# A Practical Guide to Experimentation (and Benchmarking)

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GECCO '19 Companion, July 13–17, 2019, Prague, Czech Republic

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ACM ISBN 978-14503-6748-6/19/07.

https://doi.org/10.1145/3.19810.3233207

#### Overview

- · Scientific experimentation
- Invariance
- · Display results
- · Statistical analysis
- · Performance assessment
- · What to measure
- · How to display
- Aggregation
- · Empirical distributions
- · Benchmarking with COCO
- · Using theory
- · Approaching an unknown problem
- A practical experimentation session

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A practical guide to experimentation (and benchmarking)

#### Overview

Do not hesitate to ask questions!

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# 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

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#### 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/lest "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 (quick test of code snippets) Why Most Published Research Findings Are False [loannidis 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

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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 the data, 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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#### Scientific Experimentation (dos and don'ts)

don't make minimising CPU-time a primary objective
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· Testing Heuristics: We Have it All Wrong [Hooker 1995]

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"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 decisions

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

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

Scientific Experimentation (dos and don'ts)

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Invariance is a very powerful, almost indispensable tool

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#### 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)

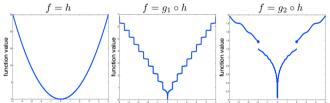
a permutation introduces structure that we may want to exploit even at the cost of abandoning invariance

Instead of 1 function, we now consider n! different but equivalent functions

 $n! \gg 2^n$ , that is, the number of permutations is even (much) larger than the size of the search space

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#### **Invariance Under Order Preserving Transformations**



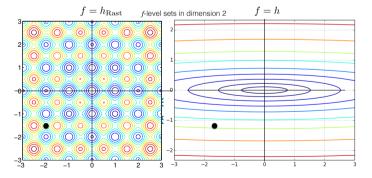
Three functions belonging to the same equivalence class

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"

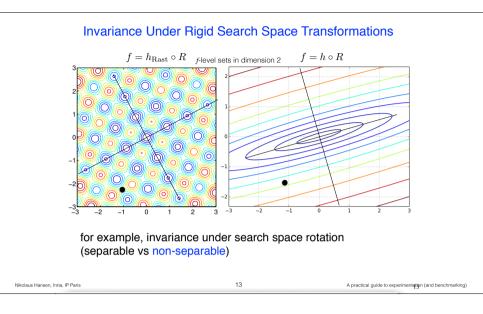
#### Invariance Under Rigid Search Space Transformations

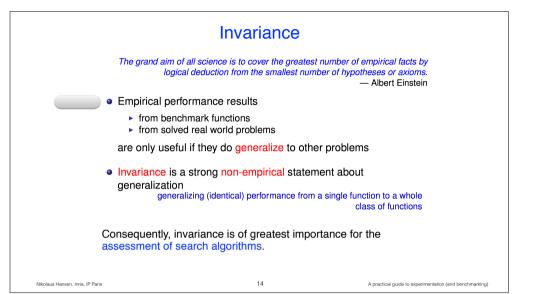


for example, invariance under search space rotation (separable vs non-separable)

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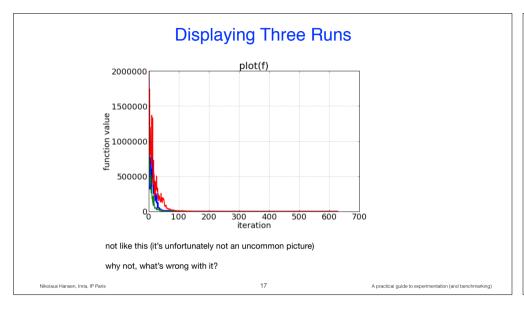
#### Displaying (Performance) Results

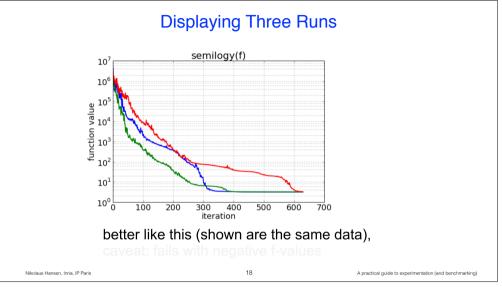
#### Empirically

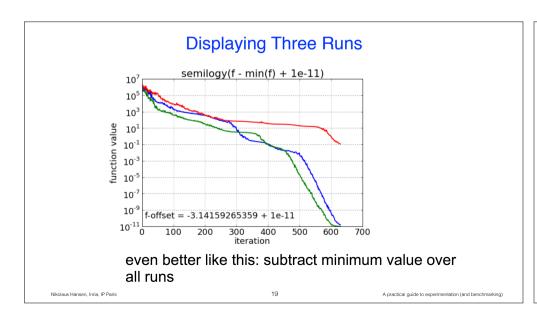
convergence graphs is all we have to start with

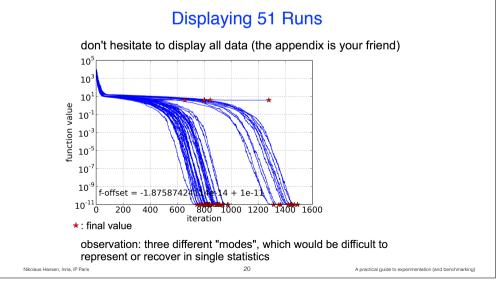
the right presentation is important!

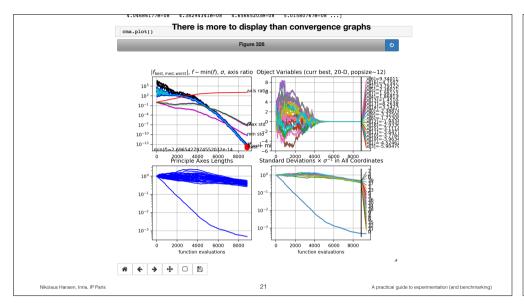
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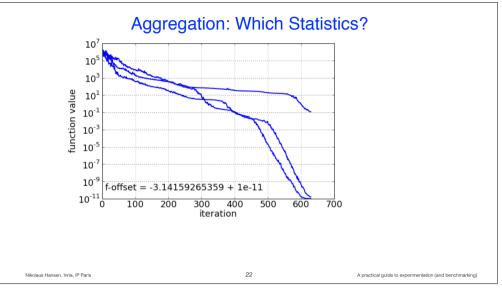


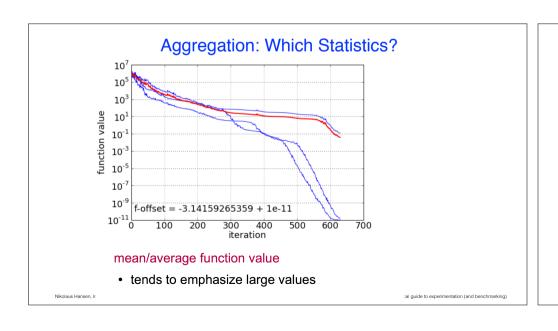








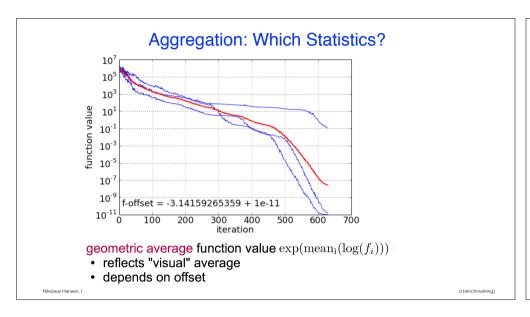


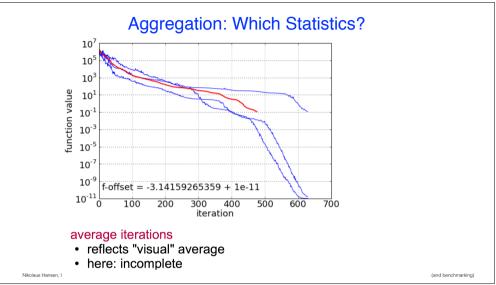


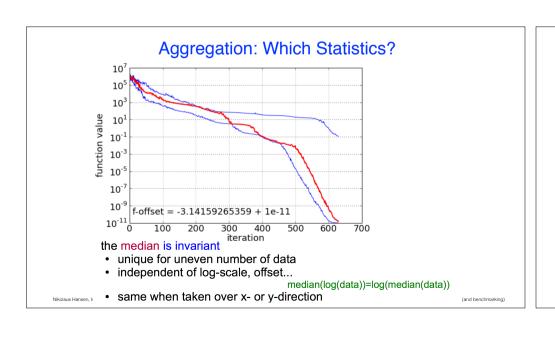
# More Caveats on Averages/Expectations

- 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

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# **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

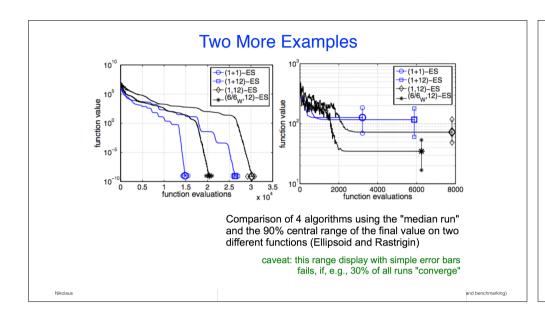
• more general: use quantiles as summary data

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

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Invariance

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· Using theory

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# 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, 2016 9 runs of two algorithms Do you agree (sounds about right) or disagree (is a little over the top) algorithm A with the quote? algorithm B 10 an experimental result (shown are all data obtained): 5 10<sup>-1</sup> 10 evaluations 32 Nikolaus Hanson Inria IP Paris A practical guide to experimentation (and benchmarking)

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#### 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: preferably 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 relevant or important or meaningful

· prefer "nonparametric" methods

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

- · Null hypothesis (H0) = both/all data come from the same distribution
- p-value = significance level = probability of a false positive outcome given H0 is true = probability H0 is rejected 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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Statistical S ecure first, check the re example of test statistics distribution density which is to be tested for sta ombinations) 0.20 le statistically a simple trick or meaninaful false positive error area prefer "nonparalme distributions • Null hypothesis (He) = polyran quara tome from the sagne distribution • p-value = significance level = probability of a false positive outcome given H0 is true = probability H0 is rejected 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

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### Statistical Significance: Methods

- use the rank-sum test (scipy.stats.ranksums, 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 for discrete data with ties: scipy.stats.mannwhitneyu(..., alternative='two-sided')

• 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: computes the sum of ranks in the ranking of all (combined) data values

 $Alg1 = [400, 422, 440] \text{ vs } Alg2 = [444, 490, 555] \Longrightarrow \text{ranks: } Alg1 = [1, 2, 3] \text{ vs } Alg2 = [4, 5, 6]$ 

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

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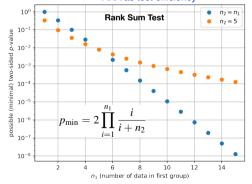
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# Statistical Significance: How many data do we need? AKA as test efficiency



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

ole and conservative: multiply the computed n-value by the number of tests

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

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

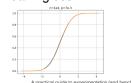
minimum number of data to possibly get two-sided p < 1%: 5+5 or 4+6 or 3+9 or 2+19 or 1+200 and p < 5%: 4+4 or 3+5 or 2+8 or 1+40

I often take two times 11 or 31 or 51

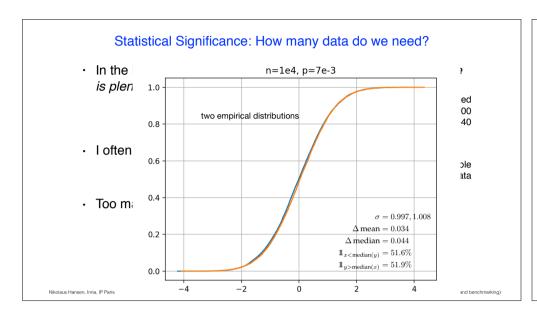
median, 5%-tile and 95%-tile are easily accessible with 11 or 31 or 51... data

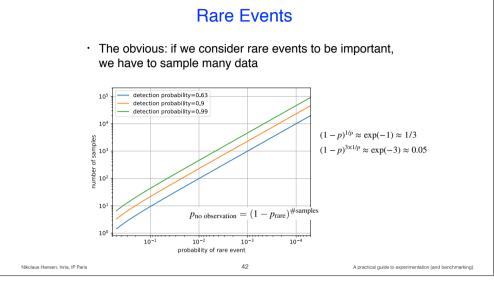
· Too many data make statistical significance meaningless

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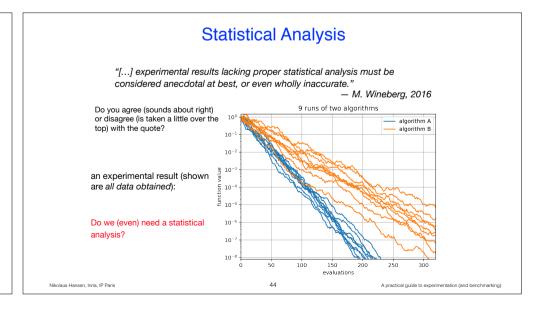


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# 



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#### 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

do not display (only) tabulated numbers subtle display changes can make a huge difference

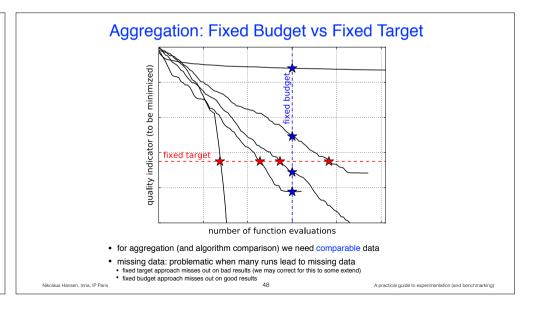
· there are surprisingly many devils in the details

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#### 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 find *where* something needs to be understood non-standard experimentation is often additionally necessary



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#### Measures for Performance Assessment

#### 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 semantically meaningful statements
- · assuming a wide range of values
- meaningful (interpretable) with regard to the real world
   transfer the measure from benchmarking to real world

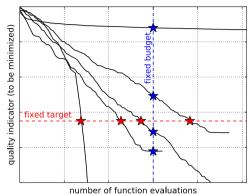
runtime or first hitting time is the prime candidate

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# Aggregation: Fixed Budget vs Fixed Target



- for aggregation (and algorithm comparison) 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

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The Problem of Missing Values

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#### Fixed Budget vs Fixed Target

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

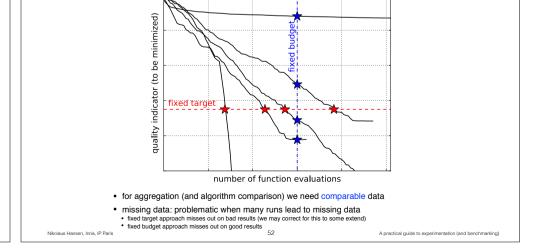
Fixed target => measuring/display needed budgets (#evaluations)

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

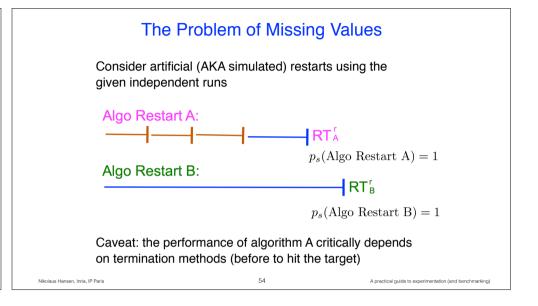
via restarts

=> fixed target is (much) preferable



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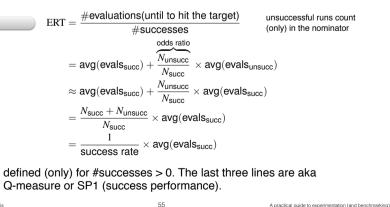
# The Problem of Missing Values how can we compare the following two algorithms? $p_s(\text{Algo A}) << 1, \text{ fast convergence}$ $p_s(\text{Algo B}) \approx 1, \text{ slow c$



#### The Problem of Missing Values

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

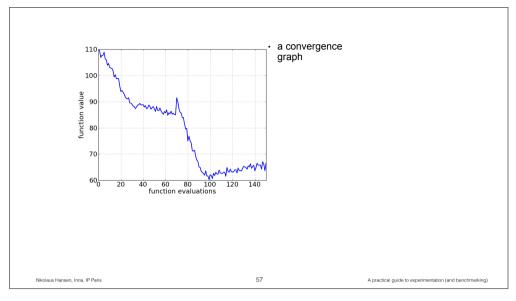
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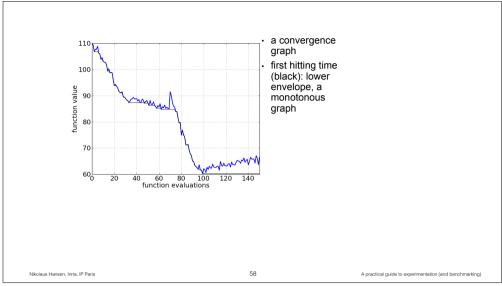


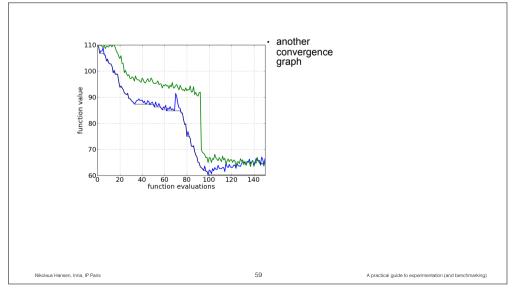
#### **Empirical Distribution Functions**

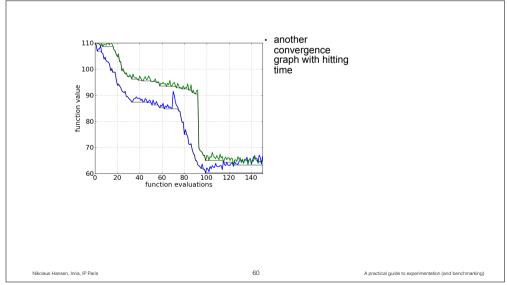
• Empirical cumulative distribution functions (ECDF, or in short, *empirical distributions*) are arguably the single most powerful tool to "aggregate" data in a display.

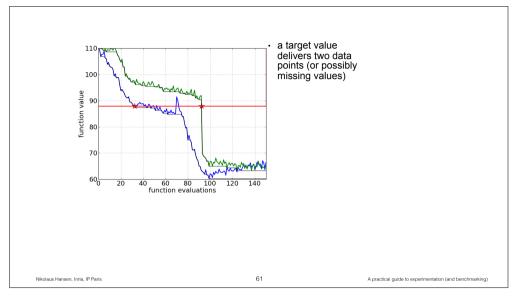
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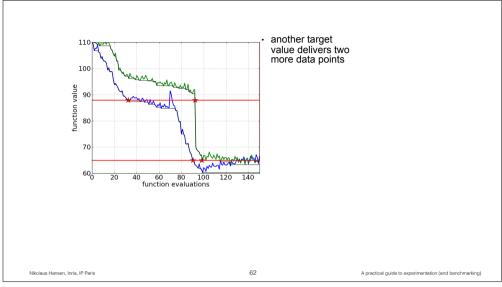


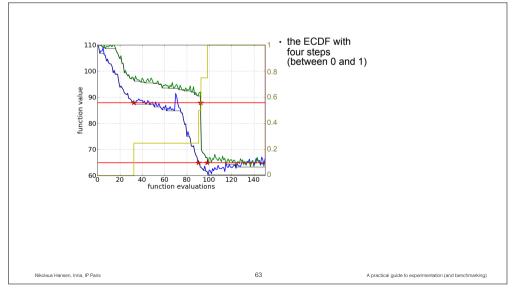


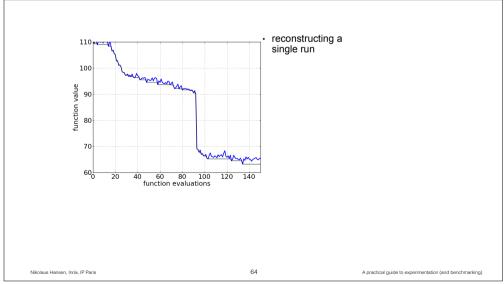


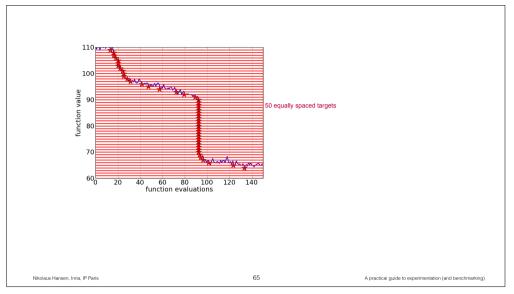


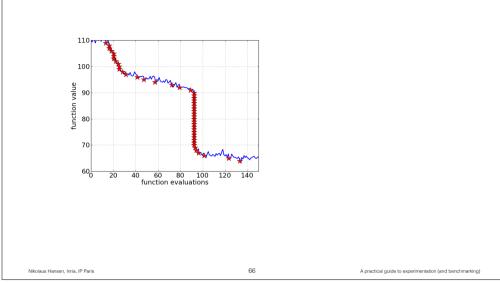


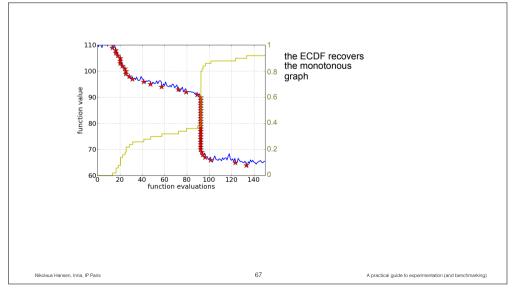


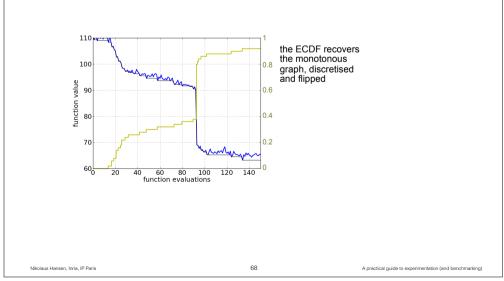


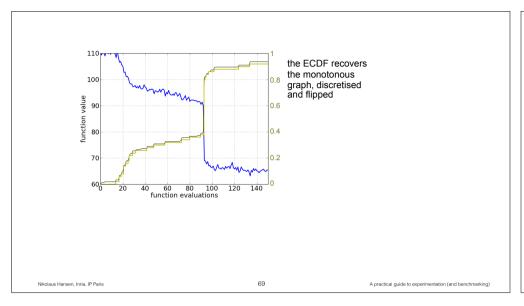


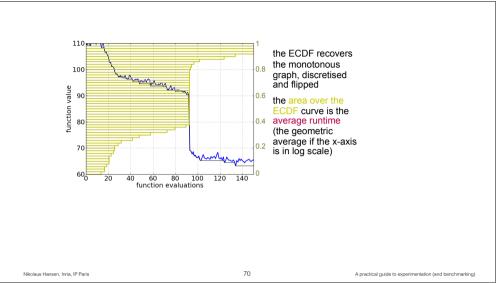












#### **Data and Performance Profiles**

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

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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

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

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#### Overview

- · Scientific experimentation
- Invariance
- · Display results
- · Statistical analysis
- · Performance assessment
- · What to measure
- · How to display
- Aggregation
- · Empirical distributions
- · Benchmarking with COCO
- · Using theory
- · Approaching an unknown problem
- A practical experimentation session

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#### 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, large-scale, mixed-integer, constrained (in beta stage)

· data of already benchmarked algorithms to compare with

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#### 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 :-)
```

```
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
```

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# Code (I blace Not. | December | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | Secrity | I height | 18 | Project AB | White | 18 | Project AB | Project AB | White | Project AB | P

#### **Benchmark Functions**

#### should (ideally) 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, in COCO we model well-identified difficulties encountered (also) in real-world problems

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#### The COCO Benchmarking Methodology

· budget-free

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

 uses 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

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#### Benchmarking Results for Algorithm ALG on the bbob Suite

Hom

Runtime distributions (ECDFs) per function

Runtime distributions (ECDFs) summary and function groups

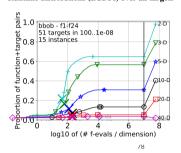
Scaling with dimension for selected targets

Tables for selected targets

Runtime distribution for selected targets and f-distributions

Runtime loss ratios

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



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**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."

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- Igor Sikorsky, airplane and helicopter designer

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#### **Using Theory in Experimentation**

- · shape our expectations and objectives
- debugging / consistency checks

theory may tell us what we expect to see

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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

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#### 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

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#### 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

• S00 https://github.com/nikohansen/GECCO-2019-experimentation-guide-notebooks

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Demonstrations

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- A somewhat typical working mode
- · A parameter investigation

FIN

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# Jupyter IPython notebook

```
| Typic | Typi
```



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