CZECH TECHNICAL UNIVERSITY IN PRAGUE

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No Free Lunch.

Empirical 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

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

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]

- Informally, for discrete spaces: "Any two (non-repeating) 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.

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.
- $P_s(t) = P[RT_{A,\pi} \leq t]$ 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

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

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

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

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

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

Runtime Behaviour for Optimization Problems

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

- A is an algorithm for a class Π of optimization problems.
- $RT_{A,\pi}$ is the runtime of algorithm A when applied to problem instance π; random variable.
- $SQ_{A,\pi}$ is the quality of the solution found by algorithm A when applied to problem instance π; random variable.
- $P_s(t, q) = P[RT_{A,\pi} \leq t, SQ_{A,\pi} \leq q]$ is the 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.
- $r \geq 1, q > 0$.

Algorithm A is r-complete if and only if

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

Algorithm A is asymptotically r-complete if and only if

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

Algorithm A is r-incomplete if and only if

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

Quiz

To which class of algorithms do local search, evolutionary algorithms, and other metaheuristics usually belong?

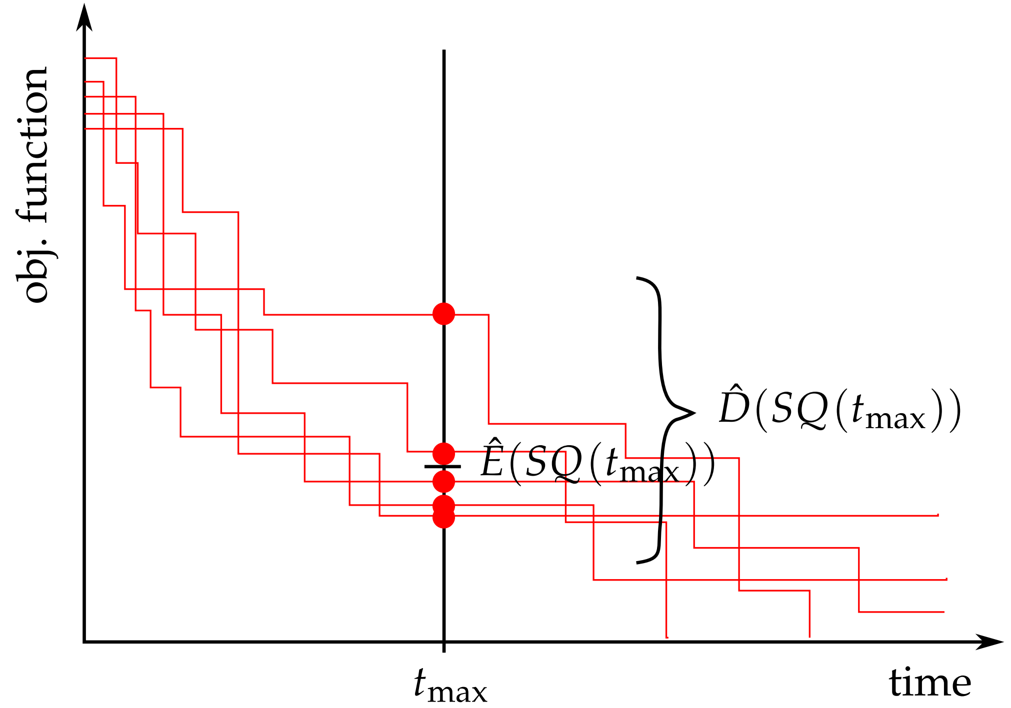
- A r-complete algorithms
- B asymptotically r-complete algorithms
- C r-incomplete algorithms
- D They do not belong to any of these classes.

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).

$\Rightarrow$ Evaluation criterion:

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



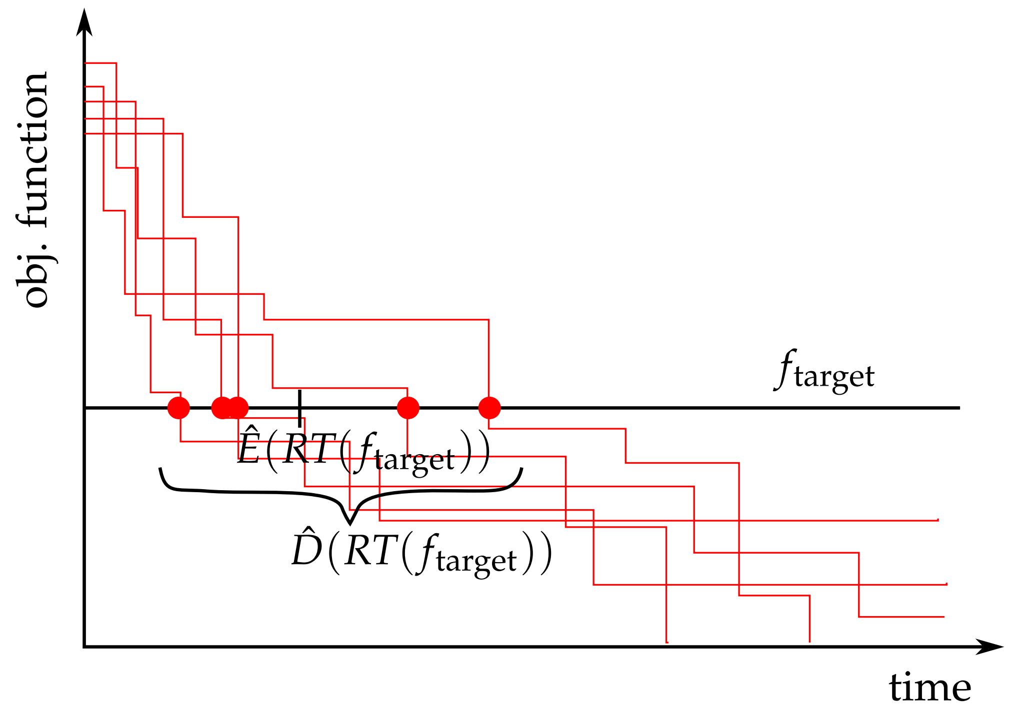
- Possible issue: What does "The expected solution quality of algorithm A is 2 times better than for algorithm B" actually mean?

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



- Is there any issue 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. problems: $U : R^+ \mapsto \langle 0, 1 \rangle$, where $U(t)$ = utility of solution found at time t
- opt. problems: $U : R^+ \times R^+ \mapsto \langle 0, 1 \rangle$, 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).

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

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

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

Monte Carlo vs. Las Vegas Algorithms

Classes of randomized algorithms:

- **Monte Carlo algorithm (MCA):** It always stops and provides a solution, but the solution may not be correct. The solution quality is a random variable. (Application scenario 1.)
- **Las Vegas algorithm (LVA):** It always produces a correct solution, but needs an unknown time to find it. The running time is a random variable. (Application scenario 2.)

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

- LVA can often be turned into MCA by bounding the allowed running time.
- MCA can often be turned into LVA by restarting the algorithm from randomly chosen states (using a restarting scheme that systematically reduces unexplored holes in the search space).

Theoretical vs. Empirical Analysis of LVAs

- Practically relevant LVAs are typically difficult to analyse theoretically.
- 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, we often **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 your model based on results

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**.
- Results of experiments should be **reproducible**.

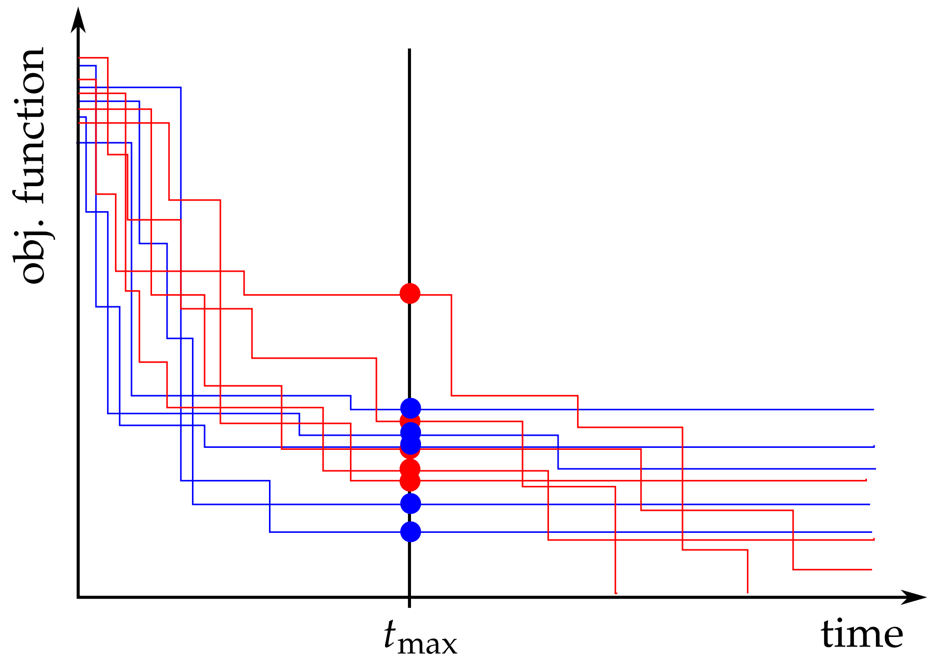
Wall-clock time

- depends on the machine configuration, computer language, and on the operating system used to run the experiments (the results are neither comparable, nor reproducible);
- produces the (disastrous) incentive to invest a long time into implementation details, because they have a huge effect on this performance measure.

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, $\text{ave}(SQ)$



Scenario 1: Limited time

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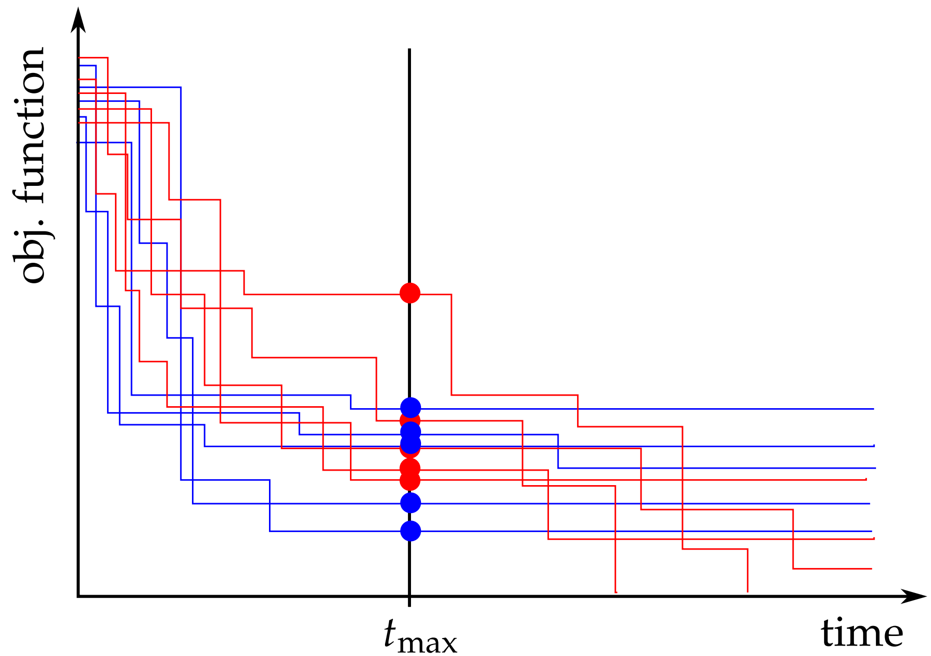

- For $t_{\max,1}$, blue algorithm is better than red.

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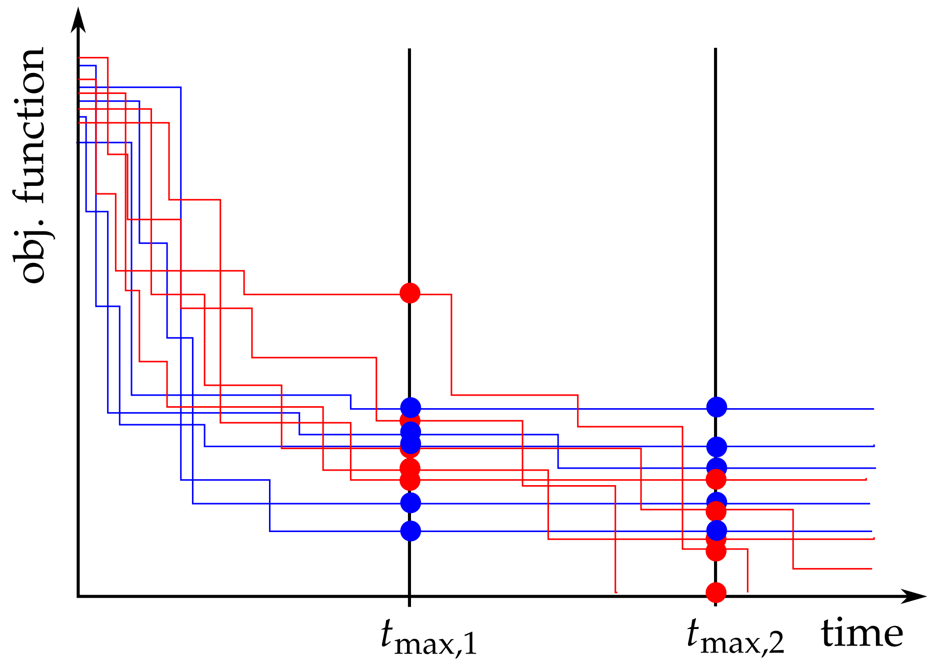
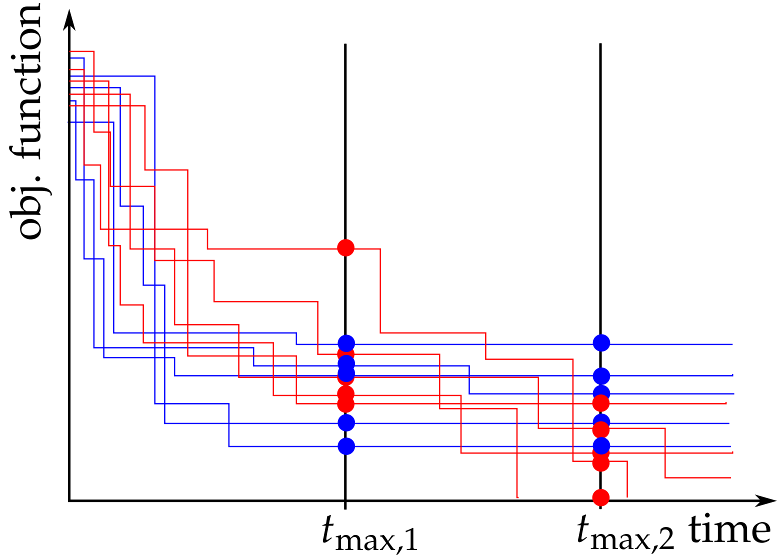


- For $t_{\max,1}$, blue algorithm is better than red.
- For $t_{\max,2}$, blue algorithm is worse than red.
- WARNING! The figure can change when $t_{\max}$ changes!!!

Quiz



OK, so for $t_{\max,2}$ it seems that there is a difference between the algorithms and that blue algorithm is worse than red.

Can our claim be false? Can we evaluate the credibility of our claim?

- **A** No, our claim cannot be false. It is evident from the picture.
- **B** Yes, our claim can be false. I have no idea how much we can trust our claim.
- **C** Yes, our claim can be false. We can evaluate the difference using Student's t-test.
- **D** Yes, our claim can be false. We can evaluate the difference using Mann-Whitney's U test.

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 with equal variances.
- 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/.

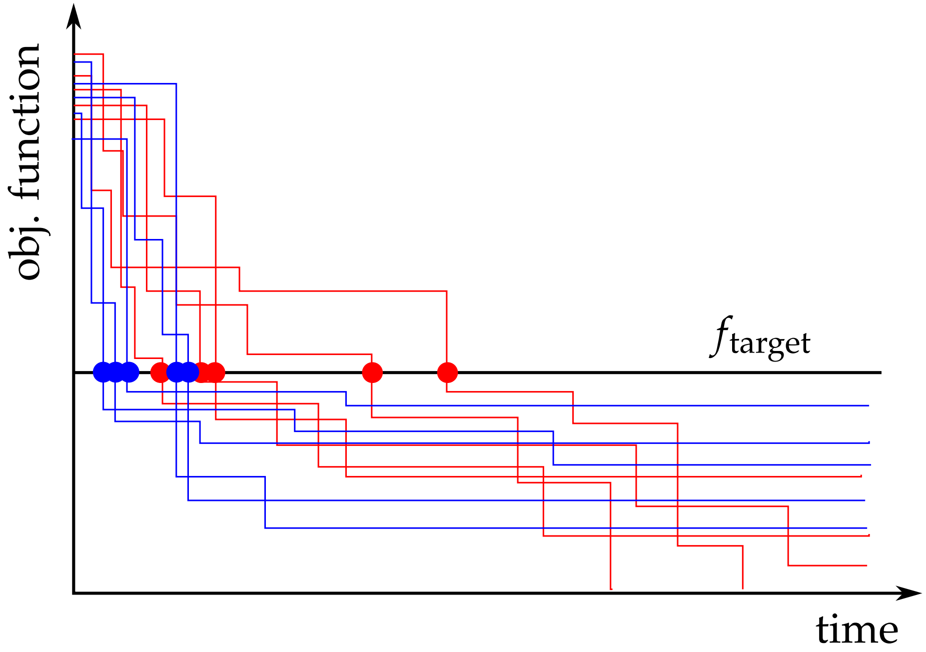
Mann-Whitney U test

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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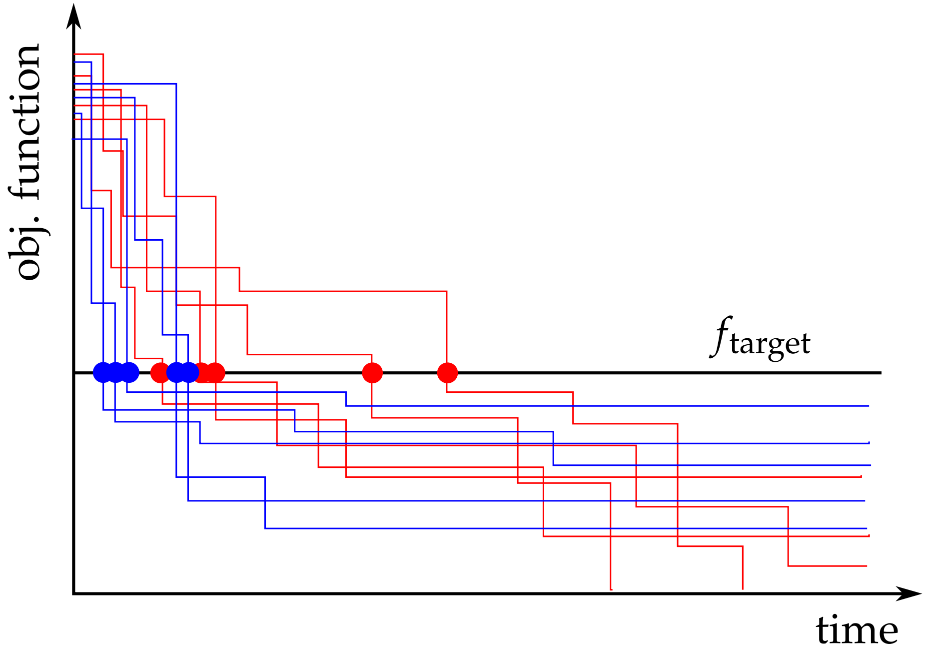

- For $f_{\text{target},1}$, blue algorithm is better than red.

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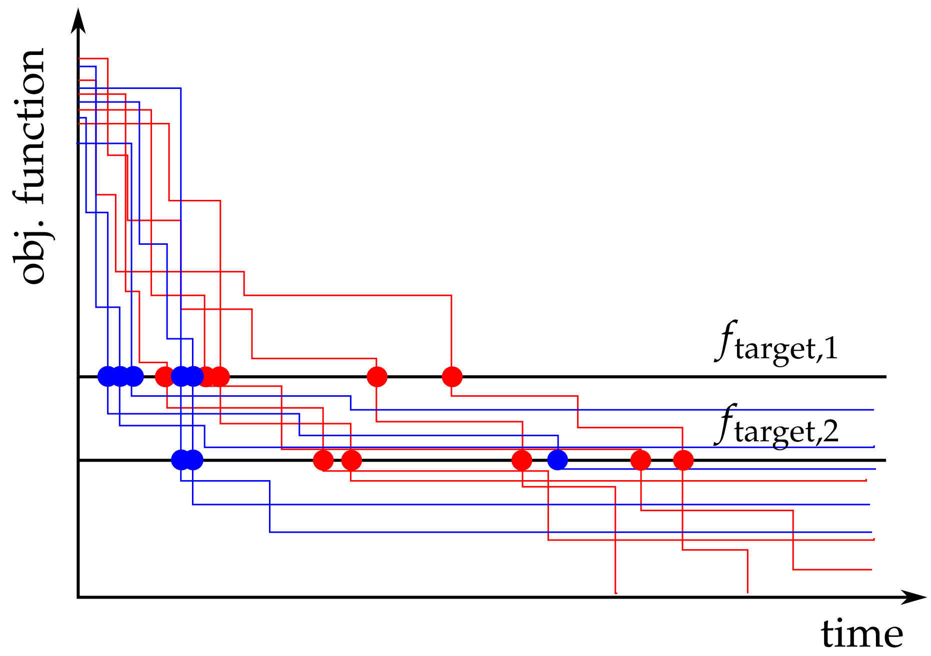

- For $f_{\text{target},1}$, blue algorithm is better than red.
- For $f_{\text{target},2}$, blue algorithm still seems to better than red (if it finds the solution, it finds it faster), but 2 blue runs did not reach the target level yet, i.e. (we are much less sure that blue is better).
- WARNING! The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

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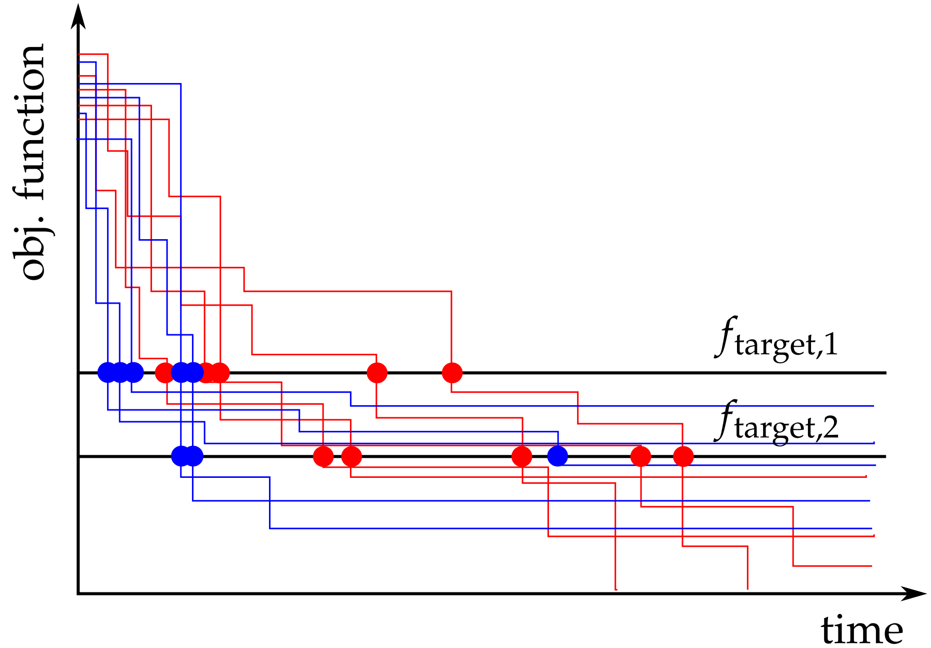

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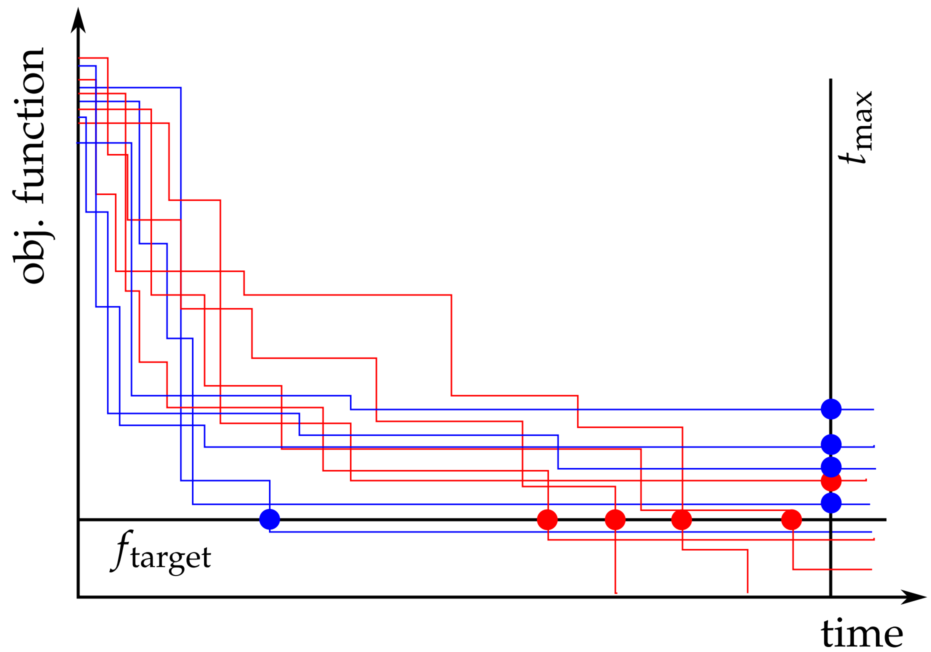
- WARNING! The figure can change when f_{target} changes!!!
- The same statistical tests as for scenario 1 can be used.

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?

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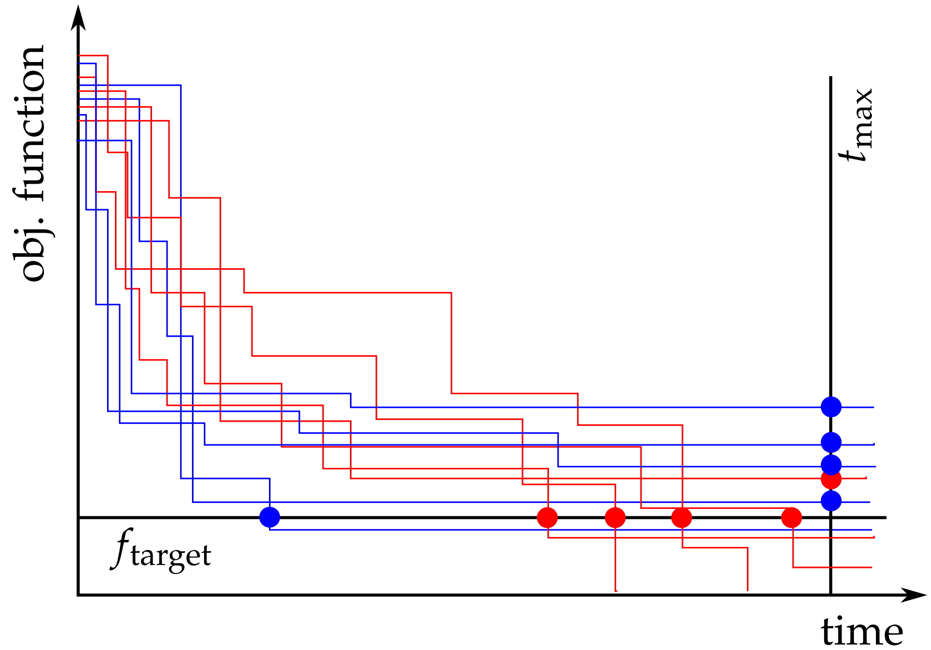

- *RT* is measured in seconds or function evaluations, *SQ* is measured in something different; now, how can we test if one algorithm is better than the other?
- The situation when the algorithm reaches f_{target} is better than when it reaches $t_{\max}$. We can still sort the values.
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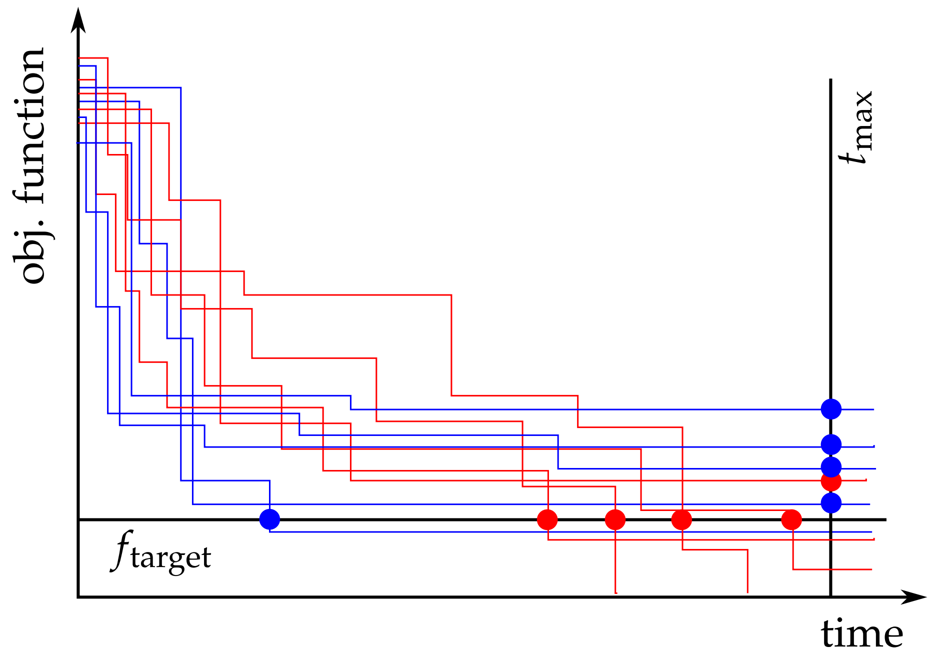

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- The situation when the algorithm reaches f_{target} is better than when it reaches $t_{\max}$. We can still sort the values.
- We can use the Mann-Whitney U-test.
- WARNING! Again, if we change f_{target} and/or $t_{\max}$, the figure can change!!!

Analysis based on runtime distribution

Runtime distributions

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

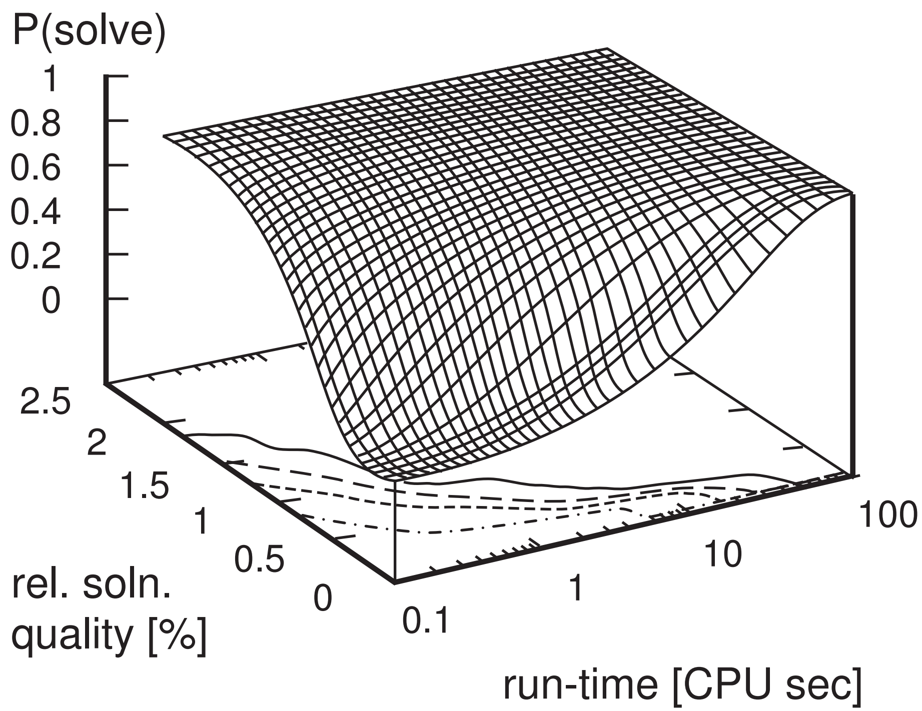
- Assume the most general scenario — type 3 with a utility function (which is often, however, unknown as well).
- Evaluate based on solution probabilities $P_s(t, q) = P[RT \leq t, SQ \leq q]$ for arbitrary runtimes t and solution qualities q.

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

RTD defintion

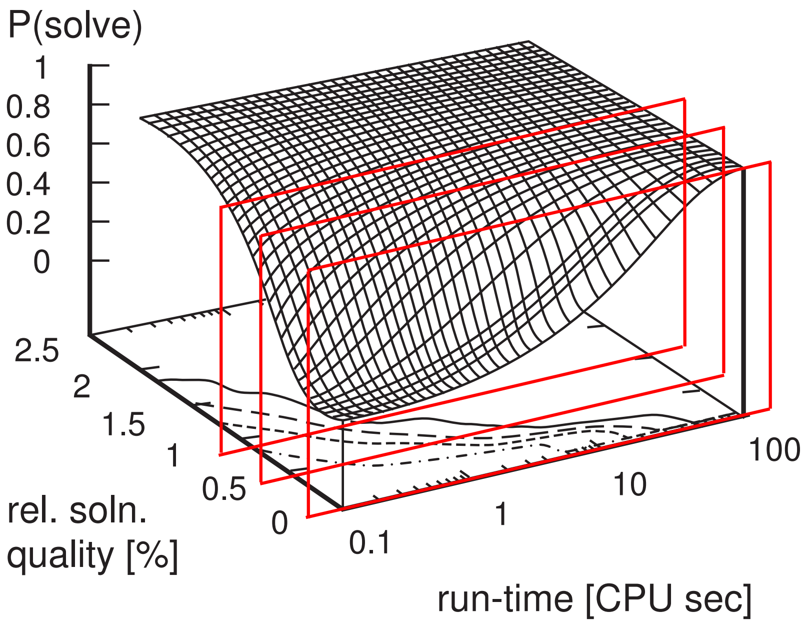
Given a Las Vegas alg. A for optimization problem π:

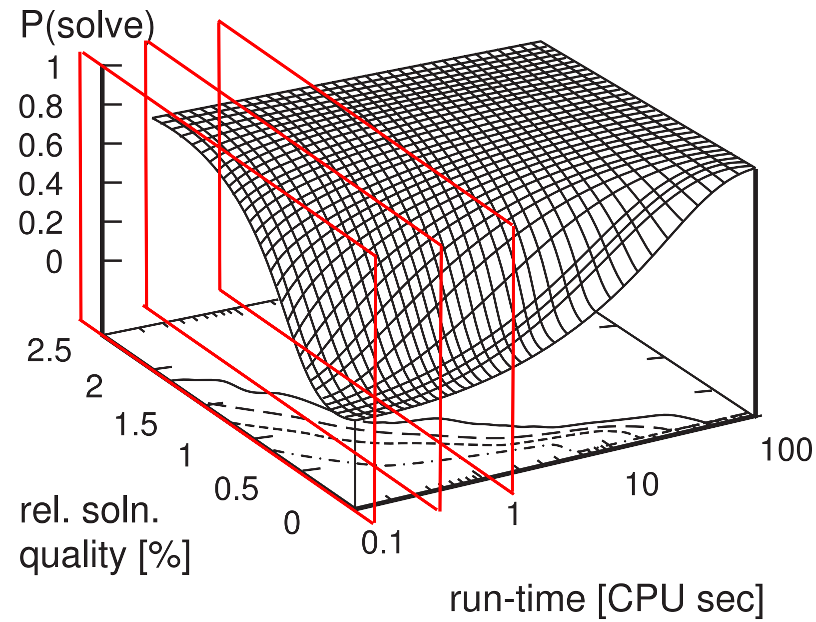
- The *success probability* $P_s(t, q) = P[RT_{A,\pi} \leq t, SQ_{A,\pi} \leq q]$ is the probability that A finds a solution for a solvable instance $\pi \in \Pi$ of quality $\leq q$ in time $\leq t$.
- The *run-time distribution* (RTD) of A on π is the probability distribution of the bivariate random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

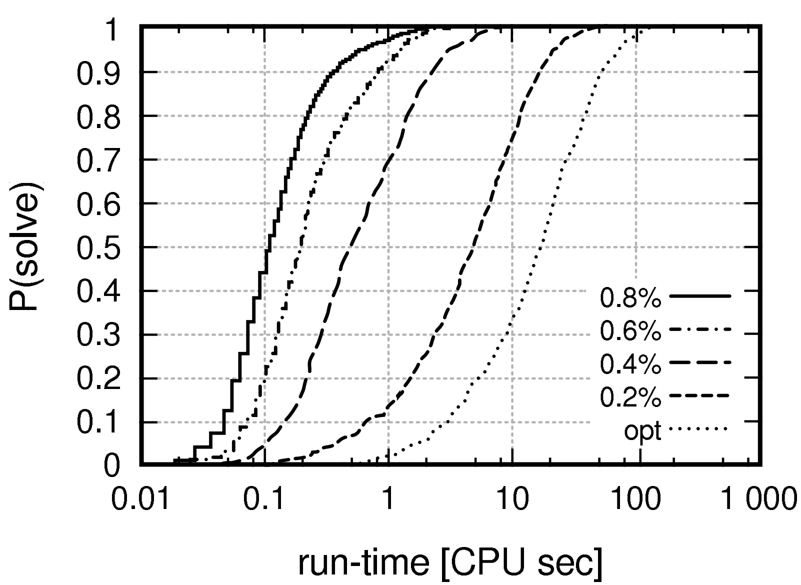


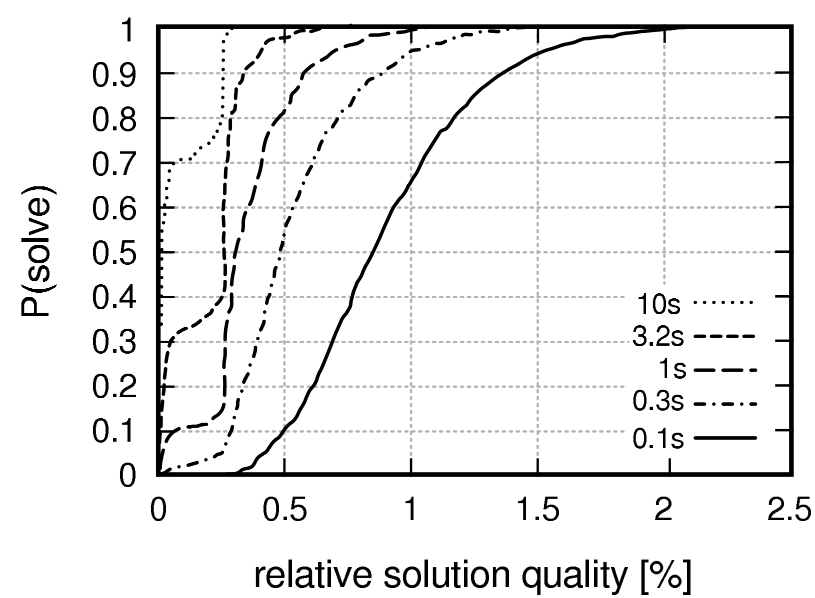
RTD cross-sections

We can study the RTD using cross-sections:



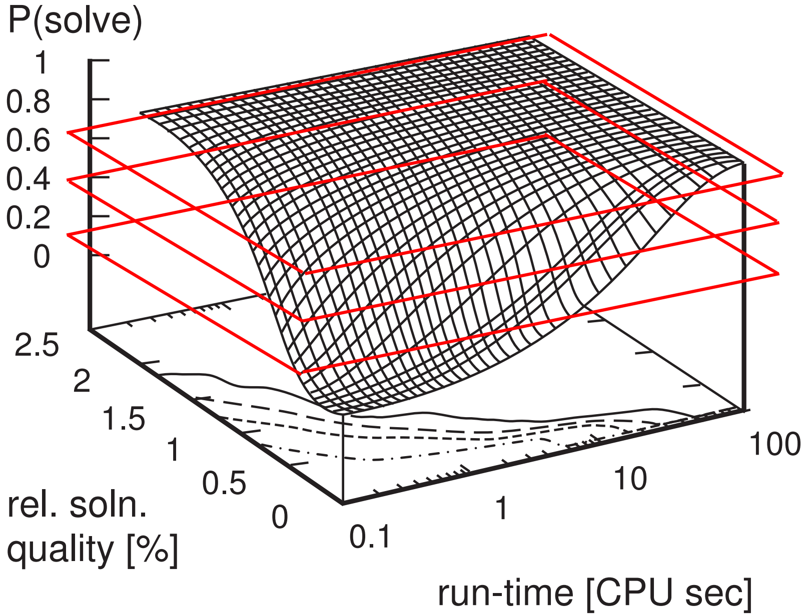


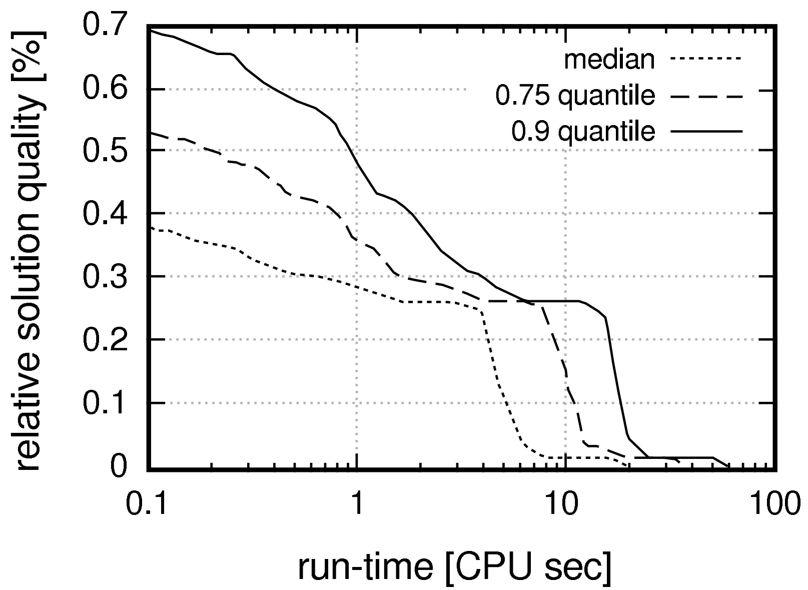




RTD cross-sections (cont.)

We can study the RTD using cross-sections:



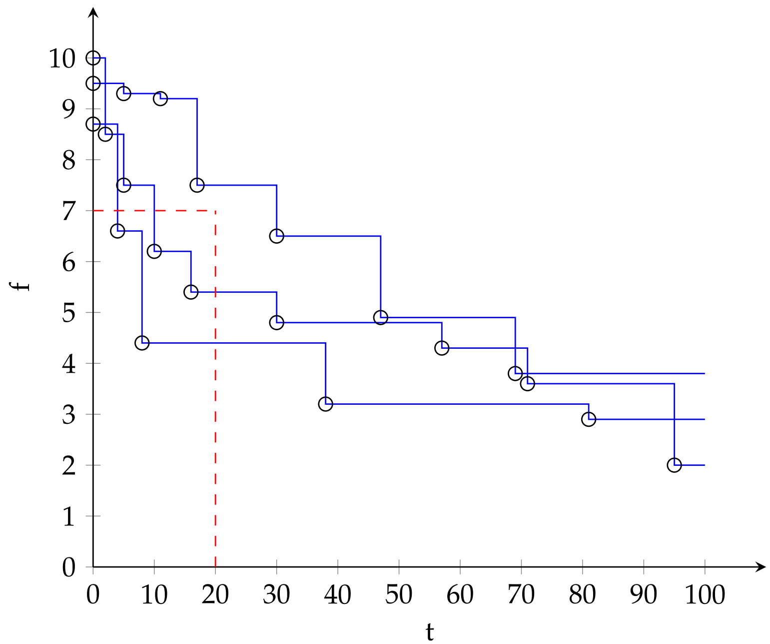


Horizontal cross-sections reveal the dependence of SQ on RT:

- 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.

Quiz

Are you able to estimate the success probability?



Based on the above convergence curves of 3 runs of the same algorithm, what is your estimate of $\hat{P}_S(20, 7)$?

- A 0
- B $\frac{1}{3}$
- C $\frac{2}{3}$
- D 1

Empirical measurement of RTDs

Empirical estimation of $P[RT \leq t, SQ \leq q]$:

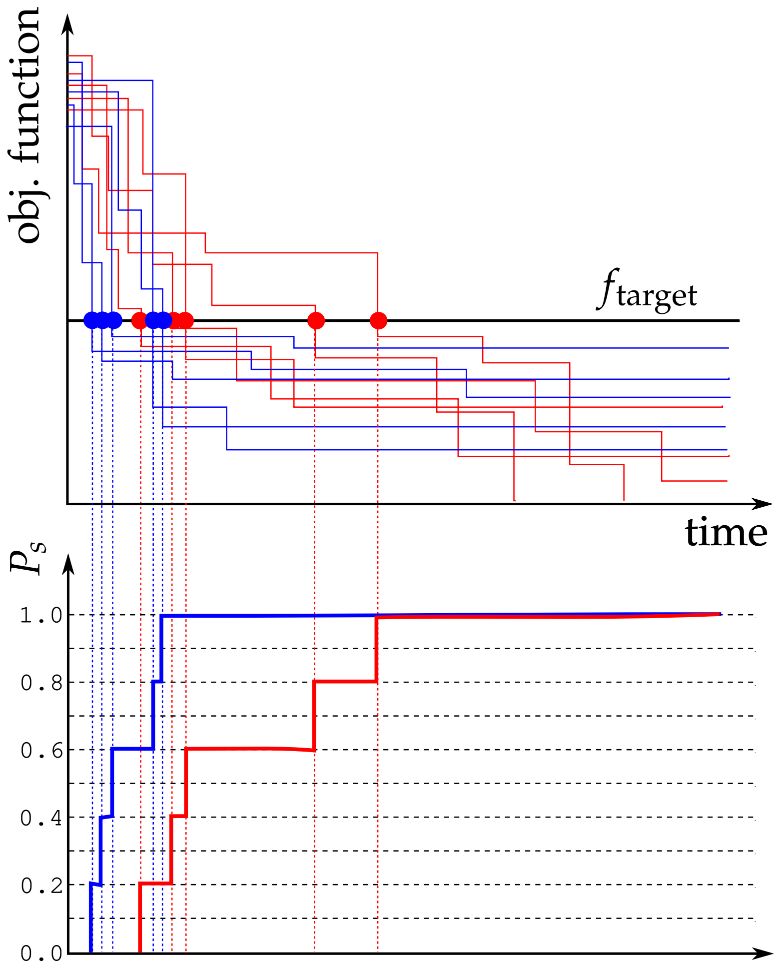
- Perform N independent runs of A on problem π.
- For n^{th} run, $n \in 1, \ldots, N$, store the so-called *solution quality trace*, i.e. $t_{n,i}$ and $q_{n,i}$ each time the quality is improved.
- $\hat{P}_s(t, q) = \dfrac{n_S(t, q)}{N}$, where $n_S(t, q)$ is the number of runs which provided at least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

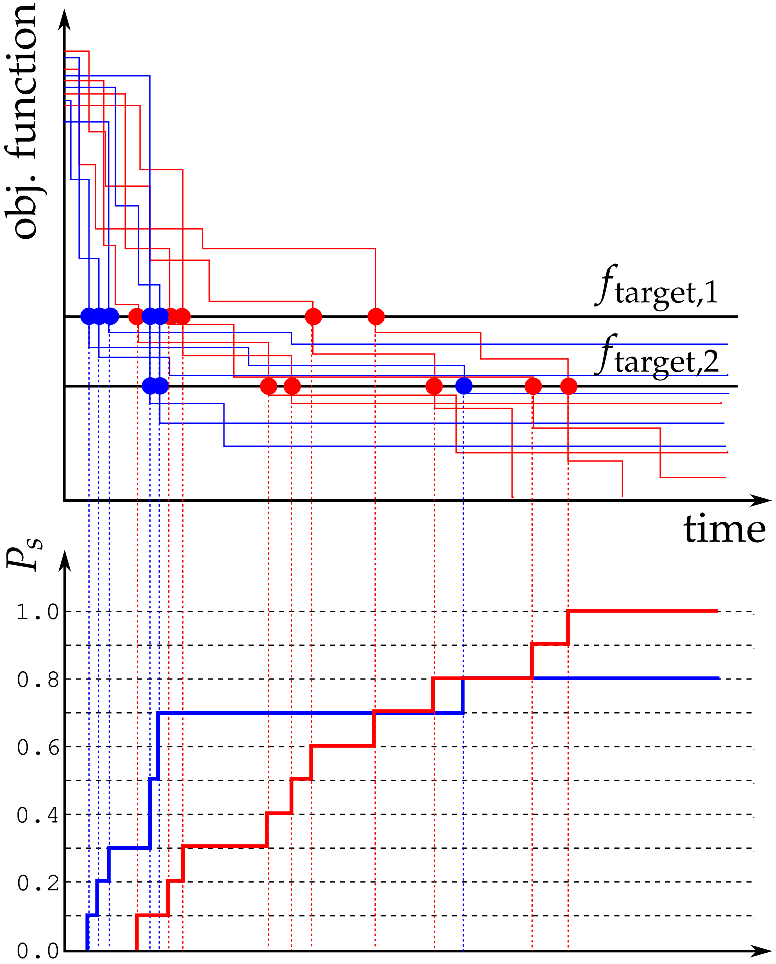
E.g. type 2 application scenario: set f_{target} and compare RTDs of the algorithms



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 …



RTD based algorithm comparisons

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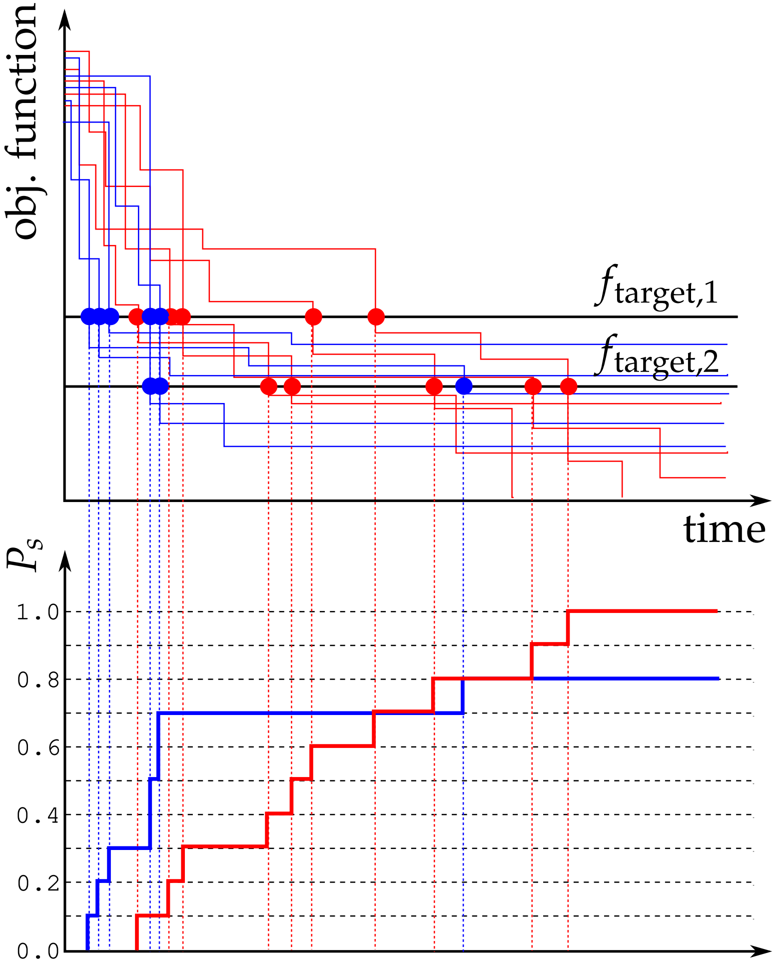


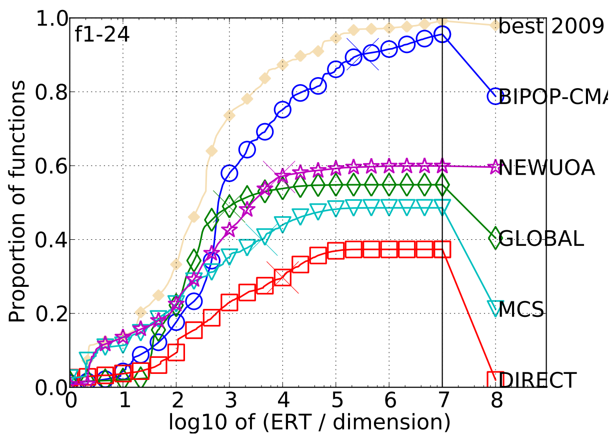
This way we can aggregate RTDs of an algorithm A not only

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

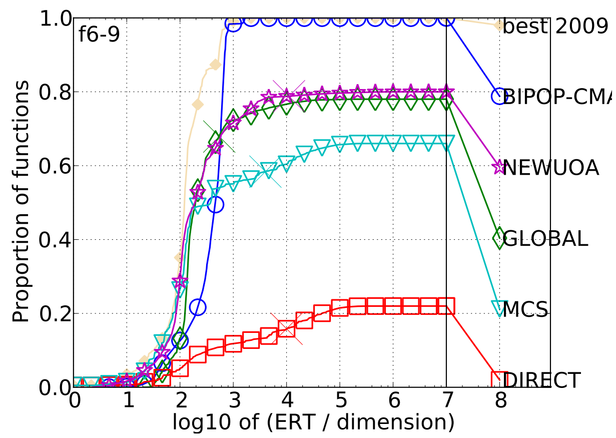
Example of comparison

COCO framework (BBOB Workshop at GECCO conference, `https://github.com/numbbo/coco`):

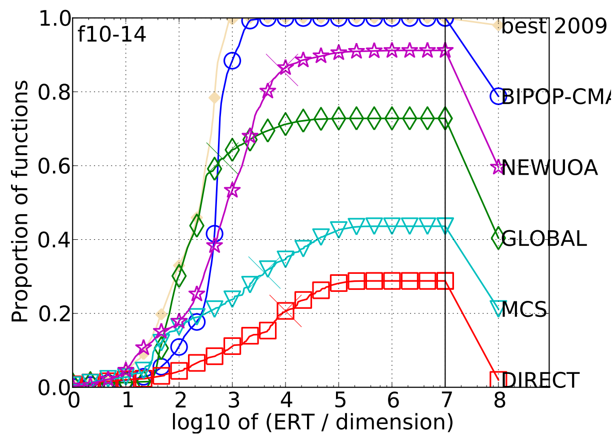
all



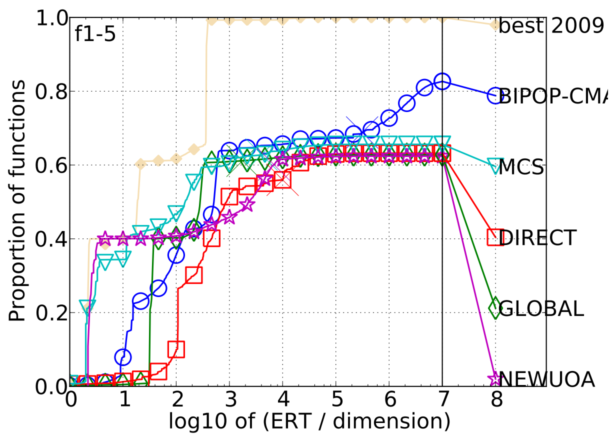
unimodal, low cond.



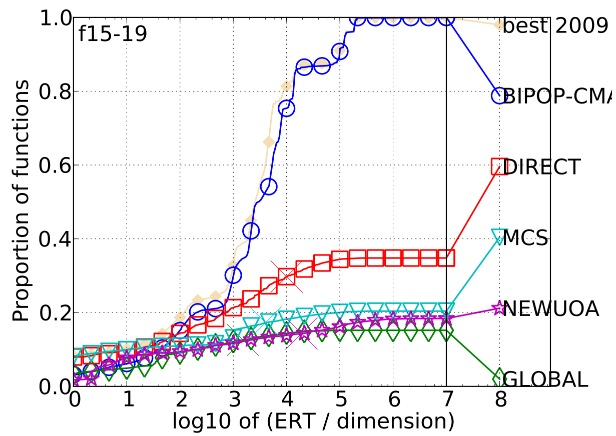
unimodal, high cond.



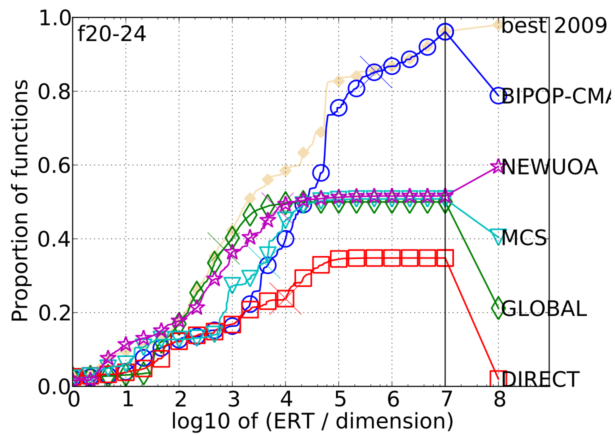
separable



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.