2. Empirical analysis and comparisons of stochastic optimization algorithms

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Substantial part of this material is based on slides provided with the book
'Stochastic Local Search: Foundations and Applications'
by Holger H. Hoos and Thomas Stützle (Morgan Kaufmann, 2004)
See www.sls-book.net for further information.

Contents

Motivation

No-Free-Lunch Theorem

"There is no such thing as a free lunch."

- ✔ Refers to the nineteenth century practice in American bars of offering a "free lunch" with drinks
- ✔ The meaning of the adage: *It is impossible to get something for nothing.*
- ✔ If something appears to be free, there is always a cost to the person or to society as a whole even though that *cost may be hidden or distributed*

No-Free-Lunch theorem in search and optimization [WM97]

- ✔ "Any two algorithms are equivalent when their performance is averaged across all possible problems."
- ✔ For a particular problem (or a particular class of problems), different search algorithms may obtain different results
- ✔ If an algorithm achieves superior results on some problems, it must pay with inferiority on other problems

It makes sense to study which algorithms are suitable for which kinds of problems!!!

[WM97] D. H. Wolpert and W. G. Macready. No free lunch theorems for optimization. *IEEE Trans. on Evolutionary Computation*, 1(1):67–82, 1997.

Monte Carlo vs. Las Vegas Algorithms

EOA belong to the class of *Monte Carlo* or *Las Vegas algorithms* (LVAs):

- ✔ **Monte Carlo algorithm:** It always stops and provides a solution, but the solution may not be correct. The solution quality is a random variable.
- ✔ **Las Vegas algorithm:** It always produces a correct solution, but needs a priori unknown time to find it. The running time is a random variable.
- ✔ LVA can be turned to MCA by bounding the allowed running time.
- ✔ MCA can be turned to LVA by restarting the algorithm from randomly chosen states.

Las Vegas algorithms

Las Vegas algorithms:

- ✔ An algorithm A for a decision problem class Π is a *Las Vegas algorithm* iff it has the following properties:
  - ✘ If A terminates for certain $\pi \in \Pi$ and returns a solution s, then s is guaranteed to be a correct solution of π.
  - ✘ For any given instance $\pi \in \Pi$, the runtime of A applied to π, $RT_{A,\pi}$, is a random variable.
- ✔ An algorithm A for an optimization problem class Π is an *optimization Las Vegas algorithm* iff it has the following properties:
  - ✘ For any given instance $\pi \in \Pi$, the runtime of A applied to π needed to find a solution with certain quality q, $RT_{A,\pi}(q)$, is a random variable.
  - ✘ For any given instance $\pi \in \Pi$, the solution quality achieved by A applied to π after certain time t, $SQ_{A,\pi}(t)$, is a random variable.
- ✔ LVAs are typically *incomplete* or at most *asymptotically complete*.

Runtime Behaviour for Decision Problems

Definitions:

- ✔ A is an algorithm for a class Π of decision problems
- ✔ $P_s\left(RT_{A,\pi} \leq t\right)$ is a probability that A finds a solution for a problem instance $\pi \in \Pi$ in time less than or equal to t.

Complete algorithm A can provably solve any solvable decision problem instance $\pi \in \Pi$ *after a finite time*, i.e. A is complete if and only if

$$\forall \pi \in \Pi,\ \exists t_{\max} : P_s\left(RT_{A,\pi} \leq t_{\max}\right) = 1. \tag{1}$$

Asymptotically complete algorithm A can solve any solvable problem instance $\pi \in \Pi$ with arbitrarily high probability *when allowed to run long enough*, i.e. A is asymptotically complete if and only if

$$\forall \pi \in \Pi : \lim_{t \to \infty} P_s\left(RT_{A,\pi} \leq t\right) = 1. \tag{2}$$

Incomplete algorithm A cannot be guaranteed to find the solution even if allowed to run indefinitely long, i.e. if it is not asymptotically complete, i.e. A is incomplete if and only if

$$\exists \text{ solvable } \pi \in \Pi : \lim_{t \to \infty} P_s\left(RT_{A,\pi} \leq t\right) < 1. \tag{3}$$

Runtime Behaviour for Optimization Problems

Simple generalization based on transforming the optimization problem to related decision problem by setting the solution quality bound to $q = r \cdot q^*(\pi)$:

- ✔ A is an algorithm for a class Π of optimization problems
- ✔ $P_s\left(RT_{A,\pi} \leq t, SQ_{A,\pi} \leq q\right)$ is a probability that A finds a solution of quality better than or equal to q for a solvable problem instance $\pi \in \Pi$ in time less than or equal to t
- ✔ $q^*(\pi)$ is the quality of optimal solution to problem π
- ✔ $r \geq 1$

Algorithm A is r-complete if and only if

$$\forall \pi \in \Pi,\ \exists t_{\max} : P_s\left(RT_{A,\pi} \leq t_{\max}, SQ_{A,\pi} \leq r \cdot q^*(\pi)\right) = 1. \tag{4}$$

Algorithm A is asymptotically r-complete if and only if

$$\forall \pi \in \Pi : \lim_{t \to \infty} P_s\left(RT_{A,\pi} \leq t, SQ_{A,\pi} \leq r \cdot q^*(\pi)\right) = 1. \tag{5}$$

Algorithm A is r-incomplete if and only if

$$\exists \text{ solvable } \pi \in \Pi : \lim_{t \to \infty} P_s\left(RT_{A,\pi} \leq t, SQ_{A,\pi} \leq r \cdot q^*(\pi)\right) < 1. \tag{6}$$

Some Tweaks

- ✔ Incompleteness of many LVAs is typically caused by their inability to escape from attractive local minima regions of the search space.
  - ✘ remedy: use diversification mechanisms such as random restart, random walk, tabu, ...
  - ✘ in many cases, these can render algorithms provably asymptotically complete, but effectiveness in practice can vary widely
- ✔ Completeness can be achived by restarting an incomplete method from a solution generated by a complete (exhaustive) algorithm.
  - ✘ typically very ineffective due to large size of the search space

Theoretical vs. Empirical Analysis of LVAs

- ✔ Practically relevant Las Vegas algorithms are typically difficult to analyse theoretically. (Algorithms are often non-deterministic.)
- ✔ Cases in which theoretical results are available are often of limited practical relevance, because they
  - ✘ rely on idealised assumptions that do not apply to practical situations,
  - ✘ apply to worst-case or highly idealised average-case behaviour only, or
  - ✘ capture only asymptotic behaviour and do not reflect actual behaviour with sufficient accuracy.

Therefore, **analyse the behaviour of LVAs using empirical methodology**, ideally based on the *scientific method*:

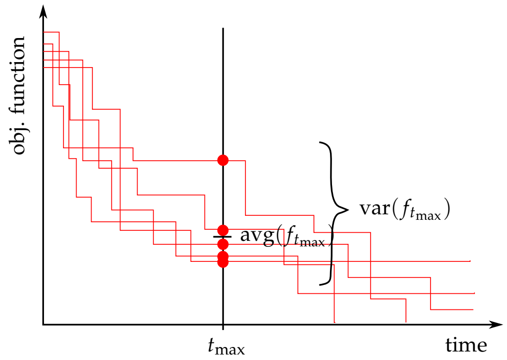
- ✔ make observations
- ✔ formulate hypothesis/hypotheses (model)
- ✔ While not satisfied with model (and deadline not exceeded):
  1. design computational experiment to test model
  2. conduct computational experiment
  3. analyse experimental results
  4. revise model based on results

Application Scenarios and Evaluation Criteria

Type 1: Hard time limit $t_{\max}$ for finding solution; solutions found later are useless (real-time environments with strict deadlines, e.g., dynamic task scheduling or on-line robot control).

⇒ Evaluation criterion:

- ✔ dec. prob.: solution probability at time $t_{\max}$, $P_s(RT \le t_{\max})$
- ✔ opt. prob.: expected quality of the solution found at time $t_{\max}$, $E(SQ(t_{\max}))$



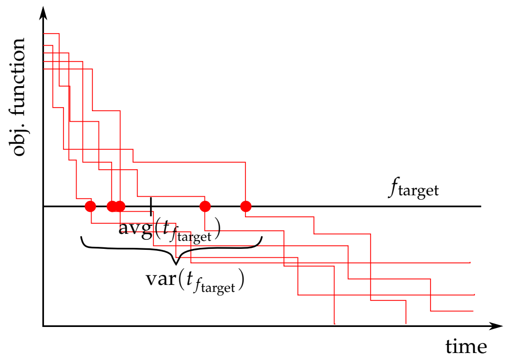
- ✔ Possible problem: What does "The expected solution quality of algorithm A is 2 times better than for algorithm B" actually mean?

Application Scenarios and Evaluation Criteria (cont.)

Type 2: No time limits given, algorithm can be run until a solution is found (off-line computations, non-realtime environments, e.g., configuration of production facility).

⇒ Evaluation criterion:

- ✔ dec. prob.: expected runtime to solve a problem
- ✔ opt. prob.: expected runtime to reach solution of certain quality



- ✔ Is there any problem with "The expected runtime of algorithm A is 2 times larger than for algorithm B"?

Application Scenarios and Evaluation Criteria (cont.)

Type 3: Utility of solutions depends in more complex ways on the time required to find them; characterised by a utility function U:

- ✔ dec. prob.: $U : R^+ \mapsto \langle 0,1 \rangle$, where $U(t)$ = utility of solution found at time t
- ✔ opt. prob.: $U : R^+ \times R^+ \mapsto \langle 0,1 \rangle$, where $U(t,q)$ = utility of solution with quality q found at time t

Example: The direct benefit of a solution is invariant over time, but the cost of computing time diminishes the final payoff according to $U(t) = \max\{u_0 - c \cdot t, 0\}$ (constant discounting).

⇒ Evaluation criterion: utility-weighted solution probability

- ✔ dec. prob.: $U(t) \cdot P_s\,(RT \leq t)$, or
- ✔ opt. prob.: $U(t,q) \cdot P_s\,(RT \leq t, SQ \leq q)$

requires detailed knowledge of $P_s\,(\ldots)$ for arbitrary t (and arbitrary q).

Empirical Algorithm Comparison

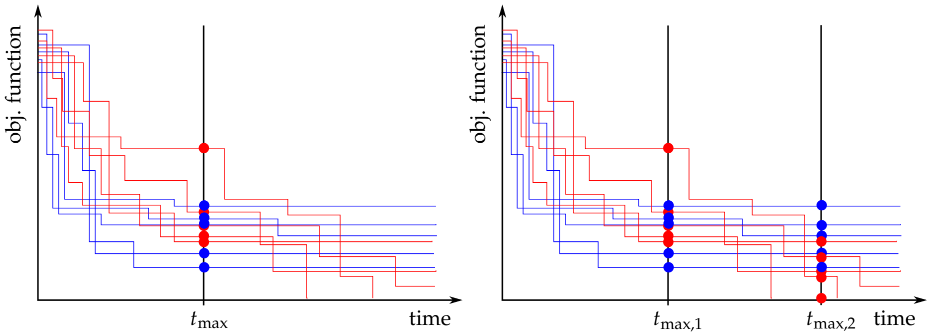
CPU Runtime vs Operation Counts

Remark: Is it better to measure the time in *seconds* or e.g. in *function evaluations*?

- ✔ Results of experiments should be comparable
- ✔ Wall-clock time depends on the machine configuration, computer language, and on the operating system used to run the experiments
- ✔ Since the objective function is often the most time-consuming operation in the optimization cycle, many authors use the *number of objective function evaluations* as the primary measure of "time"

Scenario 1: Limited time

- ✔ Let them run for certain time $t_{\max}$ and compare the average quality of returned solution, ave(SQ)



- ✔ for $t_{\max,1}$, blue algorithm is better than red
- ✔ for $t_{\max,2}$, blue algorithm is worse than red
- ✔ WARNING! The figure can change when $t_{\max}$ changes!!!
- ✔ Can our claims be false? What is the probability that our claims are wrong?

Student's t-test

Independent two-sample t-test

- ✔ Statistical method used to test if the means of 2 normally distributed populations are equal.
- ✔ The larger the difference between means, the higher the probability the means are different.
- ✔ The lower the variance inside the populations, the higher the probability the means are different.
- ✔ For details, see e.g. [**?**, sec. 11.1.2]
- ✔ Implemented in most mathematical and statistical software, e.g. in MATLAB
- ✔ Can be easily implemented in any language

Assumptions:

- ✔ Both populations should have normal distribution.
- ✔ Almost never fulfilled with the populations of solution qualities

Remedy: a non-parametric test!

[WM97] D. H. Wolpert and W. G. Macready. No free lunch theorems for optimization. *IEEE Trans. on Evolutionary Computation*, 1(1):67–82, 1997.

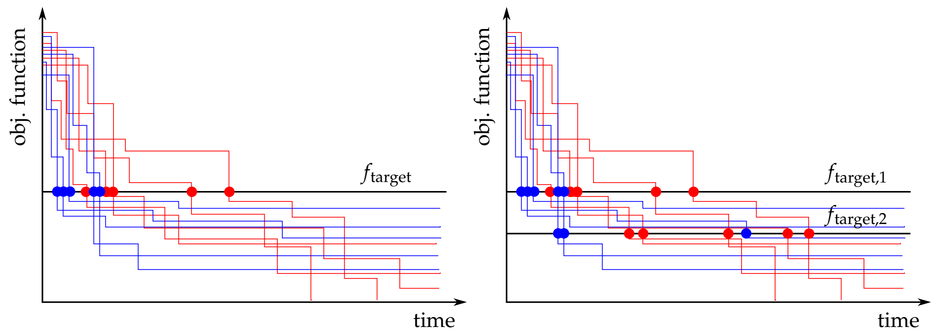
Mann-Whitney-Wilcoxon rank-sum test

Non-parametric test assessing whether two independent samples of observations have equally large values

- ✔ Virtually identical to:
  - ✘ combine both samples (for each observation, remember its original group)
  - ✘ sort the values
  - ✘ replace the values by ranks
  - ✘ use the ranks with ordinary parametric two-sample t-test
- ✔ The measurements must be at least ordinal
  - ✘ we must be able to sort them
  - ✘ this allows us to merge results from runs which reached the target level with the results of runs which did not

Scenario 2: Prescribed target level

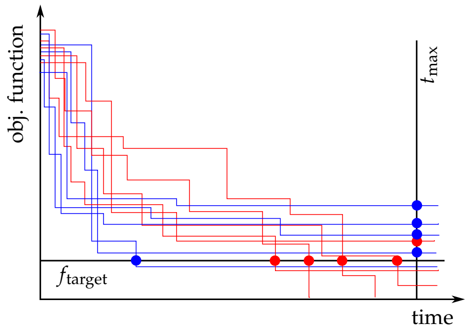
- ✔ Let them run until they find a solution of certain quality f_{target} and compare the average runtime, ave(RT)



- ✔ for $f_{\text{target,1}}$, blue algorithm is better than red
- ✔ for $f_{\text{target,2}}$, blue algorithm still seems to better than red (if it finds the solution, it finds it faster), but 2 blue runs did not reach the target level yet, i.e. (we are much less sure that blue is better)
- ✔ WARNING! The figure can change when f_{target} changes!!!
- ✔ The same statistical tests as for scenario 1 can be used

Scenarios 1 and 2 combined

- ✔ Let them run until they find a solution of certain quality f_{target} or until they use all the allowed time $t_{\max}$



- ✔ RT is measured in seconds or function evaluations, SQ is measured in something different; now, how can we test if one algorithm is better than the other?
- ✔ The situation when the algorithm reaches f_{target} is better than when it reaches $t_{\max}$. We can still sort the values.
- ✔ We can use the Mann-Whitney U-test
- ✔ WARNING! Again, if we change f_{target} and/or $t_{\max}$, the figure can change!!!

Analysis based on runtime distribution

Runtime distributions

LVAs often designed and evaluated without apriori knowledge of the application scenario:

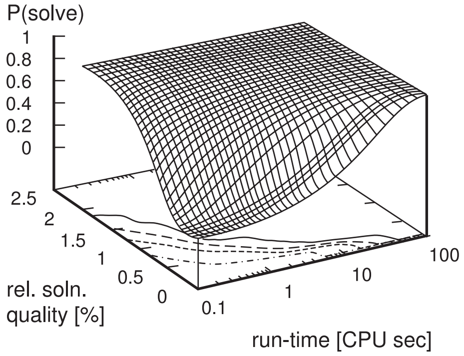
- ✔ Assume the most general scenario — type 3 with a utility function (which is often, however, unknown as well).
- ✔ Evaluate based on solution probabilities $P_s(RT \leq t, SQ \leq q)$ for arbitrary runtimes t and solution qualities q.

Study distributions of *random variables* characterising runtime and solution quality of an algorithm for the given problem instance.

RTD defintion

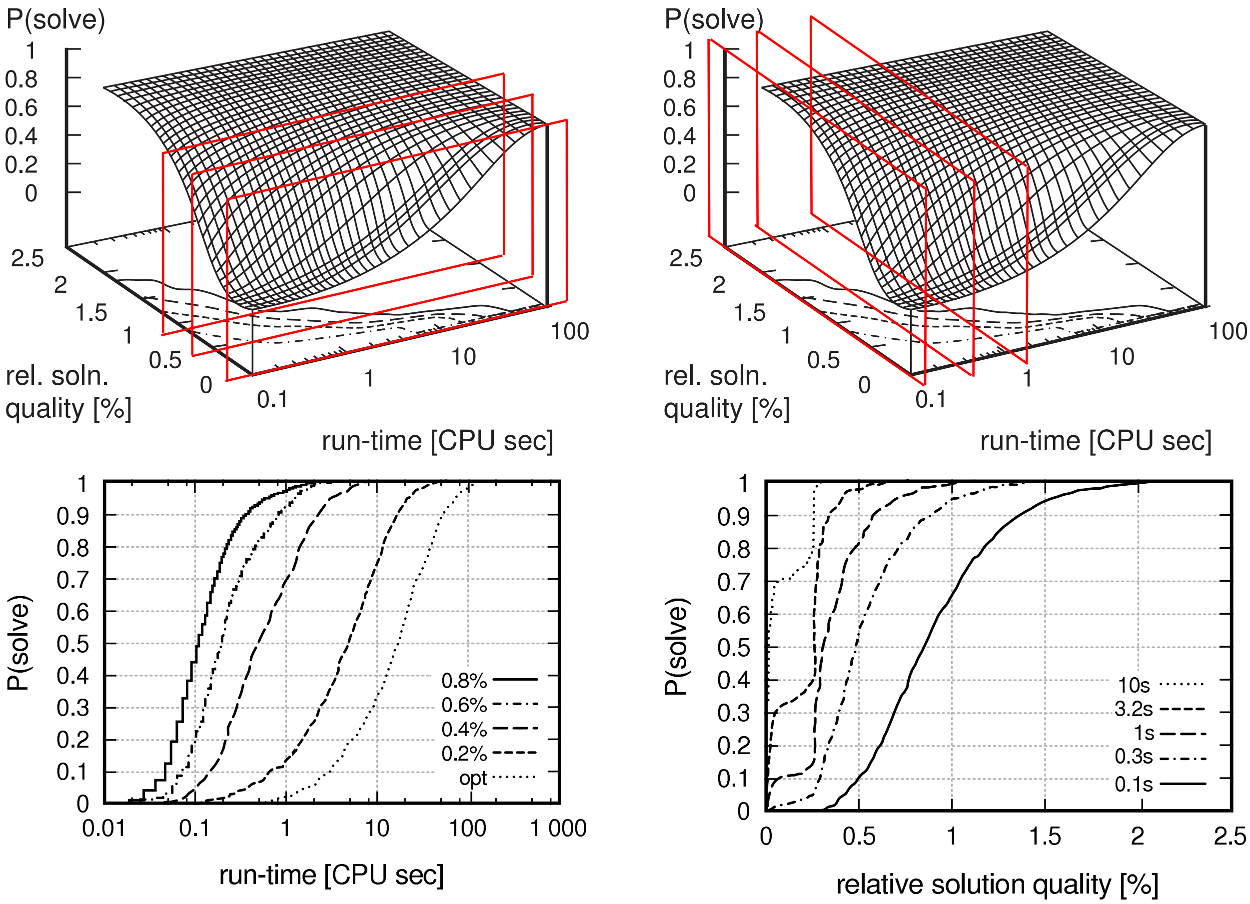
Given a Las Vegas alg. A for optimization problem π:

- ✔ The *success probability* $P_s(RT_{A,\pi} \leq t, SQ_{A,\pi} \leq q)$ is the probability that A finds a solution for a solvable instance $\pi \in \Pi$ of quality $\leq q$ in time $\leq t$.
- ✔ The *run-time distribution* (RTD) of A on π is the probability distribution of the bivariate random variable $(RT_{A,\pi}, SQ_{A,\pi})$.
- ✔ The *runtime distribution function* $rtd : R^+ \times R^+ \rightarrow [0,1]$, defined as $rtd(t,q) = P_s(RT_{A,\pi} \leq t, SQ_{A,\pi} \leq q)$, completely characterises the RTD of A on π.



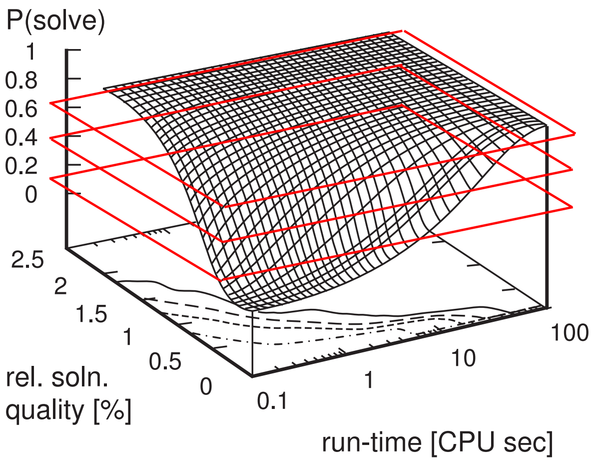
RTD cross-sections

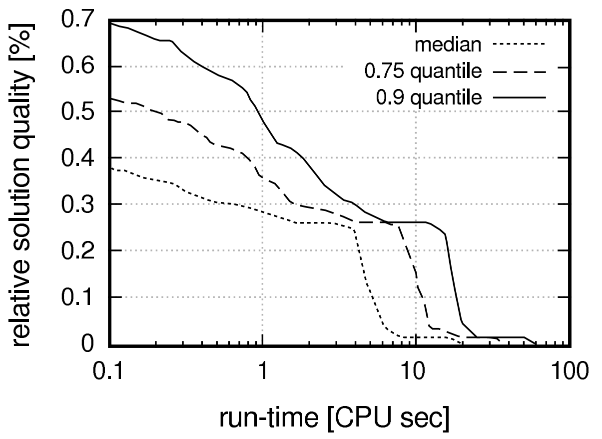
We can study the RTD using cross-sections:



RTD cross-sections (cont.)

We can study the RTD using cross-sections:





Horizontal cross-sections reveal the dependence of SQon RT:

- ✔ The lines represent various quantiles; e.g. for 75%-quantile we can expect that 75% of runs will return a better combination of SQ and RT.

Empirical measurement of RTDs

Empirical estimation of $P_s\,(RT \le t, SQ \le q)$:

- ✔ Perform N independent runs of A on problem π
- ✔ For n^{th} run, $n \in 1, \ldots, N$, store the so-called *solution quality trace*, i.e. $t_{n,i}$ and $q_{n,i}$ each time the quality is improved
- ✔ $\bar{P}_s(t,q) = \frac{n_S(t,q)}{N}$, where $n_S(t,q)$ is the number of runs which provided at least one solution with $t_i \le t$ and $q_i \le q$

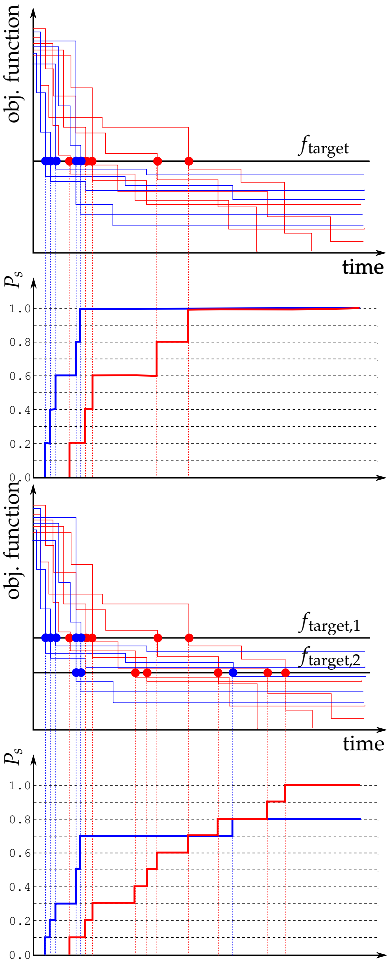
Empirical RTDs are approximations of an algorithm's true RTD:

- ✔ The larger the N, the better the approximation

RTD based algorithm comparisons

E.g. type 2 application scenario: set f_{target} and compare RTDs of the algorithms

. . . and add another f_{target} level . . .

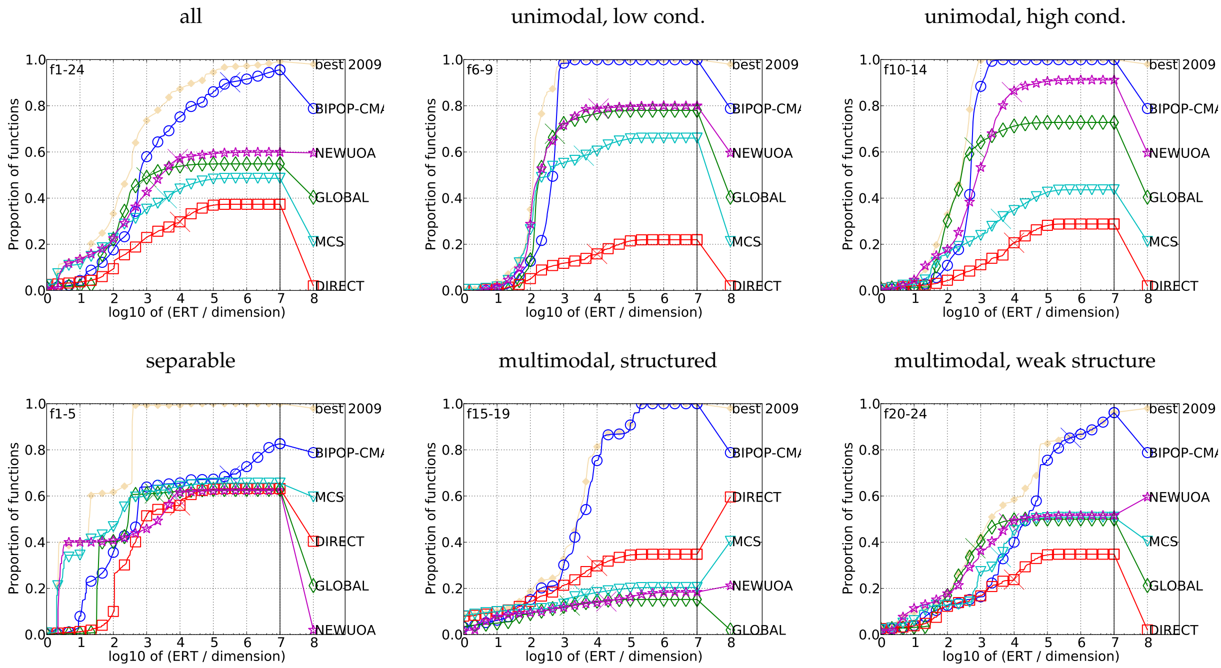


This way we can aggregate RTDs of an algorithm A not only

- ✔ over various f_{target} levels, but also
- ✔ over different problems $\pi \in \Pi$ (!!!), of course with certain loss of information

Example of comparison

Workshop on black-box optimization benchmarking (BBOB) at GECCO conference:



Summary

- ✔ No-free-lunch: all algorithms behave equally on average.
- ✔ Comparison of optimization algorithms
  - ✘ makes sense only on a well-defined class of problems,
  - ✘ is not easy since the chosen measures of algorithm quality are often random variables,
  - ✘ is often inconclusive unless the application scenario (utility function) is known.
- ✔ The most common scenario is
  - ✘ fix available runtime $t_{\max}$,
  - ✘ perform several runs and measure the solution quality at the end of each,
  - ✘ compare the algorithms based on median (or average) solution quality returned, and
  - ✘ asses statistical significance of the difference using Mann-Whitney U test.
- ✔ All measures for comparison can be derived from $rtd(t,q)$.