CZECH TECHNICAL UNIVERSITY IN PRAGUE

Faculty of Electrical Engineering
Department of Cybernetics

No Free Lunch.

Empirical comparisons of stochastic optimization algorithms

Petr Pošík

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

- No-Free-Lunch Theorem
- What is so hard about the comparison of stochastic methods?
- Simple statistical comparisons
- Comparisons based on running length distributions

Motivation

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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.

Runtime Behaviour for Decision Problems

Definitions:

- A is an algorithm for a class Π of decision problems.
- $RT_{A,\pi}$ is the runtime of algorithm A when applied to problem instance π; random variable.
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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

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

$$\exists \text{ solvable } \pi \in \Pi : \lim_{t\to\infty} P_s(t) = \lim_{t\to\infty} P[RT_{A,\pi} \leq t] < 1. \quad (3)$$

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.
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Algorithm A is r-incomplete if and only if

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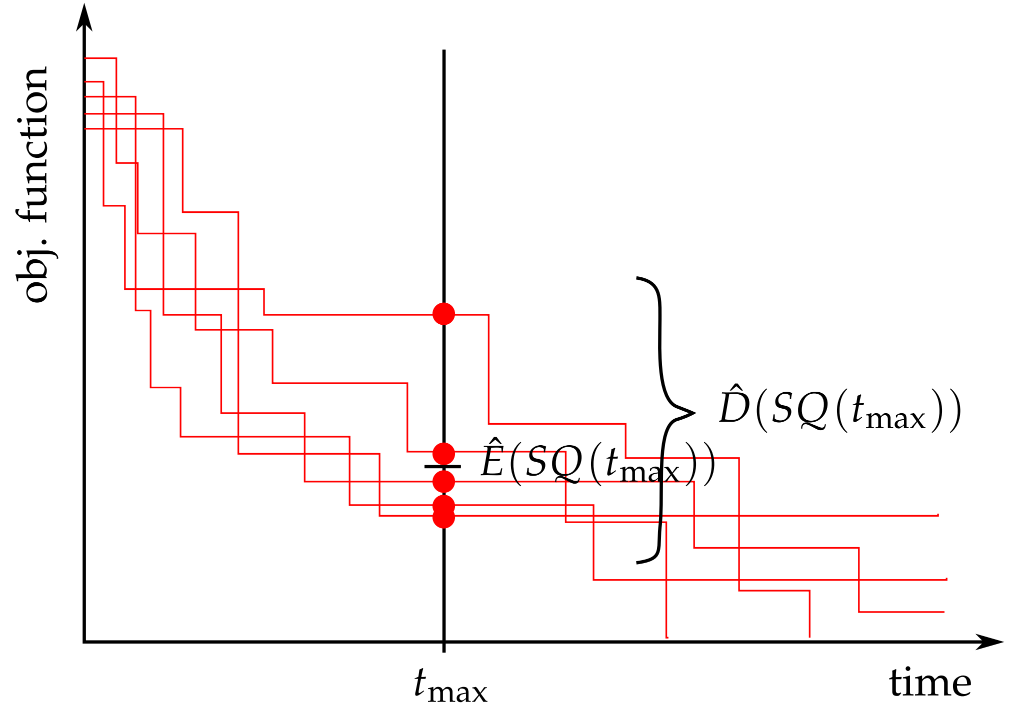
Application Scenarios and Evaluation Criteria

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



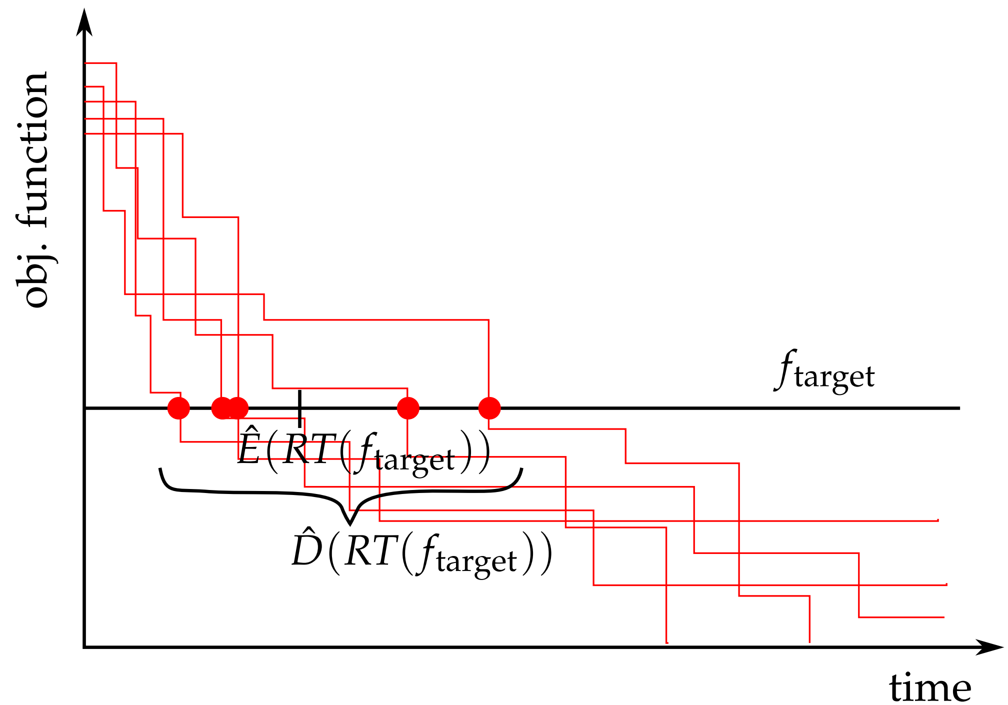
- Possible problem: What does "The expected solution quality of algorithm A is 2 times better than for algorithm B" actually mean?

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).

$\Rightarrow$ Evaluation criterion:

- dec. prob.: expected runtime to solve a problem
- opt. prob.: expected runtime to reach solution of certain quality, $E(RT(f_{\text{target}}))$



- 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
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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).

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$\Rightarrow$ Evaluation criterion: utility-weighted solution probability

- dec. prob.: $\int_0^\infty U(t) \cdot P_s(t)\, dt$, or
- opt. prob.: $\int_0^\infty \int_{-\infty}^\infty U(t, q) \cdot P_s(t, q)\, dq\, dt$

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

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How can we turn on type of algorithm into the other?

- LVA can be turned into MCA by bounding the allowed running time.
- MCA can be turned into LVA by restarting the algorithm from randomly chosen states.

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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

Empirical Algorithm Comparison

CPU Runtime vs Operation Counts

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- depends on the machine configuration, computer language, and on the operating system used to run the experiments (the results are neither comparable, nor reproducible);
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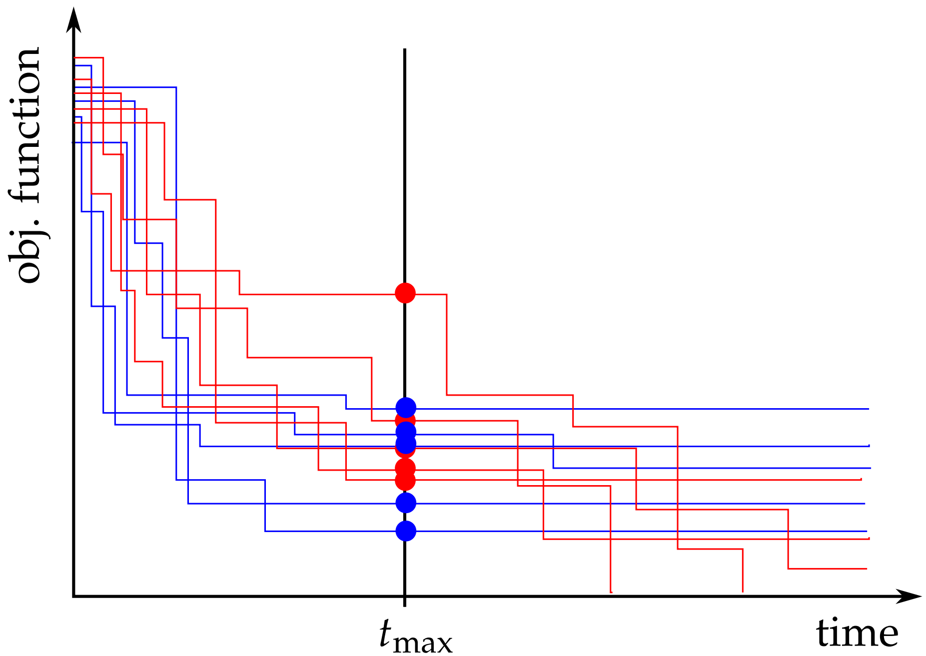
Since the objective function is often the most time-consuming operation in the optimization cycle, many authors use the **number of objective function evaluations** as the primary measure of "time".

Scenario 1: Limited time

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



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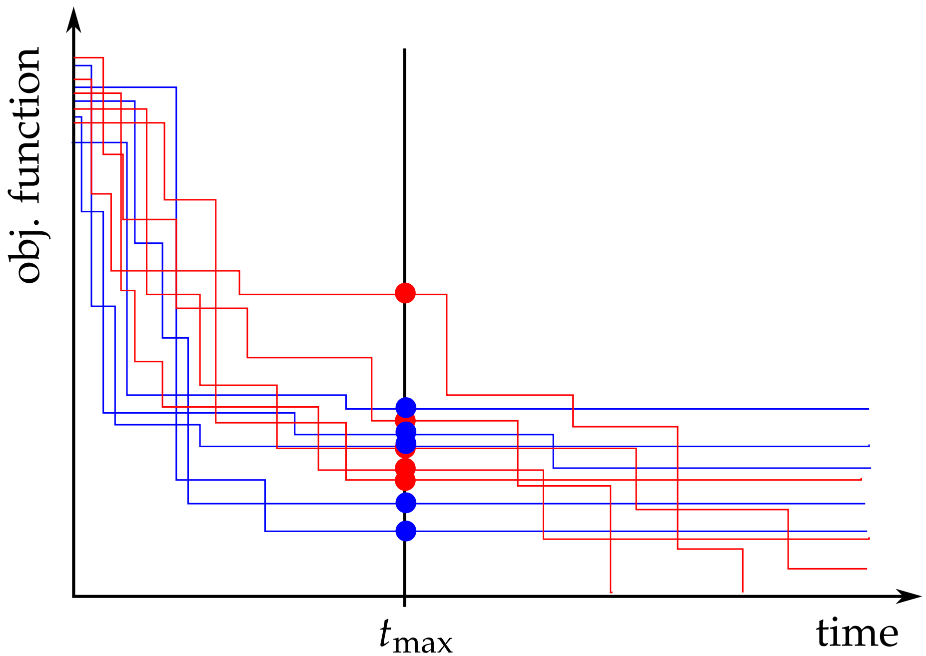

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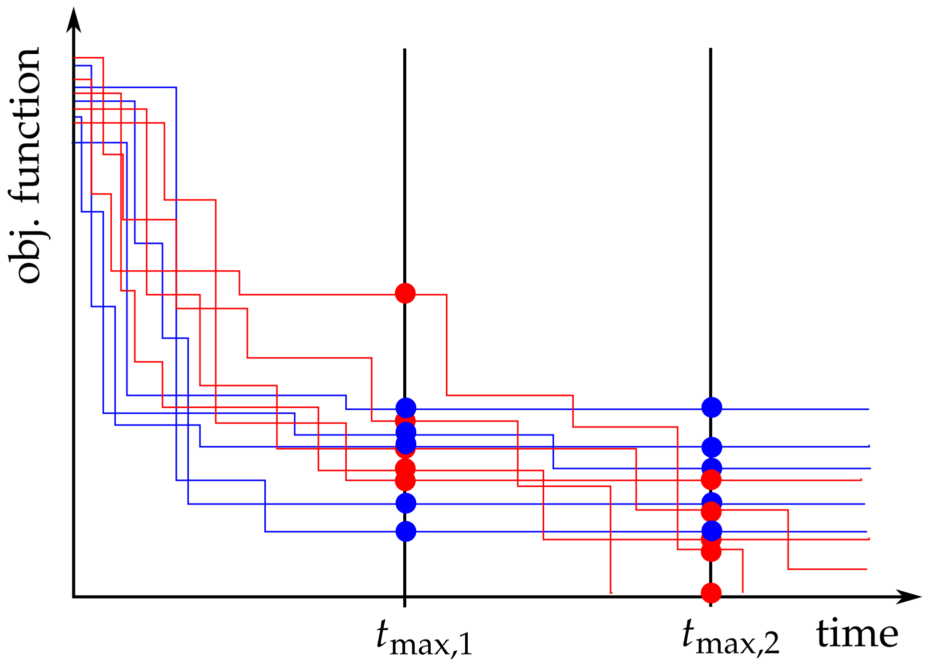

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Motivation

Empirical Comparisons
- Seconds vs counts
- Scenario 1
- Student's t-test
- MWUT
- Scenario 2
- S1 and S2 combined

RTD Analysis

Summary

Scenario 1: Limited time

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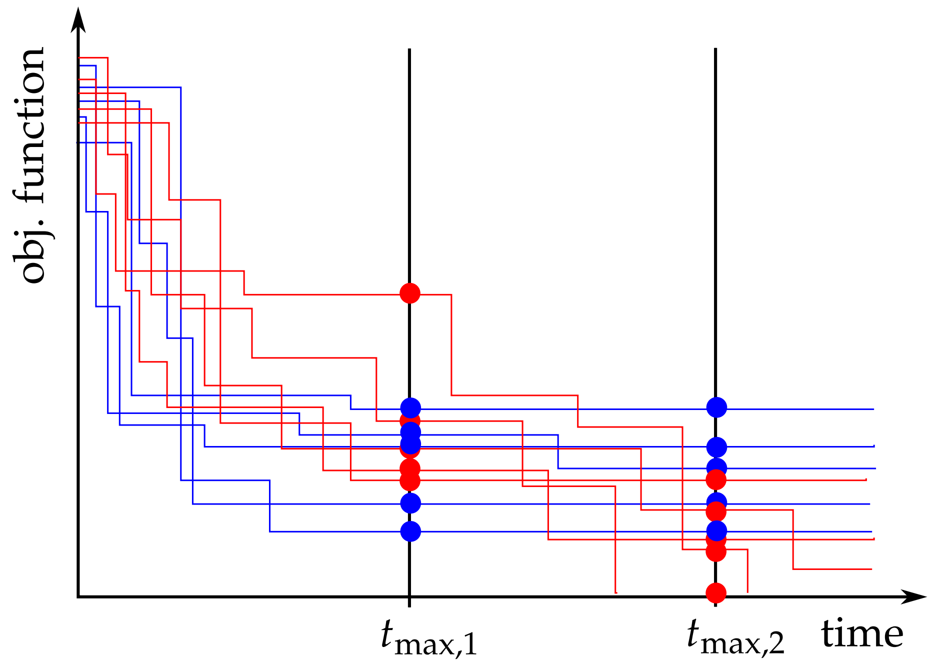

- For $t_{\max,1}$, blue algorithm is better than red.
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- Can our claims be false? What is the probability that our claims are wrong?

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. [Luk09, 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!

[Luk09] Sean Luke. *Essentials of Metaheuristics*. 2009. available at http://cs.gmu.edu/~sean/book/metaheuristics/.

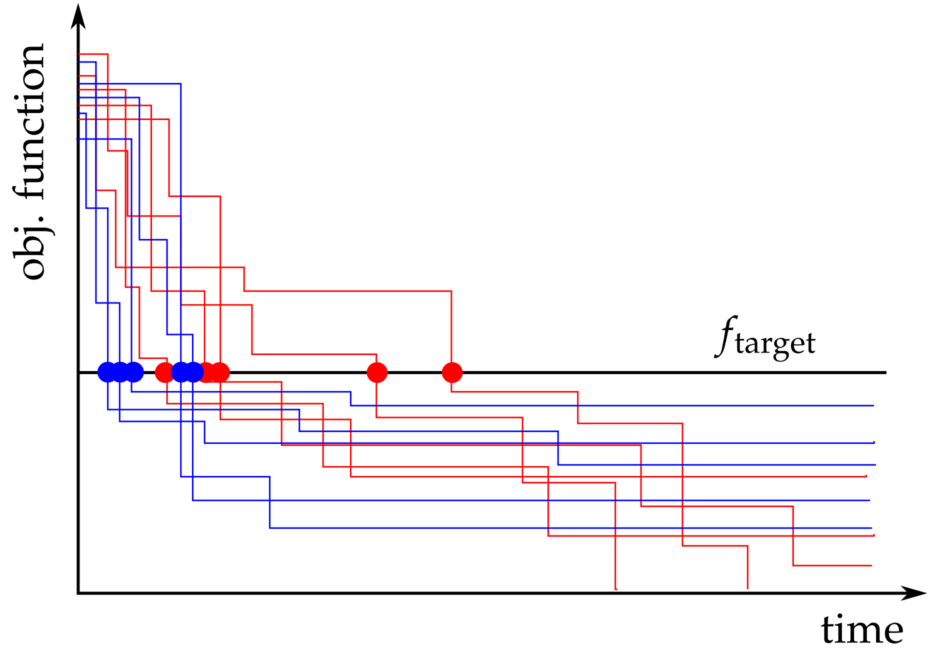
Mann-Whitney U test

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, $\text{ave}(RT)$



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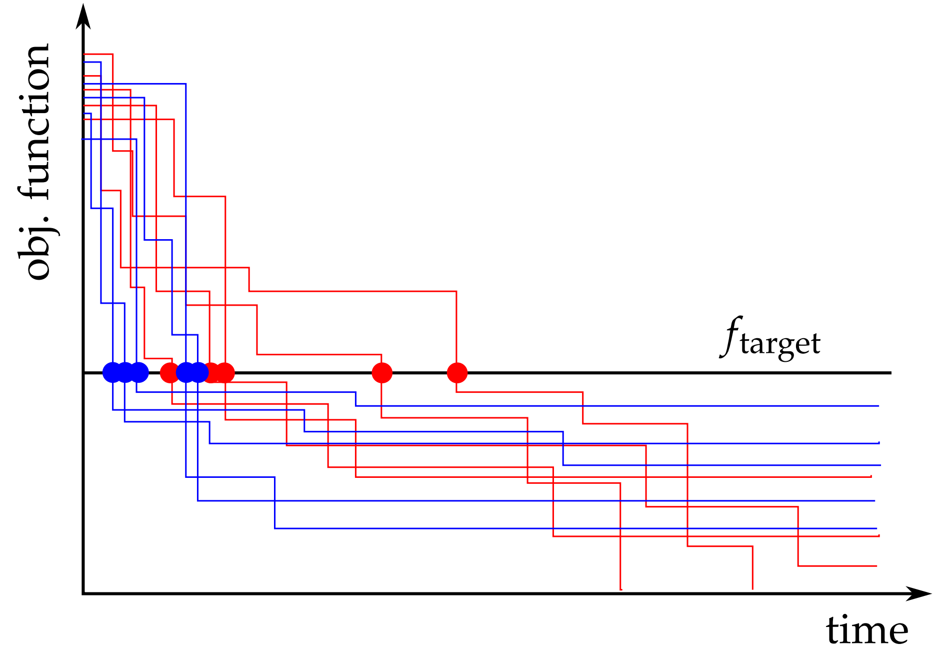

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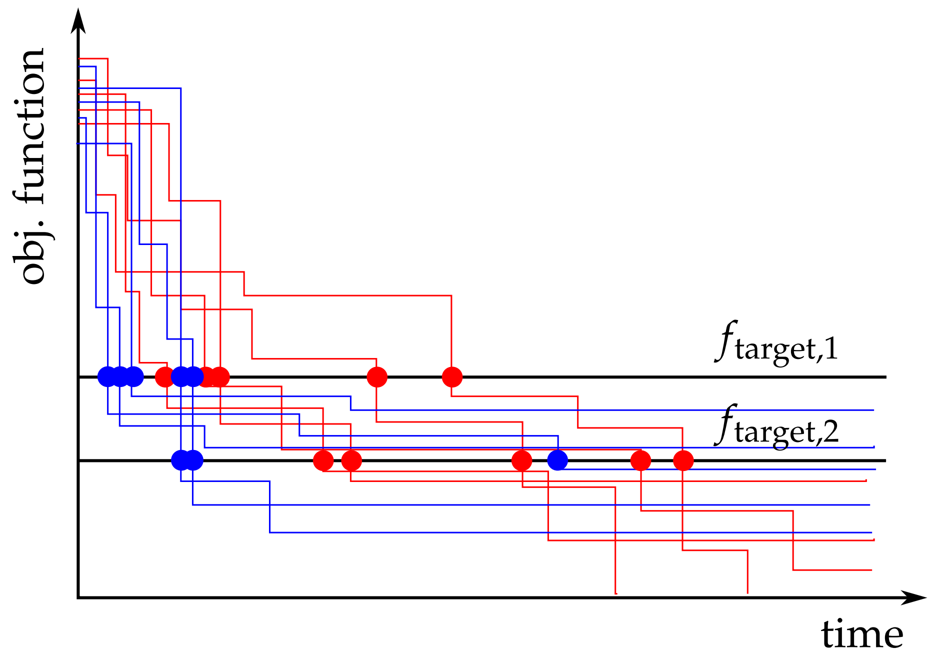

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- For $f_{\text{target},2}$, blue algorithm still seems to better than red (if it finds the solution, it finds it faster), but 2 blue runs did not reach the target level yet, i.e. (we are much less sure that blue is better).
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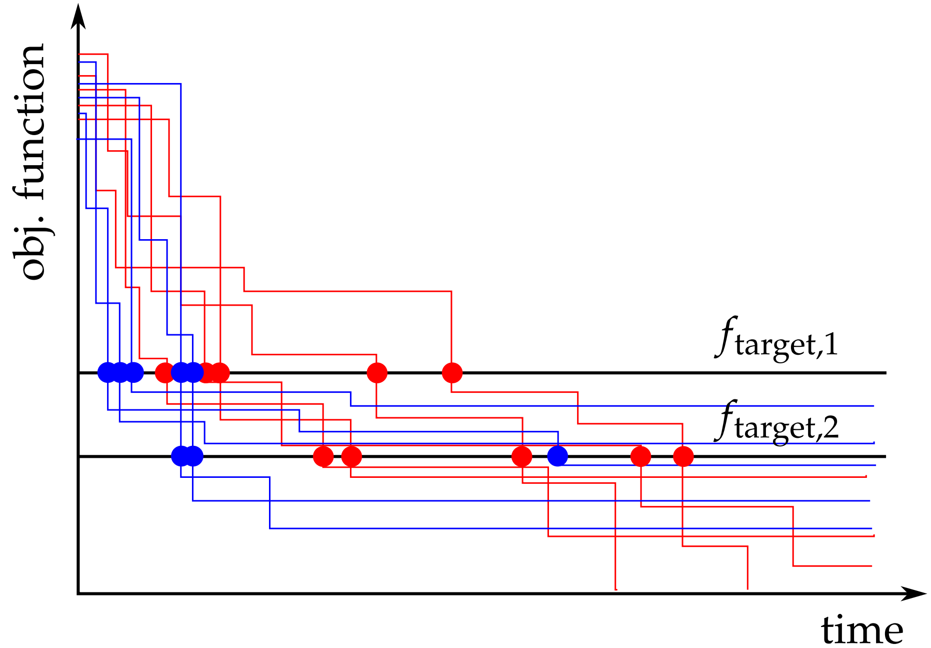

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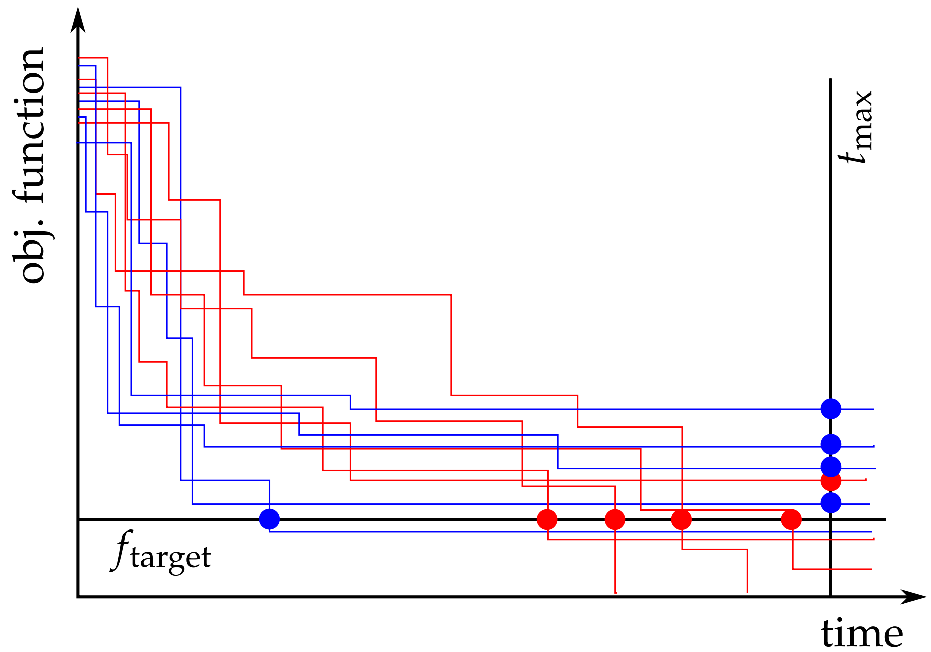
- The same statistical tests as for scenario 1 can be used.

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 $t_{\max}$.



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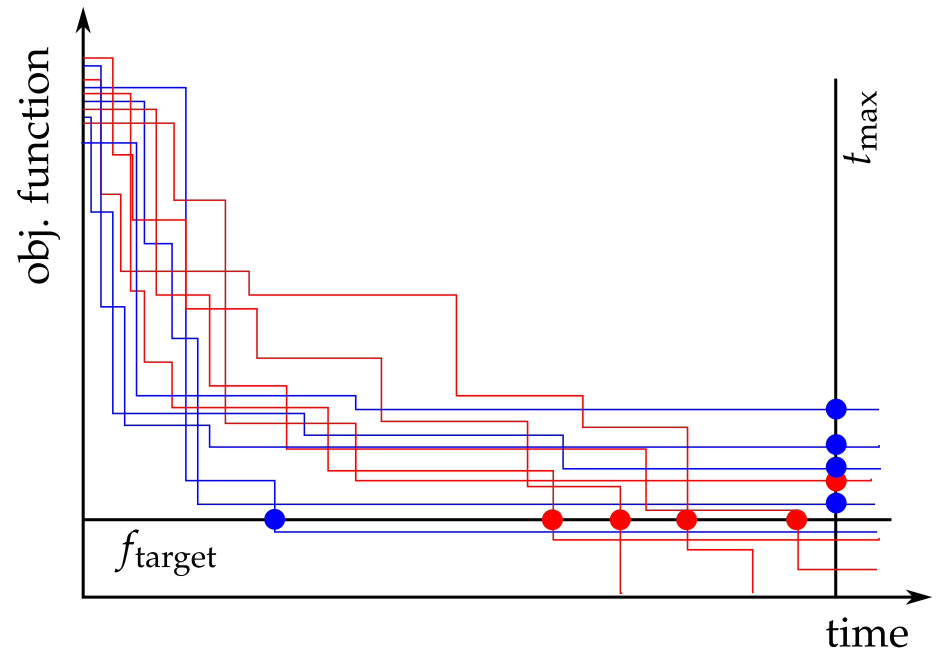
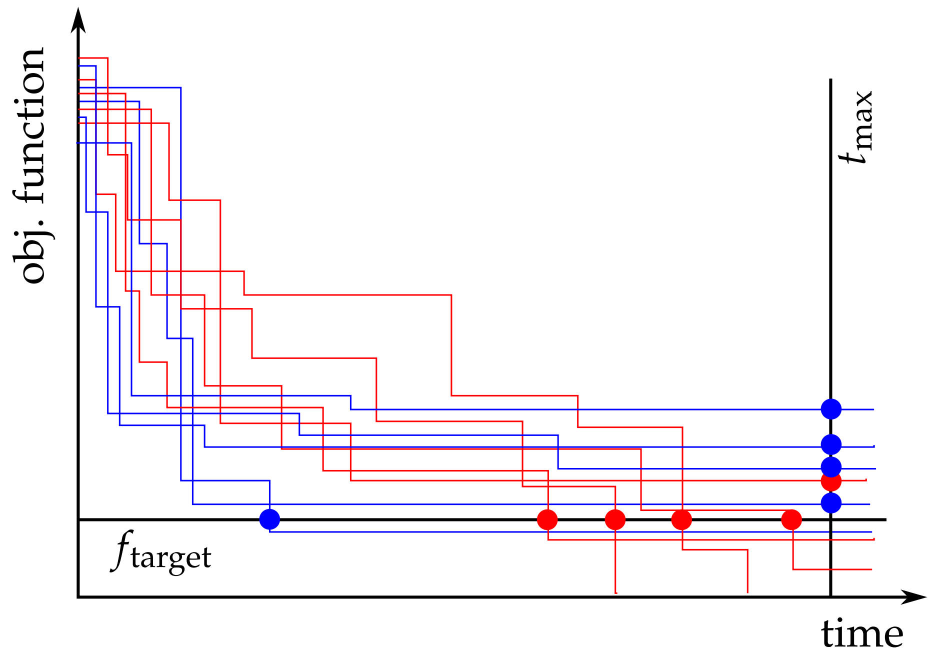


- *RT* is measured in seconds or function evaluations, *SQ* is measured in something different; now, how can we test if one algorithm is better than the other?
- The situation when the algorithm reaches f_{target} is better than when it reaches t_{max}. We can still sort the values.
- We can use the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

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 are 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 $P_s(t, q) = P[RT \leq t, SQ \leq q]$ 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* $P_s(t, q) = P[RT_{A,\pi} \leq t, SQ_{A,\pi} \leq q]$ is the probability that A finds a solution for a solvable instance $\pi \in \Pi$ of quality $\leq q$ in time $\leq t$.

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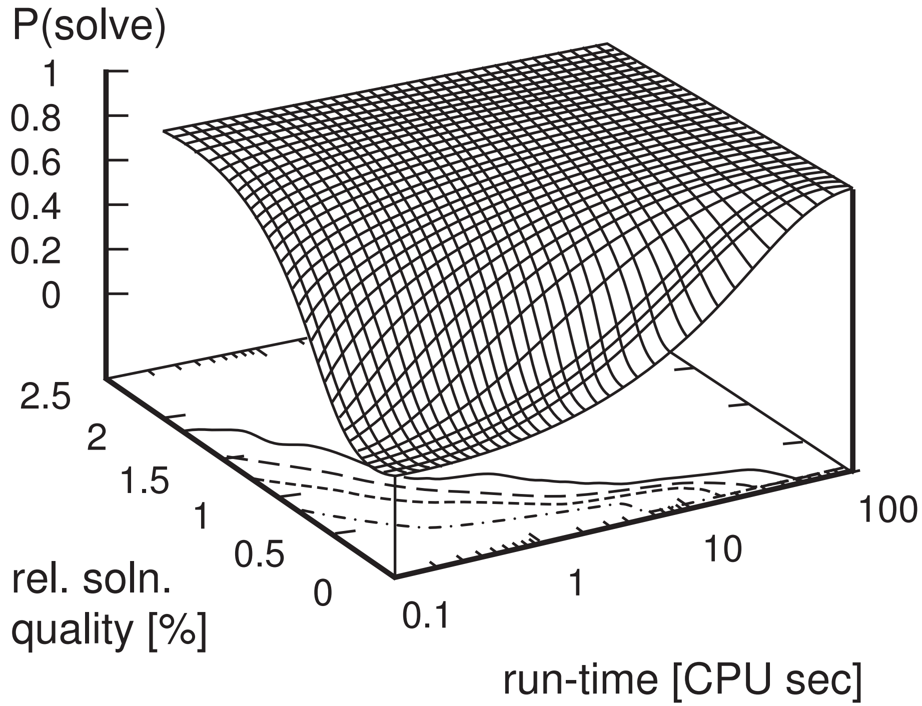
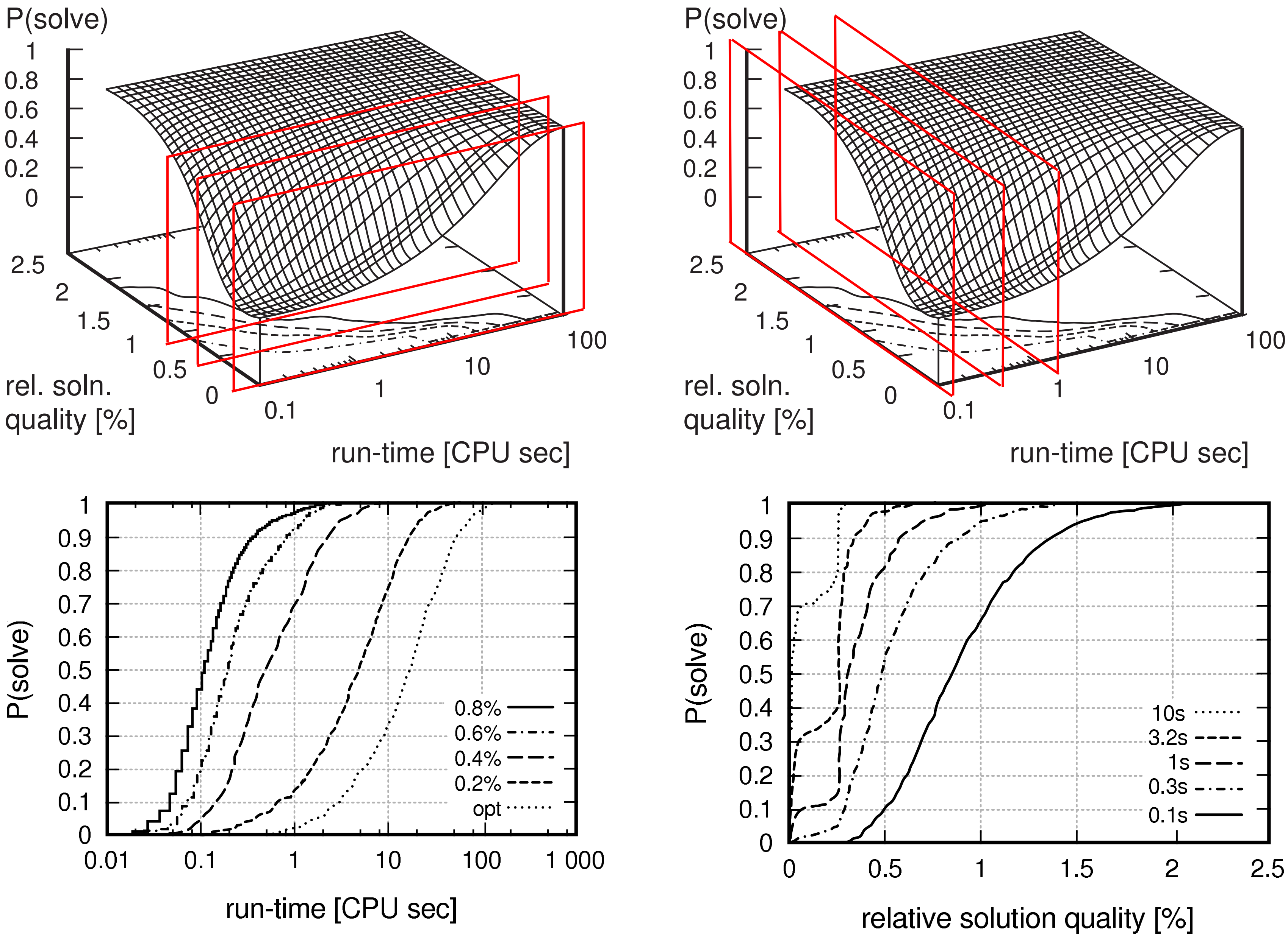


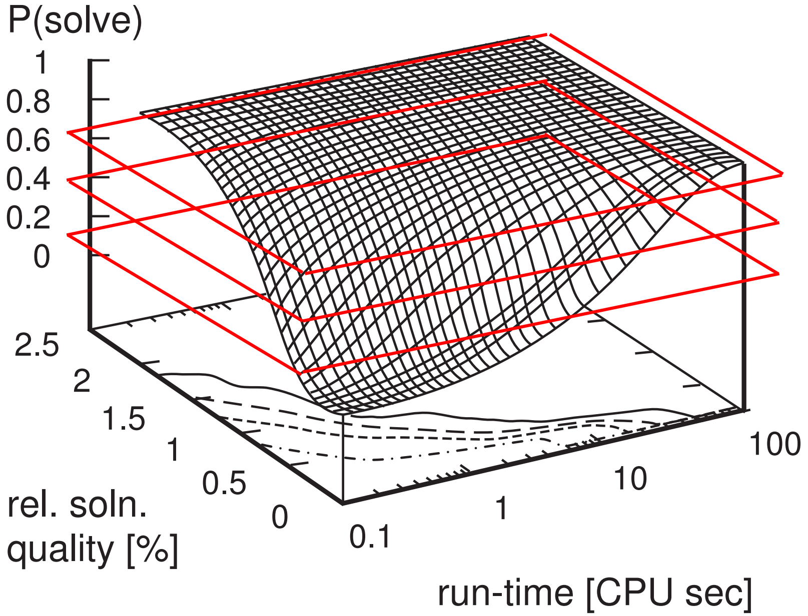
RTD cross-sections

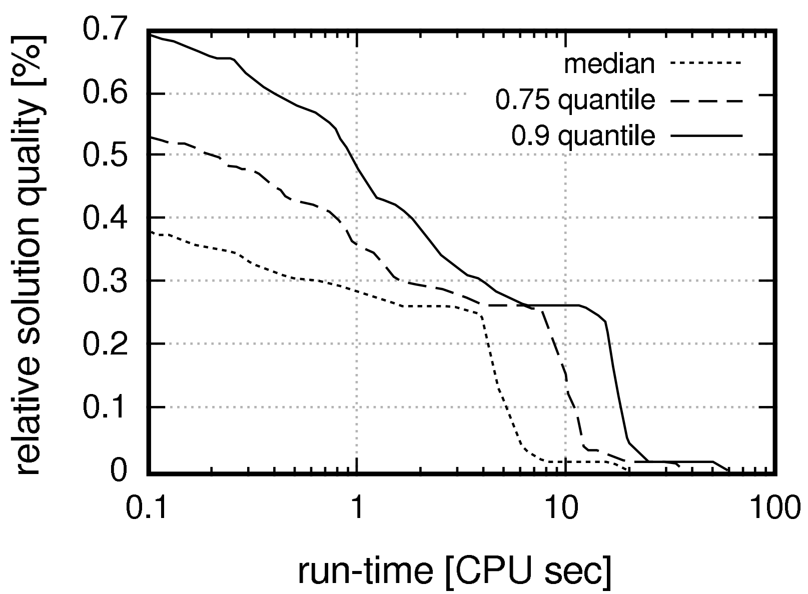
We can study the RTD using cross-sections:



RTD cross-sections (cont.)

We can study the RTD using cross-sections:





Horizontal cross-sections reveal the dependence of SQ on 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 $P[RT \leq t, SQ \leq q]$:

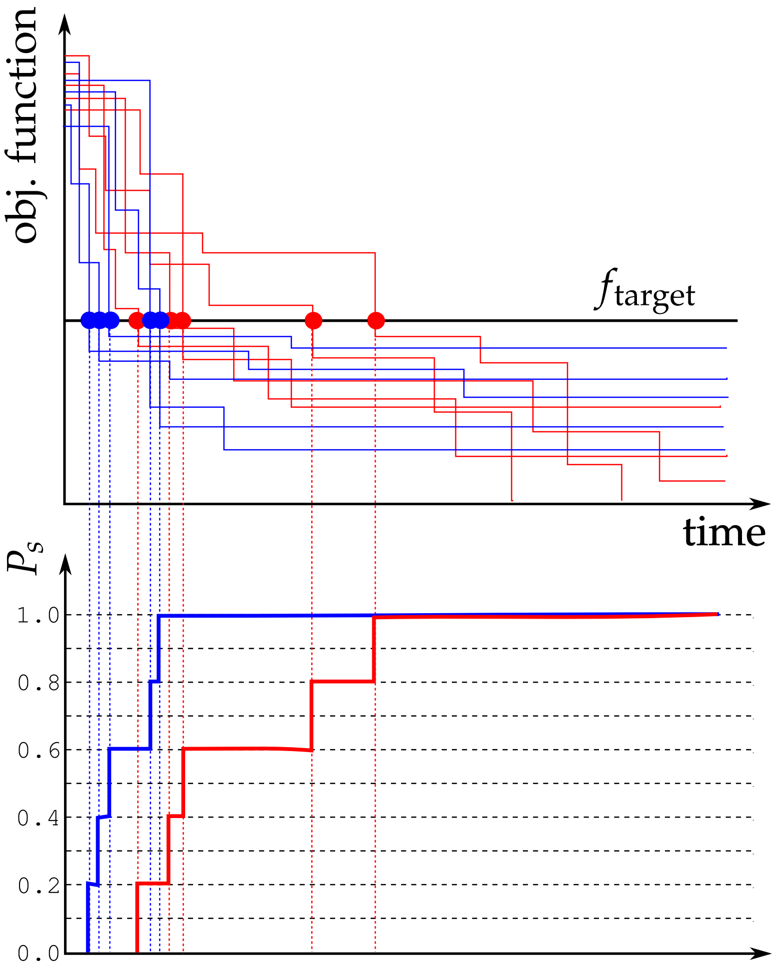
- Perform N independent runs of A on problem π.
- For n^{th} run, $n \in 1, \ldots, N$, store the so-called *solution quality trace*, i.e. $t_{n,i}$ and $q_{n,i}$ each time the quality is improved.
- $\hat{P}_s(t, q) = \dfrac{n_S(t, q)}{N}$, where $n_S(t, q)$ is the number of runs which provided at least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

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

- The larger the N, the better the approximation.

RTD based algorithm comparisons

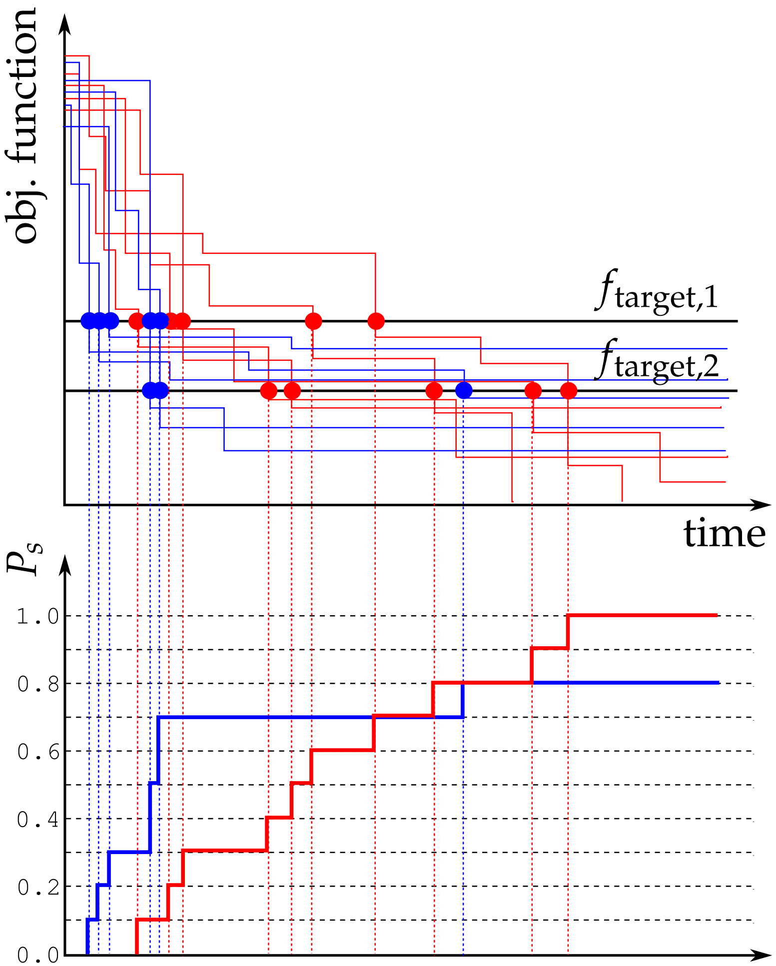
E.g. type 2 application scenario: set f_{target} and compare RTDs of the algorithms



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 …



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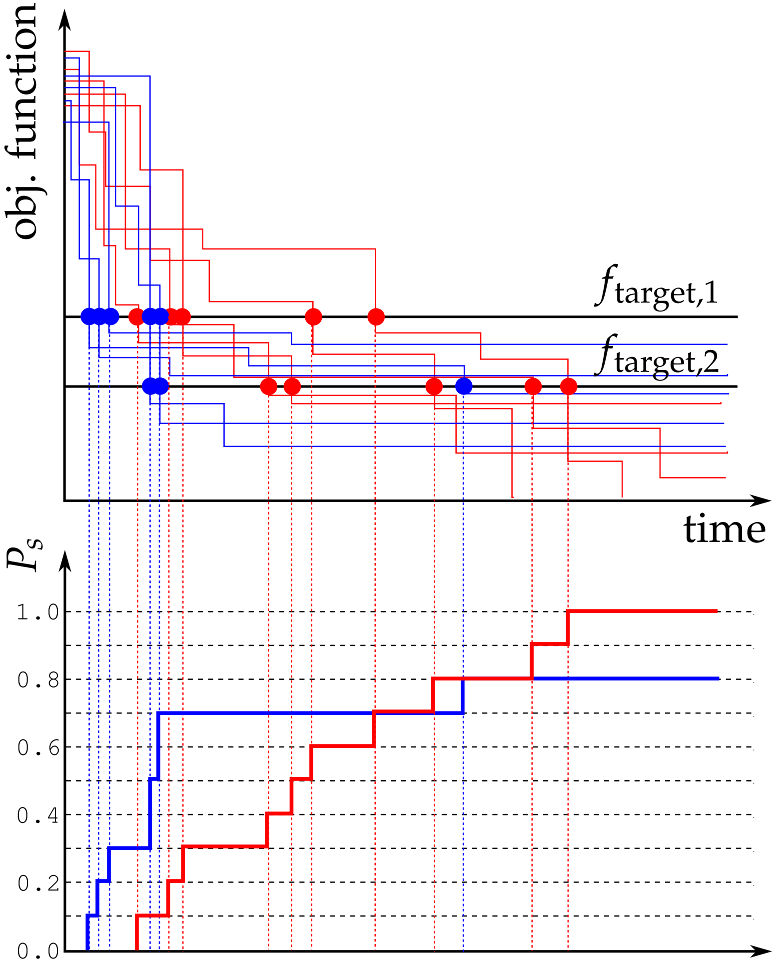

This way we can aggregate RTDs of an algorithm A not only

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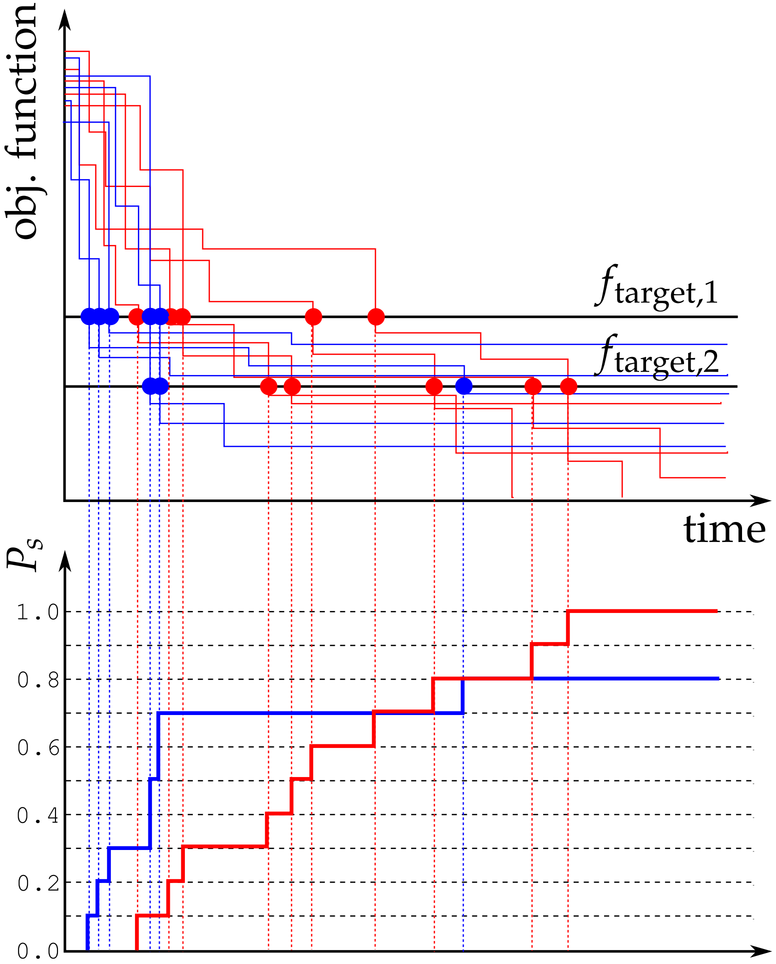


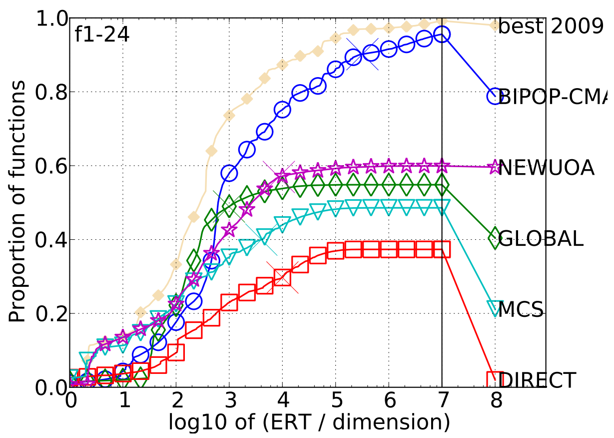
This way we can aggregate RTDs of an algorithm A not only

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

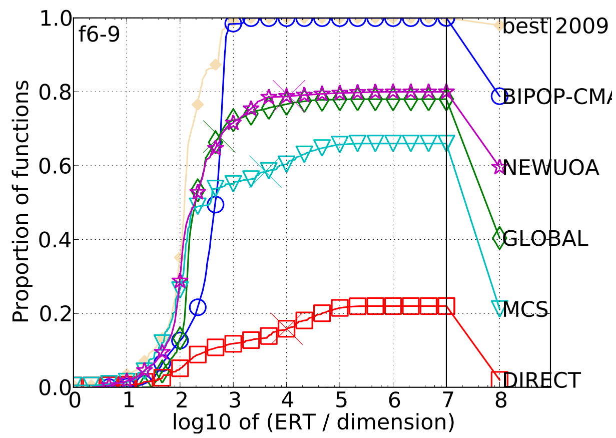
Example of comparison

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

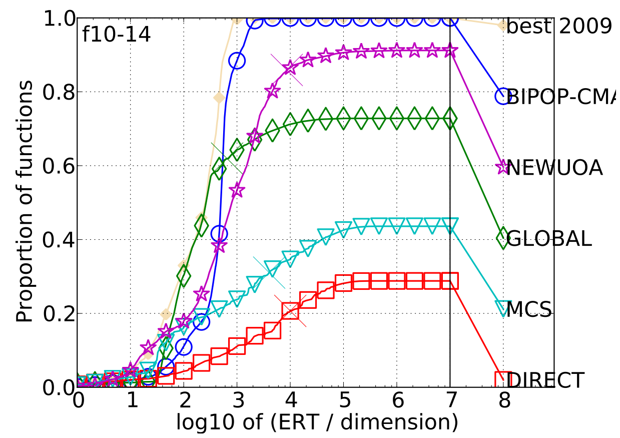
all



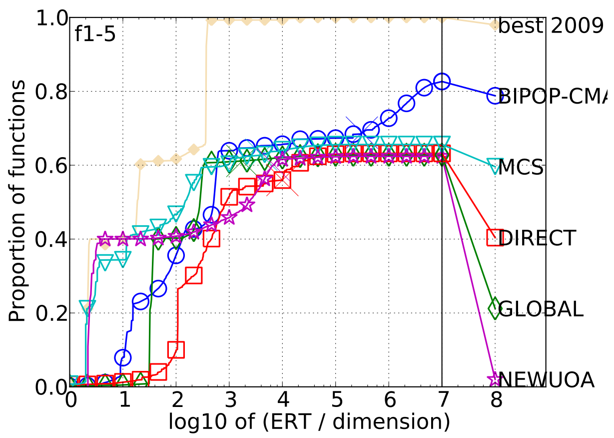
unimodal, low cond.



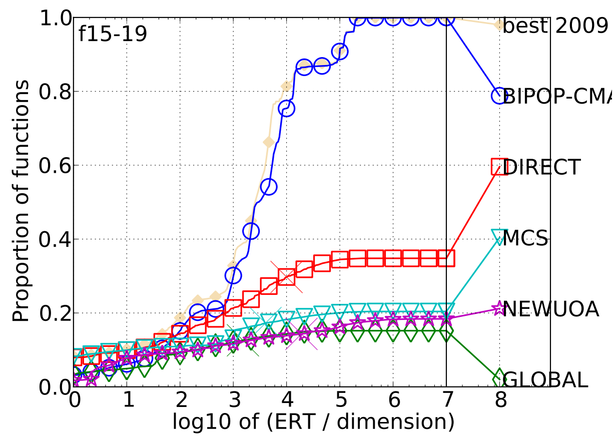
unimodal, high cond.



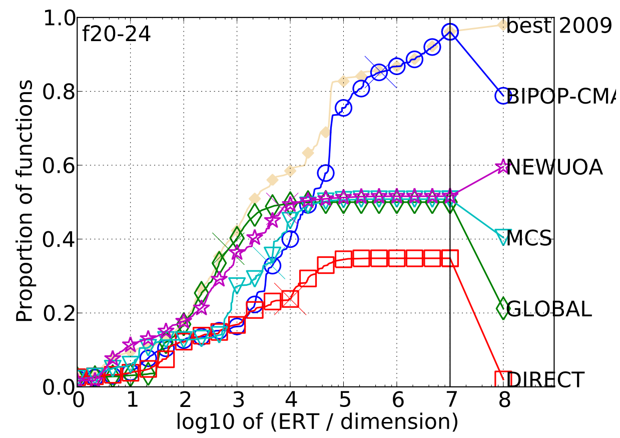
separable



multimodal, structured



multimodal, weak structure



Summary

Learning outcomes

After this lecture, a student shall be able to

- explain No Free Lunch Theorem, and its consequences;
- explain the concepts of success probability, runtime distribution, solution quality, and their relationship;
- define r-complete, asymptotically r-complete, and r-incomplete algorithms;
- describe 3 usual scenarios of applying an algorithm to an optimizaton problem, and explain their differences;
- explain differences between Monte Carlo and Las Vegas algorithms;
- name the advantages and disadvantages of measuring time in seconds vs measuring time in the number of performed operations;
- explain what errorneous conclusions can be drawn from the results of an experiment when comparing algorithms using a single time limit, and/or a single required target level;
- know a few statistical test that can be used to compare 2 algorithms;
- exemplify what kind of characteristics we can get when taking cross-sections of the runtime distribution function;
- explain how the runtime distributions can be aggregated over different target levels, different problem instances and different problems;
- derive valid conclusions when presented with runtime distributions of two or more algorithms.