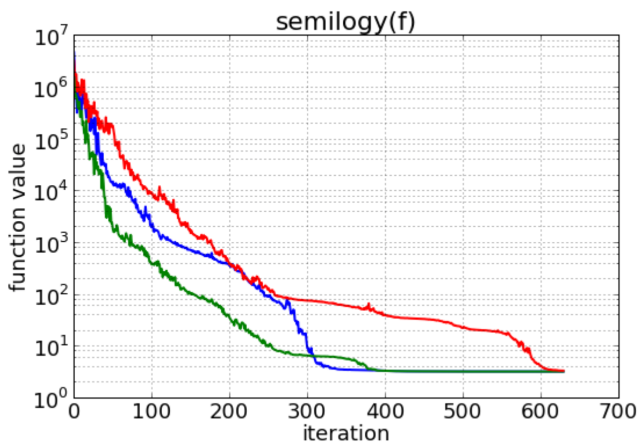
Displaying Three Runs



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

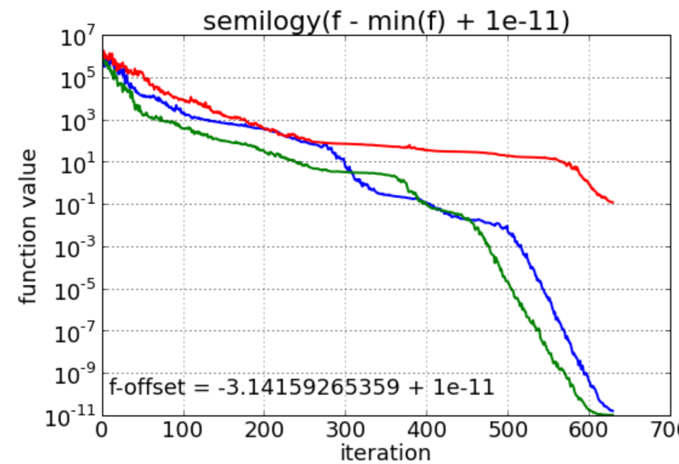
why not, what's wrong with it?

Displaying Three Runs



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

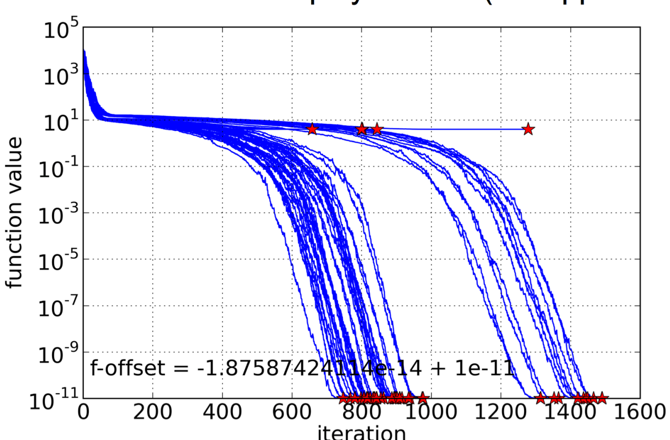
Displaying Three Runs



even better like this: subtract minimum value over all runs

Displaying 51 Runs

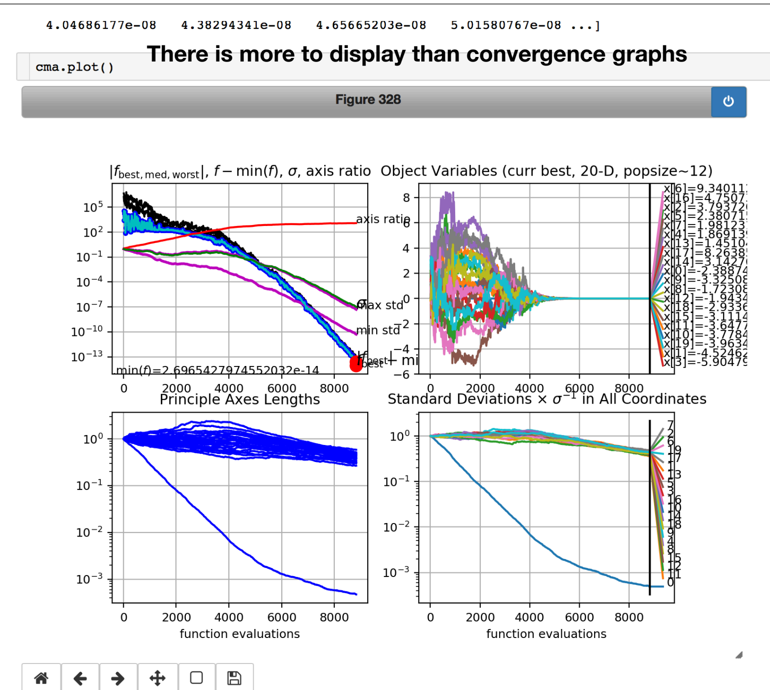
don't hesitate to display all data (the appendix is your friend)



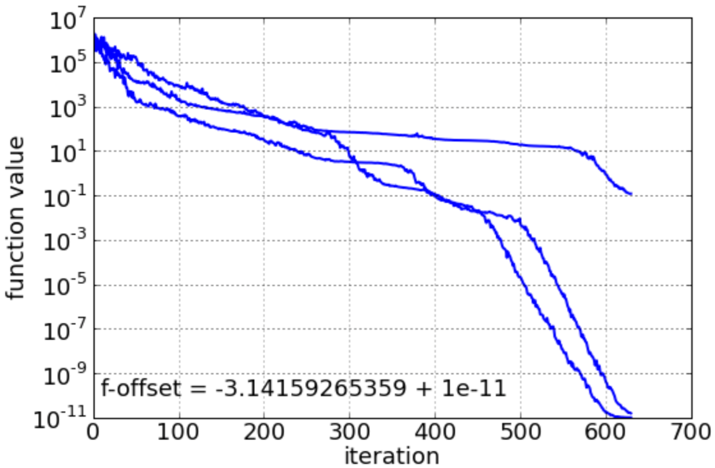
★ : final value

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

There is more to display than convergence graphs



Aggregation: Which Statistics?



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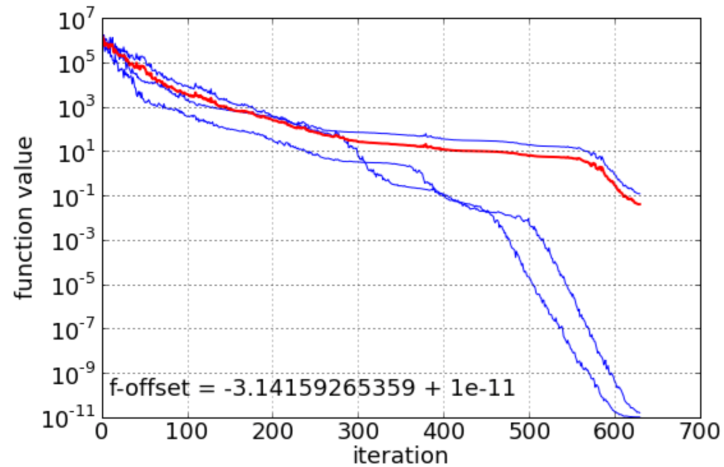


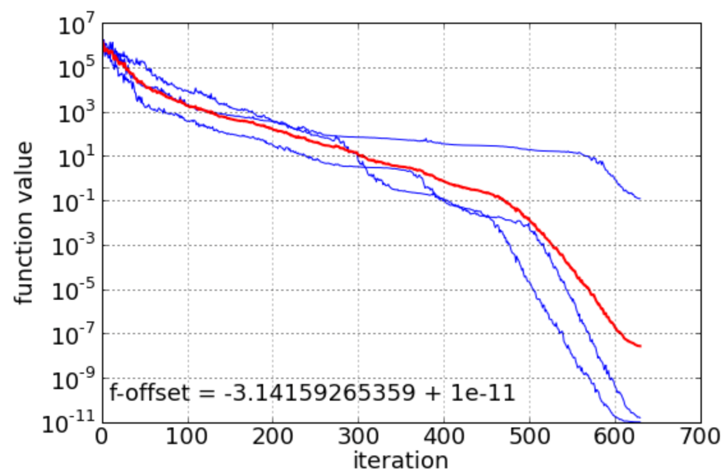
mean/average function value

- tends to emphasize large values

More Caveats on Averages/Expectations

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

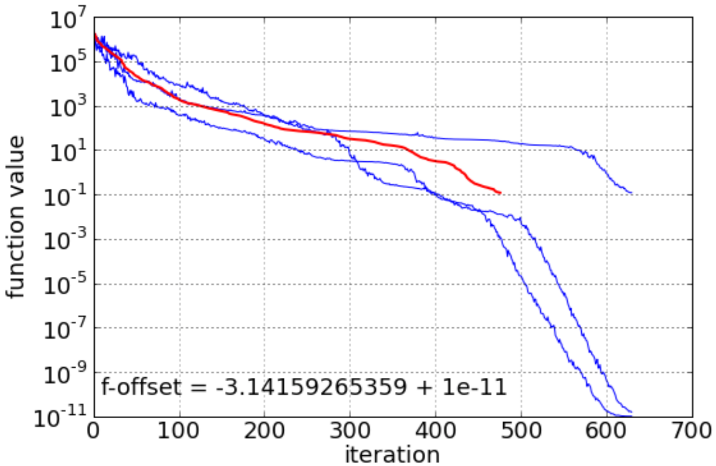
Aggregation: Which Statistics?



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

- reflects "visual" average
- depends on offset

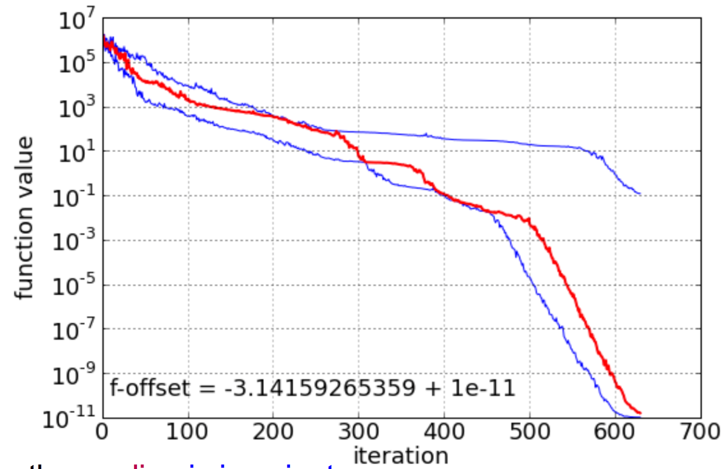
Aggregation: Which Statistics?



average iterations

- reflects "visual" average
- here: incomplete

Aggregation: 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

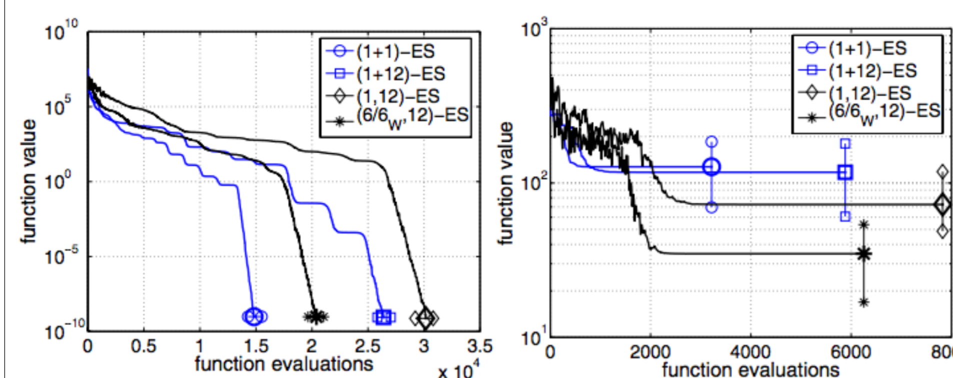
- use the median as summary datum

  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

Two More 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"

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

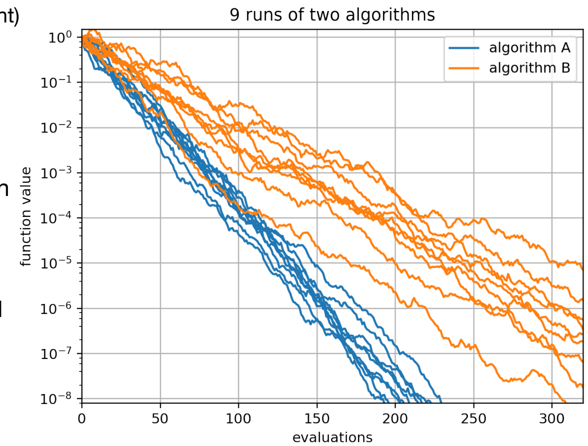
"experimental results lacking proper statistical analysis must be considered anecdotal at best, or even wholly inaccurate"

— M. Wineberg

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

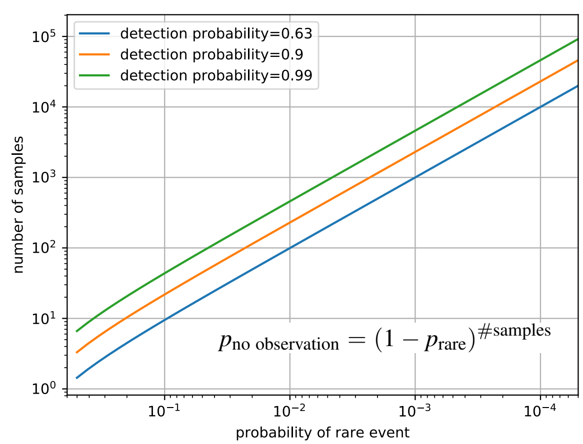
an experimental result (shown are *all data obtained*):

Do we (even) need a statistical analysis?



Rare Events

- The obvious: if we consider rare events to be important, we have to sample many data



Statistical Significance: General Prodecure

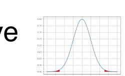
- *first*, check *the relevance* of the result, for example of the difference which is to be tested for statistical significance

  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

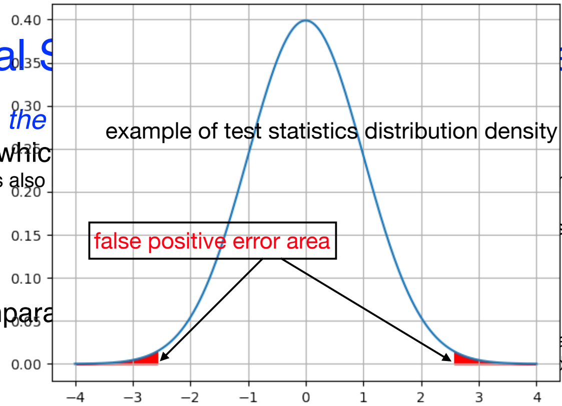
  

  smaller p-values are better
  <0.1% or <1% or <5% is usually considered as *statistically significant*

- *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

Statistical S… …ecure



- *first*, check *the* … difference whic…
  this also … …mbinations) … *statistically* … simple trick, … *meaningful*
- prefer "nonpara… …*arametrised* …istributions
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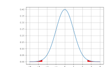

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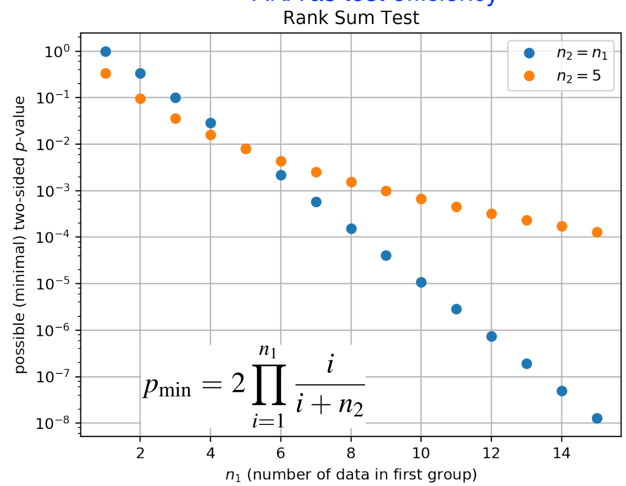
Statistical Significance: Methods

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

Statistical Significance: How many data do we need?

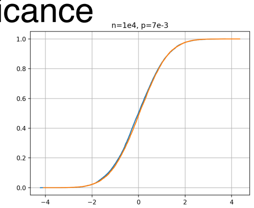
- In the best case: at least ten (two times five) and *two times nine is plenty*

  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



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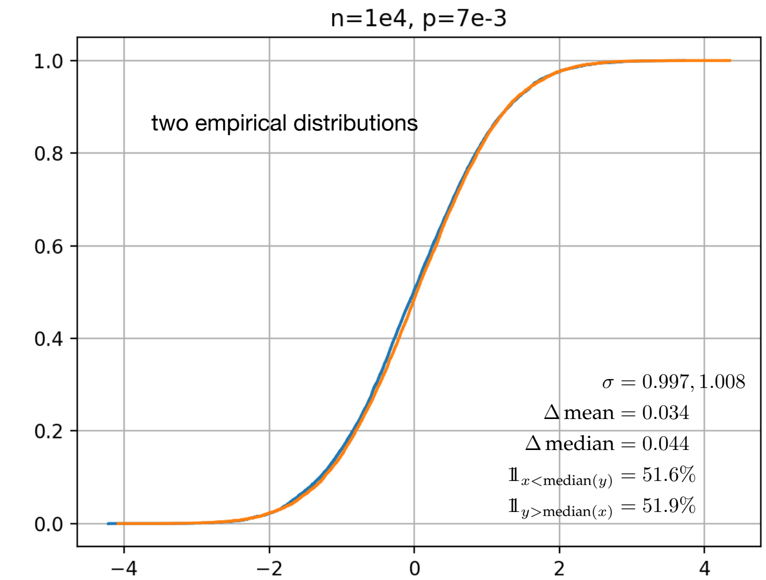

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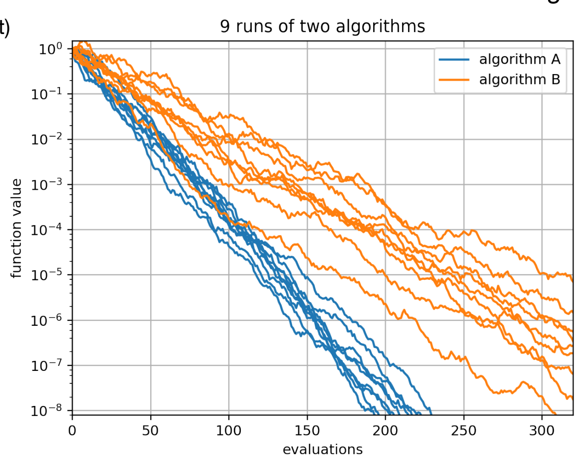


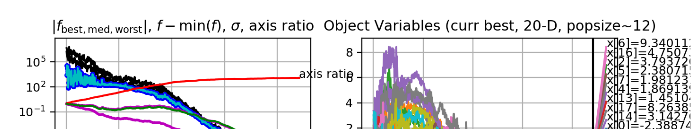
Jupyter IPython notebook

```
%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()
```

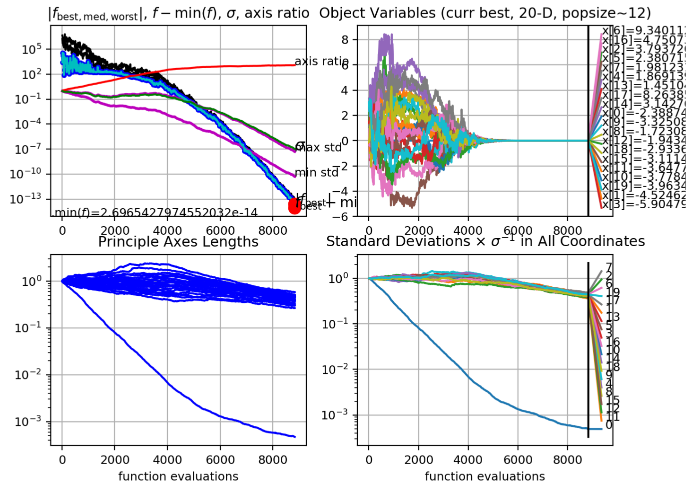
Figure 328



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

```
cma.plot()
```

Figure 328



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 https://github.com/nikohansen/GECCO-2019-experimentation-guide-notebooks
- 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".
- Create sections plots (f vs x on a line)
  one-dimensional grid search is cheap
- 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 http://cma.gforge.inria.fr/cmaes_sourcecode_page.html#practical

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

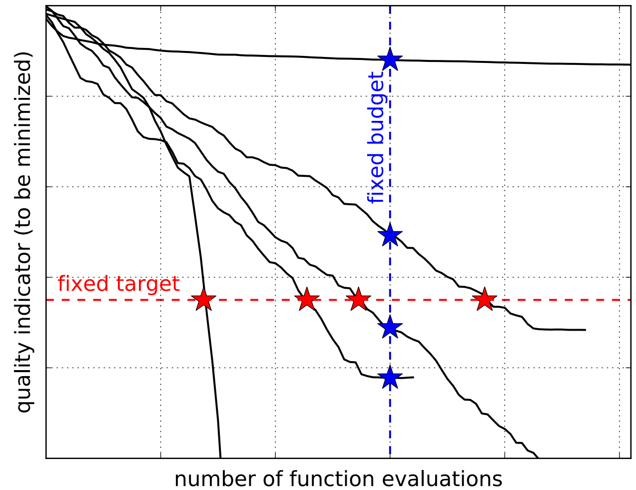
- regression testing after (small) changes

  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

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

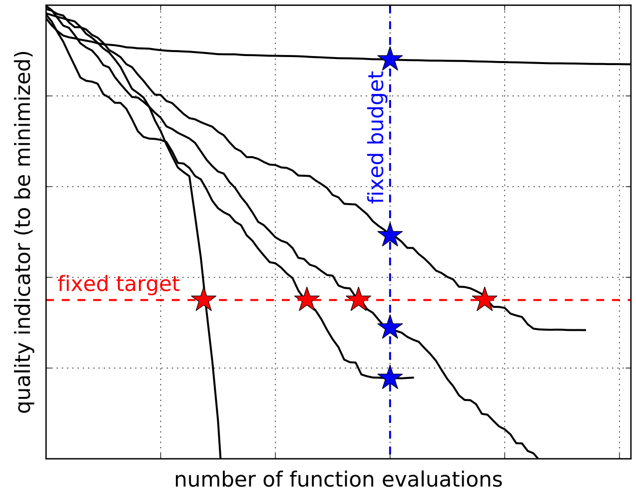
Performance Measures for Evaluation

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



- 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

Fixed Budget vs Fixed Target

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

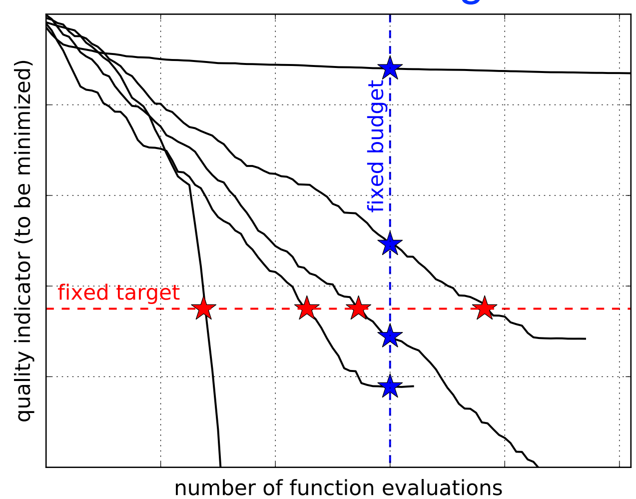
Fixed target => *measuring/display* *needed* budgets (#evaluations)

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

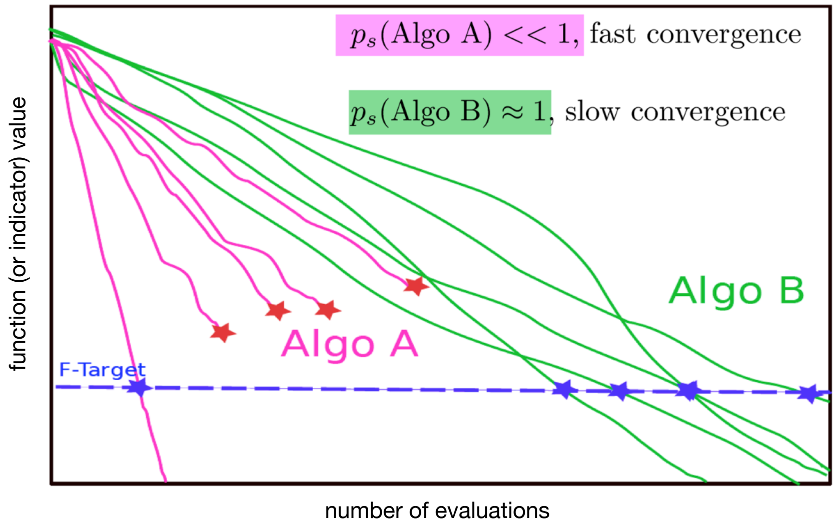
The Problem of Missing Values



- 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

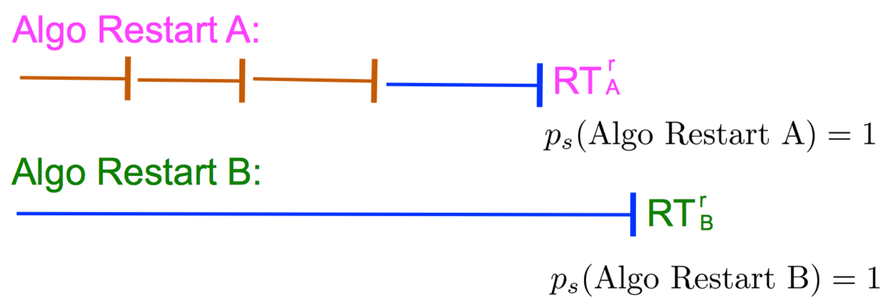
The Problem of Missing Values

how can we compare the following two algorithms?



The Problem of Missing Values

Consider simulated (artificial) restarts using the given independent runs



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

The Problem of Missing Values

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

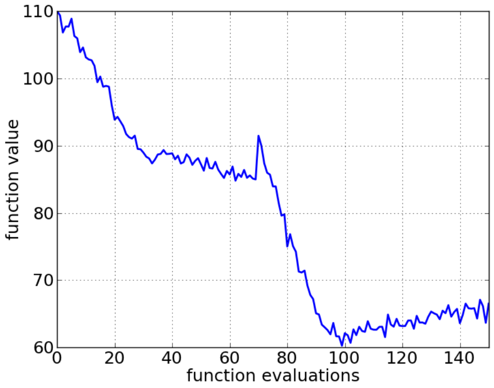
$$\begin{aligned}
\text{ERT} &= \frac{\text{\#evaluations(until to hit the target)}}{\text{\#successes}} \\
&= \text{avg}(\text{evals}_{\text{succ}}) + \overbrace{\frac{N_{\text{unsucc}}}{N_{\text{succ}}}}^{\text{odds ratio}} \times \text{avg}(\text{evals}_{\text{unsucc}}) \\
&\approx \text{avg}(\text{evals}_{\text{succ}})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

unsuccessful runs count (only) in the nominator

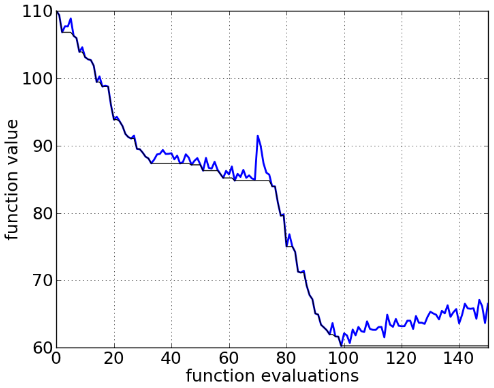
defined (only) for #successes > 0. The last three lines are aka Q-measure or SP1 (success performance).

Empirical Distribution Functions

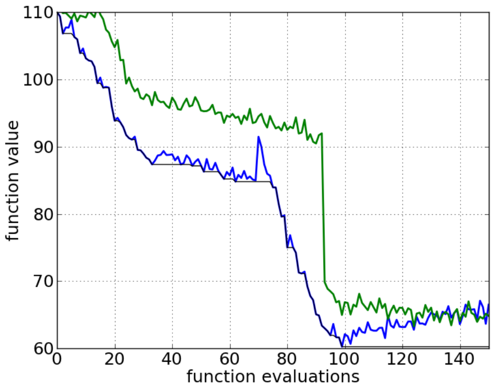
- Empirical cumulative distribution functions (ECDF, or in short, *empirical distributions*) are arguably the single most powerful tool to "aggregate" data in a display.



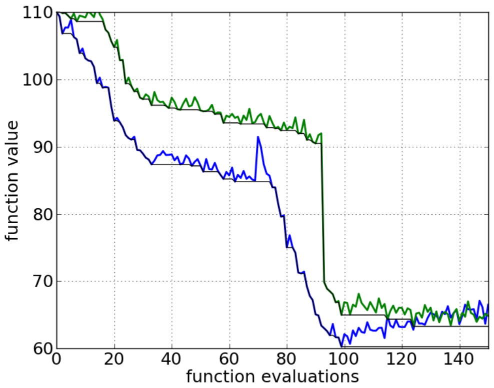
- a convergence graph



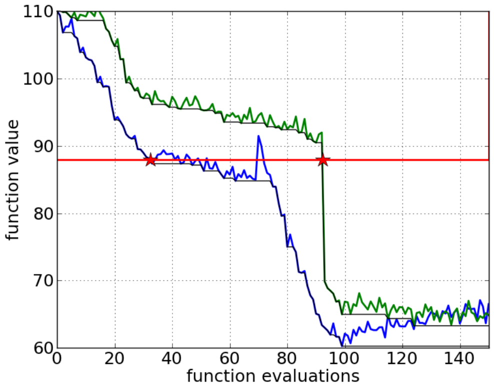
- a convergence graph
- first hitting time (black): lower envelope, a monotonous graph



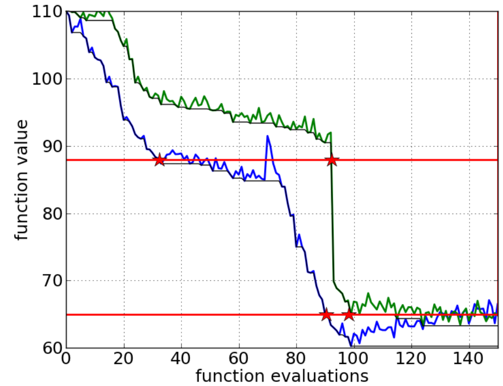
- another convergence graph



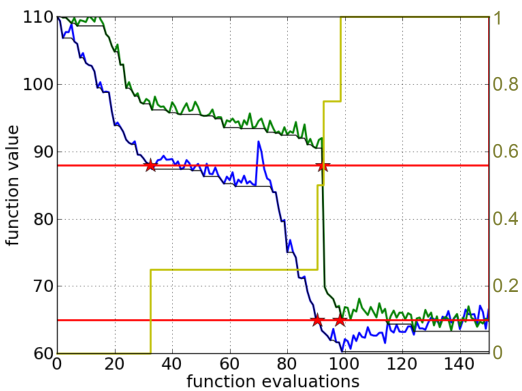
- another convergence graph with hitting time



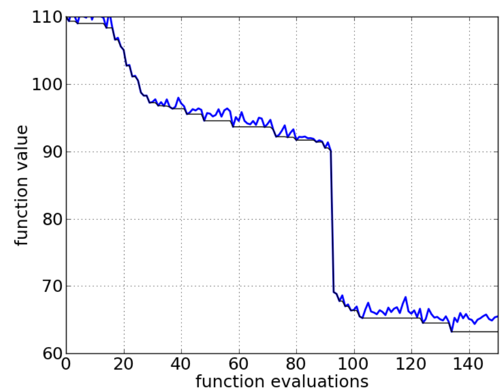
- a target value delivers two data points (or possibly missing values)



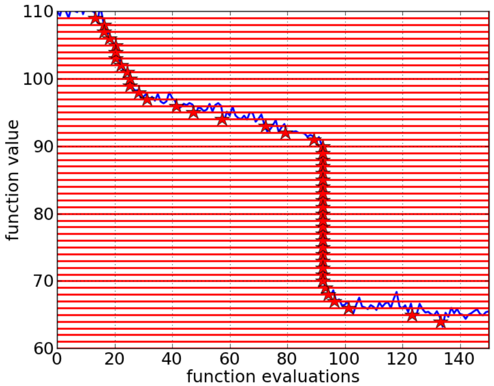
- another target value delivers two more data points



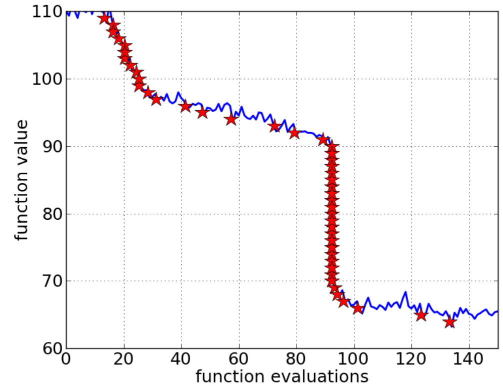
- the ECDF with four steps (between 0 and 1)

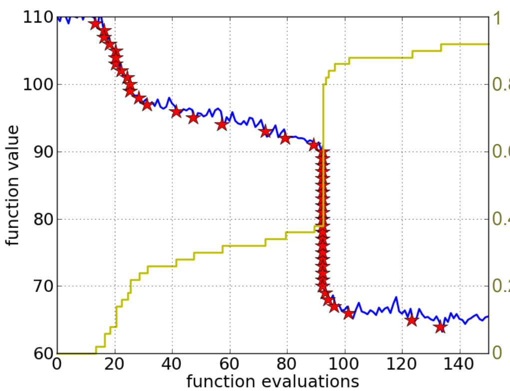


- reconstructing a single run

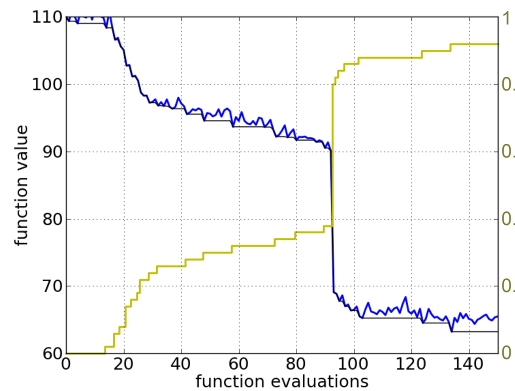


50 equally spaced targets

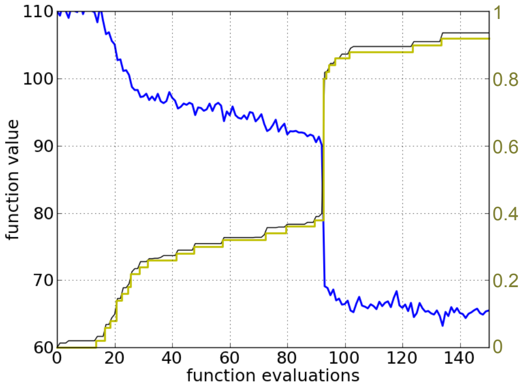




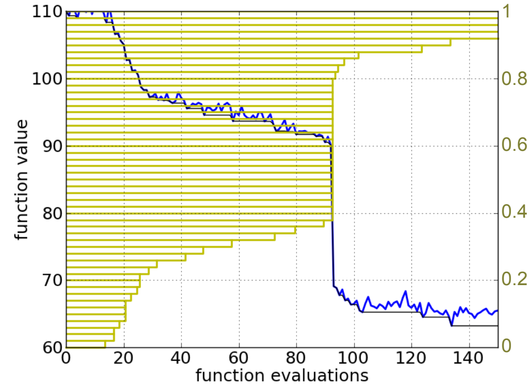
the ECDF recovers
the monotonous
graph



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 :-)
```

```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

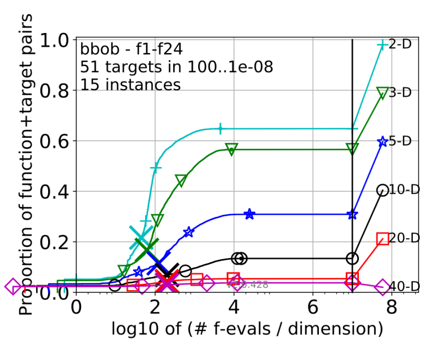
Scaling with dimension for selected targets

Tables for selected targets

Runtime distribution for selected targets and f-distributions

Runtime loss ratios

Runtime distributions (ECDFs) over all targets



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