

STOCHASTIC LOCAL SEARCH
FOUNDATIONS AND APPLICATIONS

Empirical Analysis of SLS Algorithms

Holger H. Hoos & Thomas Stützle

Outline

1. Las Vegas Algorithms
2. Run-Time Distributions
3. RTD-Based Analysis of LVA Behaviour
4. Characterising and Improving LVA Behaviour

Las Vegas Algorithms

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But: For decision problems, any solution returned is guaranteed to be correct.

Also: The run-time required for finding a solution (in case one is found) is subject to random variation.

↔ These properties define the class of (*generalised*) *Las Vegas algorithms*, of which SLS algorithms are a subset.

Definition: (Generalised) Las Vegas Algorithm (LVA)

An algorithm A for a problem class Π is a *(generalised) Las Vegas algorithm (LVA)* iff it has the following properties:

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Note: This is a slight generalisation of the definition of a Las Vegas algorithm known from theoretical computing science (our definition includes algorithms that are not guaranteed to return a solution).

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- ▶ Las Vegas algorithms can be deterministic, since deterministic run-time is modelled by a *degenerate probability distribution* (aka *Dirac delta distribution*).

Note: For SLS algorithms for optimisation problems, the *solution quality achieved within bounded run-time* as well as the *run-time required for reaching a given solution quality* are random variables.

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- ▶ There are successful types of LVAs other than SLS algorithms, *e.g.*, *randomised systematic search algorithms*.
- ▶ LVAs can be seen as special cases of *Monte Carlo Algorithms*, *i.e.*, randomised algorithms that can sometimes return an incorrect solution to the given problem instance (*false positive result*).

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 - ▶ capture only *asymptotic behaviour* and do not reflect *actual behaviour* with sufficient accuracy.

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- ▶ *essential incompleteness:*

for some soluble problem instances, the probability for finding a solution is strictly smaller than 1 for run-time $\rightarrow \infty$.

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- ▶ *Iterative Improvement* is essentially incomplete.

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In many cases, these can render algorithms provably PAC; but effectiveness in practice can vary widely.

Asymptotic behaviour of OLVAs

- ▶ Simple generalisation based on associated decision problems for given solution quality bound $q := r \cdot q^*$, where q^* = optimal solution quality for given problem instance:
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- ▶ Terminology for optimal solution qualities:
complete = 1-complete, *PAC* = 1-PAC,
essentially incomplete = *essentially 1-incomplete*.

Application scenarios and evaluation criteria (1)

Evaluation criteria for LVAs depend on the application context:

- ▶ **Type 1:** 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).

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- ▶ **Type 2:** 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: solution probability at time t_{max}

Application scenarios and evaluation criteria (2)

In many real applications, utility of solutions depends in more complex ways on time required for finding them:

- ▶ **Type 3:** Characterised by *utility function* $U : \mathbb{R}^+ \mapsto [0, 1]$, where $U(t)$ = utility of solution found at time t .

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Evaluation criterion for type 3 scenario:

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Note: Type 3 is a generalisation of types 1 and 2.

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- ▶ Run-time is unconstrained, given solution quality threshold must be reached (generalisation of type 1 scenario)
- ▶ Hard time-limit is given, during which best possible solution quality should be found (generalisation of type 2 scenario).

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- ▶ **Generalisation of type 3 scenario:** Utility of solution depends on quality and time needed for finding it; characterised by utility function $U : \mathbb{R}^+ \times \mathbb{R}^+ \mapsto [0, 1]$, where $U(t, q) =$ utility of solution of quality q found at time t .

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Evaluation criterion: utility-weighted solution probability

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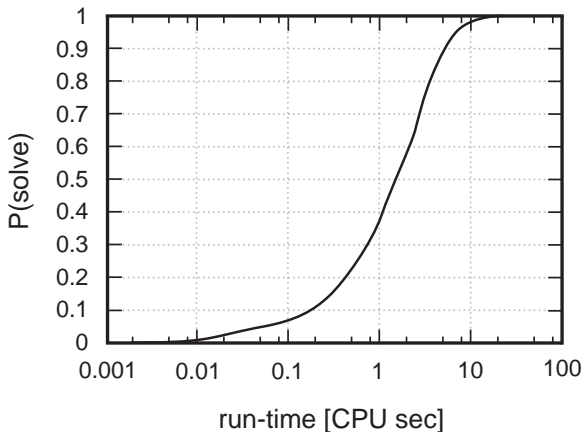
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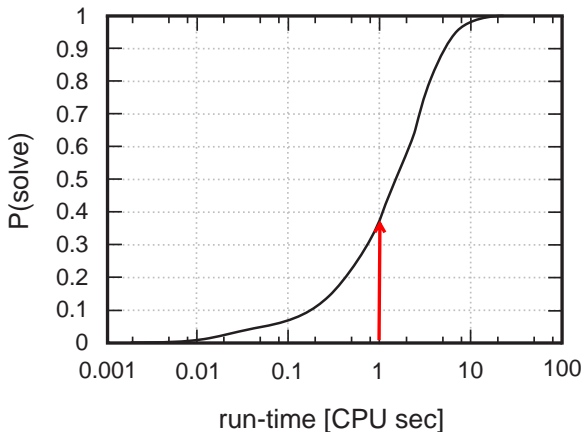
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- ↪ study distributions of *random variables* characterising run-time and solution quality of algorithm on given problem instance.

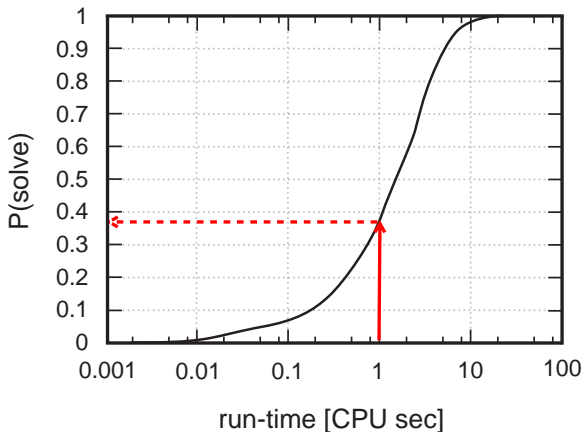
Typical run-time distribution for SLS algorithm applied to hard instance of combinatorial decision problem:



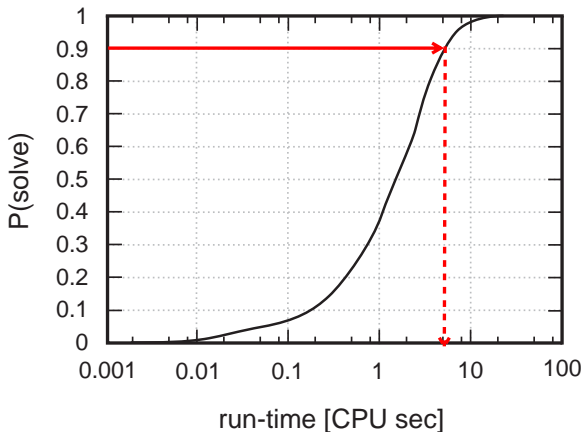
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- ▶ The *run-time distribution function rtd* : $\mathbb{R}^+ \mapsto [0, 1]$, defined as $rtd(t) = P_s(RT_{A,\pi} \leq t)$, completely characterises the RTD of A on π .

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Given OLVA A' for optimisation 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 soluble instance $\pi' \in \Pi'$ of quality $\leq q$ in time $\leq t$.

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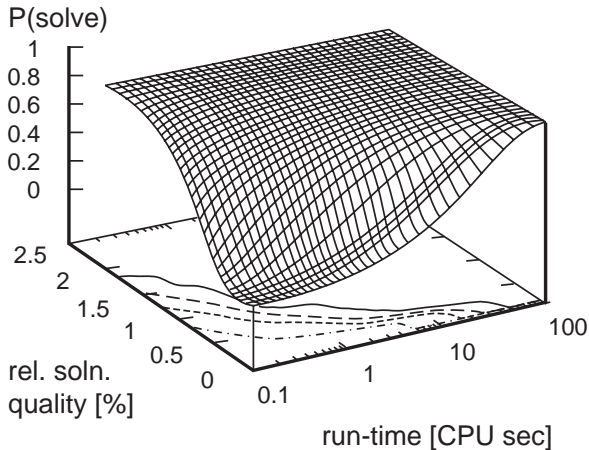
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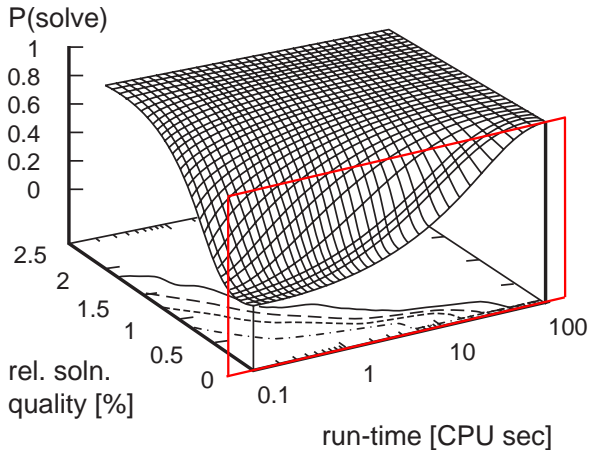
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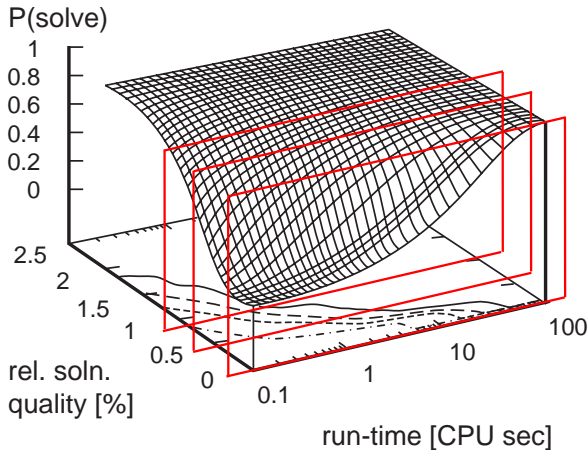
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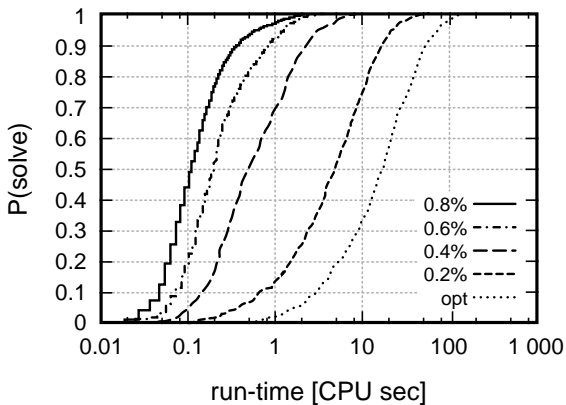
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Qualified RTDs for various solution qualities:



Qualified run-time distributions (QRTDs)

- ▶ A *qualified run-time distribution (QRTD)* of an OLVA A' applied to a given problem instance π' for solution quality q' is a marginal distribution of the bivariate RTD $rtd(t, q)$ defined by:

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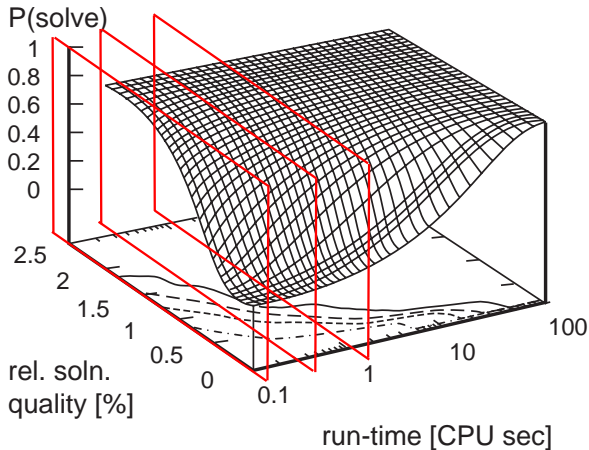
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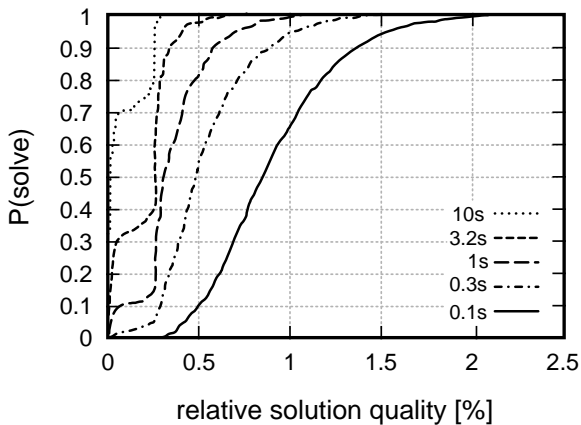
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Note: Solution qualities q are often expressed as *relative solution qualities* $q/q^* - 1$, where q^* = optimal solution quality for given problem instance.

Typical solution quality distributions for SLS algorithm applied to hard instance of combinatorial optimisation problem:



Solution quality distributions for various run-times:



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- ▶ SQDs correspond to cross-sections of the two-dimensional bivariate RTD graph.
- ▶ SQDs characterise the solution qualities achieved by a given SLS algorithm for a combinatorial optimisation problem within a given run-time bound (useful for type 2 application scenarios).

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- ▶ For sufficiently long run-times, increase in mean solution quality is often accompanied by decrease in solution quality variability.
- ▶ For PAC algorithms, the SQDs for very large time-limits t' approach degenerate distributions that concentrate all probability on the optimal solution quality.
- ▶ For any essentially incomplete algorithm A' (such as Iterative Improvement) applied to a problem instance π' , the SQDs for sufficiently large time-limits t' approach a non-degenerate distribution called the *asymptotic SQD of A' on π'* .

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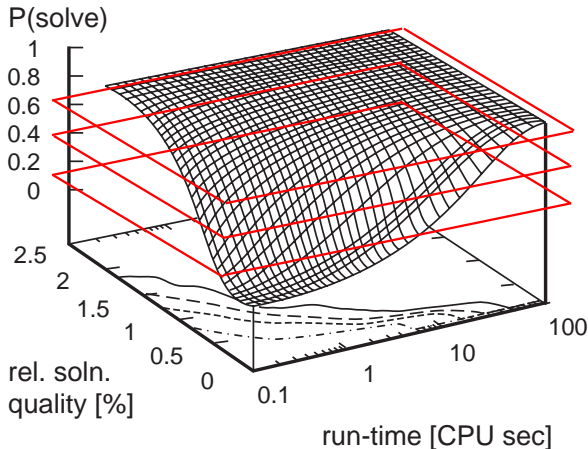
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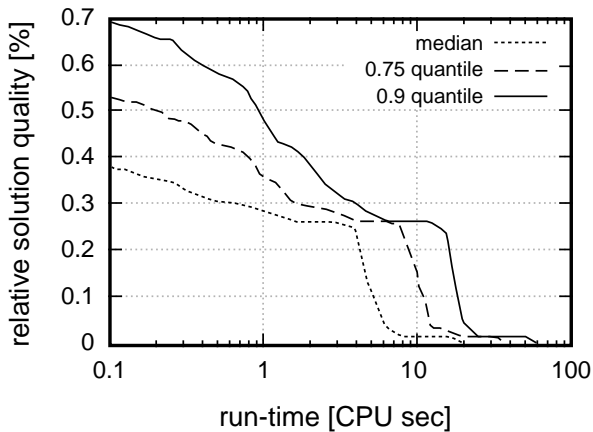
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- ▶ **But:** Important aspects of an algorithm's run-time behaviour may be easily missed when basing an analysis solely on a single SQT curve.

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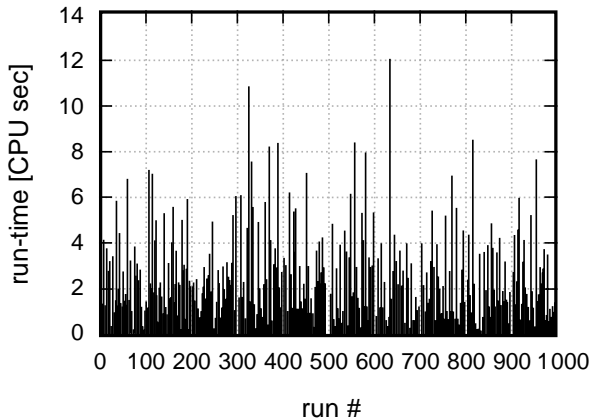
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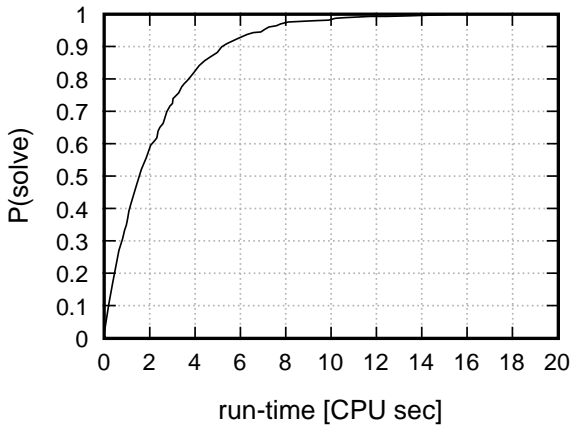
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Typical sample of run-times for an SLS algorithm applied to an instance of a hard decision problem:



Corresponding empirical RTD:



Protocol for obtaining the empirical RTD for an LVA A applied to a given instance π of a decision problem:

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- ▶ Plot the graph $(rt(j), j/k)$, *i.e.*, the cumulative empirical RTD of A on π .

Note:

- ▶ The fraction of successful runs, $sr := k'/k$, is called the *success ratio*; for large run-times t' , it approximates the *asymptotic success probability* $p_s^* := \lim_{t \rightarrow \infty} P_s(RT_{a,\pi} \leq t)$.

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The mean run-time for a variant of the algorithm that restarts after time t' can be estimated as:

$$\widehat{E}(RT_s) + (1/sr - 1) \cdot \widehat{E}(RT_f)$$

where $\widehat{E}(RT_s)$ and $\widehat{E}(RT_f)$ are the average times of successful and failed runs, respectively.

Note: $1/sr - 1$ is the expected number of failed runs required before a successful run is observed.

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- ▶ Let $sq(t', j)$ denote the best solution quality encountered in run j up to time t' . The cumulative empirical RTD of A' on π' is defined by $\hat{P}_s(RT \leq t', SQ \leq q') := \#\{j \mid sq(t', j) \leq q'\} / k$.

Note: Qualified RTDs, SQDs and SQT curves can be easily derived from the same solution quality traces.

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When reporting CPU times, the run-time environment should be specified (at least CPU type, model, speed and cache size; amount of RAM; OS type and version); ideally, the implementation of the algorithm should be made available.

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- ▶ *cost models* that specify the CPU time for each such operation for a given implementation and run-time environment.

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when running the algorithm on an Intel Xeon 2.4GHz CPU with 512KB cache and 1GB RAM running Red Hat Linux, Version 2.4smp (*run-time environment*).

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- ▶ Elementary operations commonly used as the basis for RLD and other run-time measurements of SLS algorithms include search steps, objective function evaluations and updates of data structures used for implementing the step function.

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RTD-based empirical analysis in combination with proper statistical techniques (hypothesis tests) is a state-of-the-art approach in empirical algorithmics.

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- ▶ *Semi-log plots* give a better view of the distribution over its entire range.

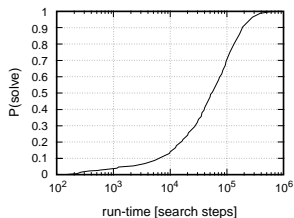
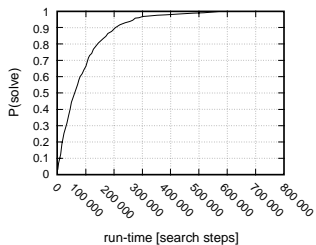
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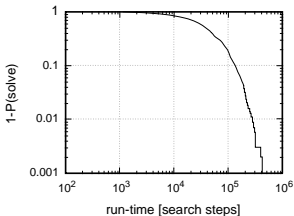
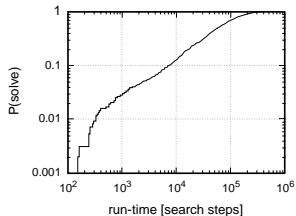
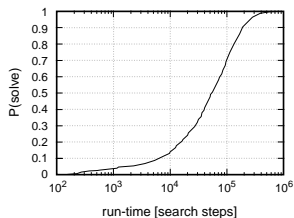
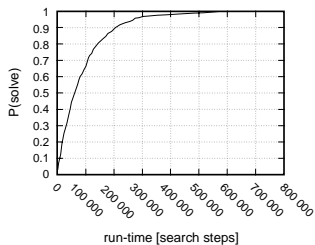
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Various graphical representations of a typical RTD:



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Note: SLS algorithms typically show very high variability in run-time; therefore, reporting a measure of variability along with the mean or median run-time is important.

Example:

The empirical RLD of a given SLS algorithm for SAT on a specific SAT instance is characterised by the following basic descriptive statistics:

mean	57 606.23	median	38 911
min	107	$q_{0.25}; q_{0.1}$	16 762; 5 332
max	443 496	$q_{0.75}; q_{0.9}$	80 709; 137 863
stddev	58 953.60	$q_{0.75}/q_{0.25}$	4.81
vc	1.02	$q_{0.9}/q_{0.1}$	25.86

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- ▶ Obtaining sufficiently stable descriptive statistics requires the same number of runs of the given algorithm as measuring reasonably accurate empirical RTDs.
- ▶ QRTDs and SQDs can be handled analogously to RTDs; along with SQT curves they can be easily determined from the same solution quality traces that provide the basis for empirical bivariate RTDs of a given optimisation LVA.

Basic quantitative analysis for ensembles of instances (1)

- ▶ In principle, the same approach as for individual instances is applicable: Measure empirical RTD for each instance, analyse using RTD plots or descriptive statistics.

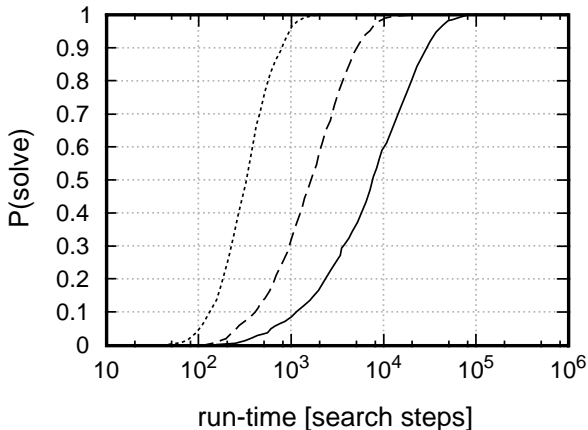
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 - ↪ Select typical instance for presentation or further analysis, briefly summarise data for remaining instances.

RTDs for WalkSAT/SKC, a prominent SLS algorithm for SAT, on three hard 3-SAT instances:



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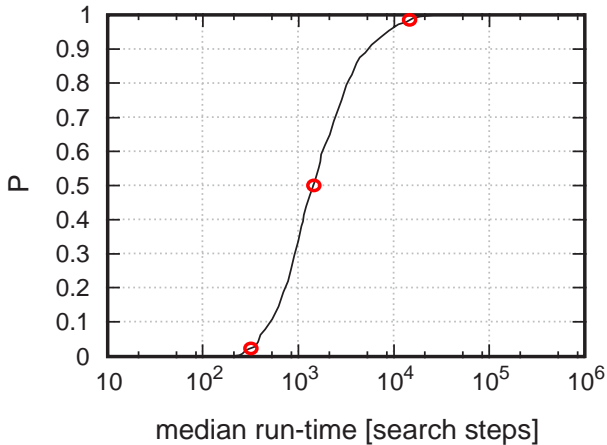
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Useful fact: *Exponential* and *polynomial functions* appear as straight lines in *semi-log plots* and *log-log plots*, respectively.

Distribution of median search cost for WalkSAT/SKC over set of 1000 randomly generated, hard 3-SAT instances:



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 - ▶ encodings of various other types of problems (e.g., SAT-encodings of graph colouring problems)

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Careful selection and good understanding of benchmark sets are often crucial for the relevance of an empirical study!

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- ▶ For an instance of an optimisation problem, OLVA A' probabilistically dominates OLVA B' on a given problem instance iff for all solution quality bounds, A' probabilistically dominates B' on the respective associated decision problem.

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- ▶ To assess the *statistical significance* of observed performance differences, an appropriate *statistical hypothesis test* must be applied.

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Typical values of α are 0.05 or 0.01.

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The null hypothesis is rejected iff this p-value is smaller than the previously chosen significance level.

Background: Statistical hypothesis tests (2)

- ▶ The *power* of the test provides a lower bound for the probability of correctly accepting the null hypothesis. The desired power of a test determines the required *sample size*.
Typical power values are at least 0.8; in many cases, sample size calculations for given power values are difficult.

- ▶ The application of a test to a given data set results in a *p-value*, which represents the probability that the null hypothesis is incorrectly rejected.

The null hypothesis is rejected iff this p-value is smaller than the previously chosen significance level.

- ▶ Most common statistical hypothesis tests and other statistical analyses can be performed rather conveniently in the free *R software environment* (see <http://www.r-project.org/>).

Comparing algorithms based on RTDs (3)

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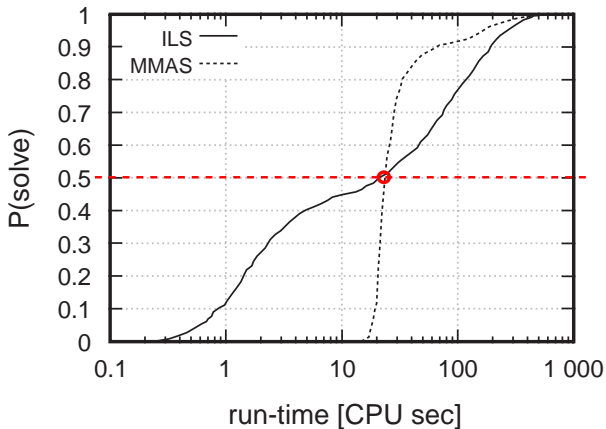
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- ▶ The more specific hypothesis whether the theoretical RTDs (or SQDs) of two algorithms are identical can be tested using the *Kolmogorov-Smirnov test*.

Performance differences detectable by the Mann-Whitney U-test for various sample sizes (sign. level 0.05, power 0.95):

sample size	m_1/m_2
3010	1.1
1000	1.18
122	1.5
100	1.6
32	2
10	3

m_1/m_2 is the ratio between the medians of the two empirical distributions.

Example of crossing RTDs for two SLS algorithms for the TSP applied to a standard benchmark instance (1000 runs/RTD):



Comparative analysis for instance ensembles (1)

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The size of these subsets gives a rather detailed picture of the algorithms' relative performance on the given ensemble.

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- ▶ **Note:** This test *does not* capture qualitative performance differences such as different shapes of the underlying RTDs and can easily miss interesting variation in relative performance across the ensemble.

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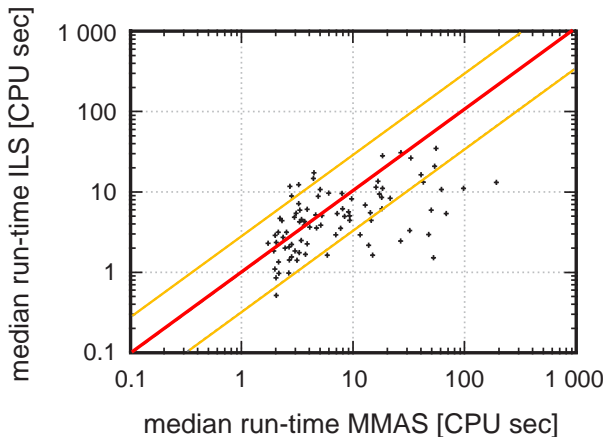
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- ▶ For qualitative correlation analyses, *scatter plots* in which each instance π is represented by one point whose x and y co-ordinates correspond to the performance of A and B on π .

Correlation between median run-time for two SLS algorithms for the TSP over a set of 100 randomly generated instances:



10 runs per instance.

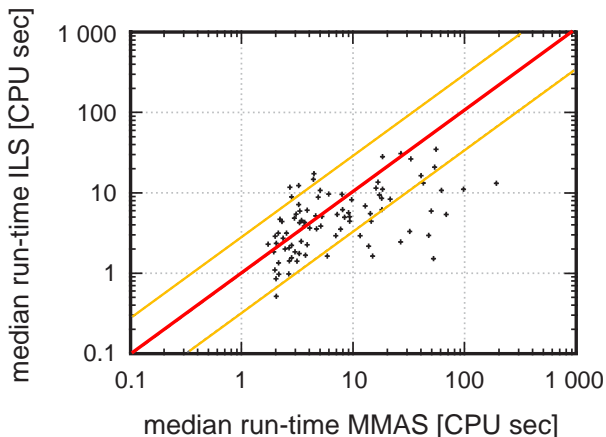
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- ▶ To test the statistical significance of an observed *monotonic* relationship, use non-parametric tests such as *Spearman's rank order test*.

Correlation between median run-time for two SLS algorithms for the TSP over a set of 100 randomly generated instances:



10 runs per instance; correlation coefficient 0.39, significant according to Spearman's rank order test at $\alpha = 0.05$; p-value = $9 \cdot 10^{-11}$.

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Note: Peak performance is a measure of *potential performance*.

- ▶ **Pitfall:** *Unfair parameter tuning*, i.e., the use of unevenly optimised parameter settings in comparative studies.

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- ▶ **Note:**
 - ▶ Optimal parameter settings often vary substantially between problem instances or instance classes.
 - ▶ Effects of multiple parameters are typically *not* independent.
- ▶ *Performance robustness*, i.e., the variation in performance due to deviations from optimal parameter settings, is an important performance criterion.

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- ▶ More general notions of robustness include performance variation over
 - ▶ multiple runs for fixed input (captured in RTD),
 - ▶ different problem instances or domains.
- ▶ Advanced empirical studies should attempt to relate the latter type of variations to features of the respective instances or domains (*e.g.*, *scaling studies* relate LVA performance to instance size).

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Asymptotic behaviour and stagnation

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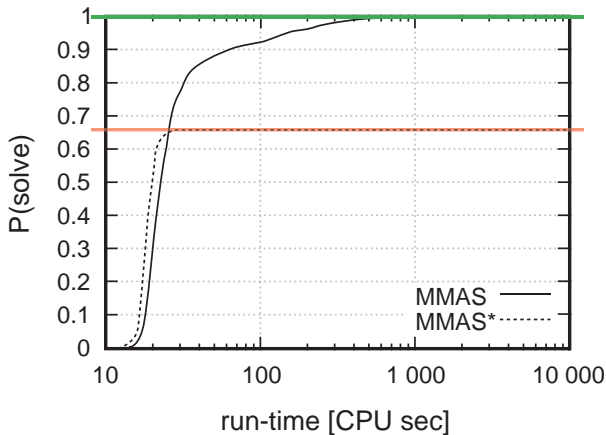
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- ▶ Neither the *PAC property*, nor *essential incompleteness* can be empirically verified or falsified.
- ▶ **But:** Empirical RTDs can provide *evidence* (rather than proof) for essential incompleteness or PAC behaviour.

Example of asymptotic behaviour in empirical RTDs:



Note: $\mathcal{M}\mathcal{M}\mathcal{A}\mathcal{S}$ is provably PAC, $\mathcal{M}\mathcal{M}\mathcal{A}\mathcal{S}^*$ is essentially incomplete.

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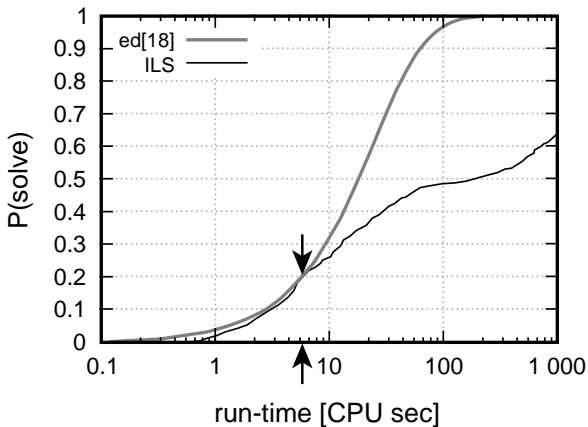
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- ▶ A drop in $\lambda_{A,\pi}(t)$ indicates *stagnation* of algorithm A 's progress towards finding a solution of instance π .
- ▶ Stagnation can be detected by comparing the RTD against an exponential distribution.

Evidence of stagnation in an empirical RTD:



'ed[18]' is the CDF of an exponential distribution with median 18; the arrows mark the point at which stagnation behaviour becomes apparent.

Note:

- ▶ The formal definition of LVA *efficiency* and *stagnation* is based on the idea that an LVA A suffers from stagnation iff its success probability can be increased by restarting A after an appropriately chosen cutoff time.

(For details, see Definition 4.9 on page 187 of SLS:FA.)

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- ▶ Efficiency and stagnation are *relative measures*; they cannot indicate all situations in which a given LVA's behaviour can be further improved.

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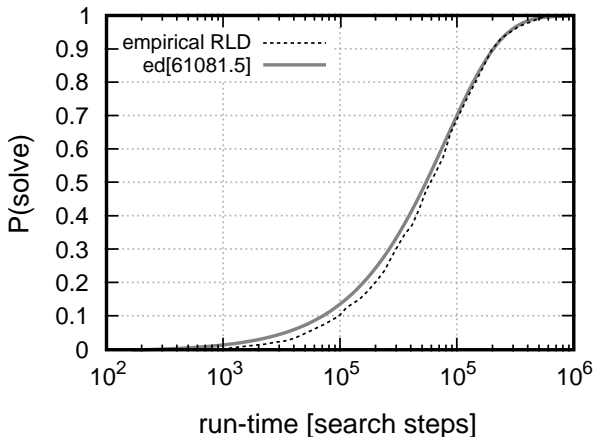
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- ▶ Approximations with parameterised families of continuous distribution functions known from statistics, such as exponential or normal distributions, are particularly useful.

Approximation of an empirical RTD with an exponential distribution $ed[m](x) := 1 - 2^{-x/m}$:



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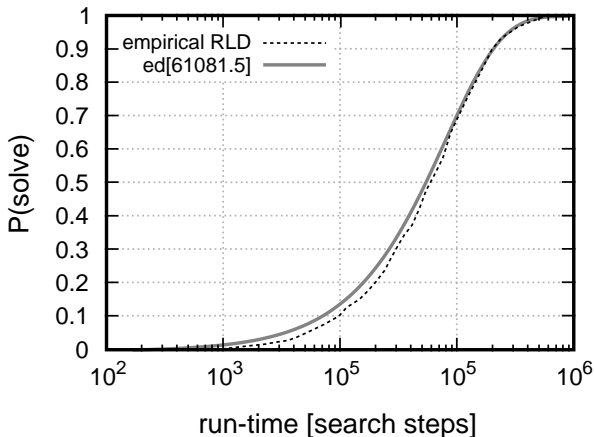
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- ▶ This approach can be easily generalised to ensembles of problem instances.

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The optimal fit exponential distribution obtained from the Marquardt-Levenberg algorithm passes the χ^2 goodness-of-fit test at $\alpha = 0.05$.

Performance improvements based on static restarts (1)

- ▶ Detailed RTD analyses can often suggest ways of improving the performance of a given SLS algorithm.

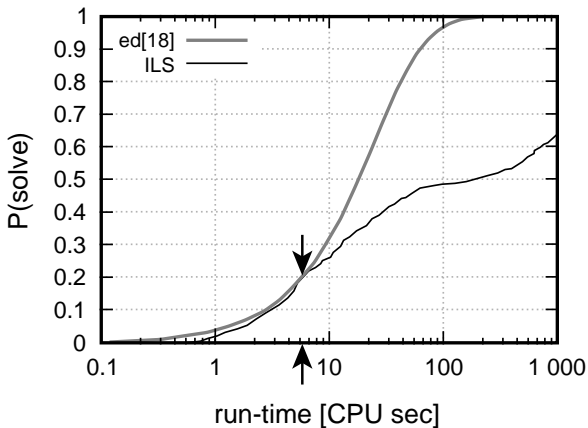
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- ▶ A static restart strategy is effective, *i.e.*, leads to increased solution probability for some run-time t'' , if the RTD of the given algorithm and problem instance is less steep than an exponential distribution crossing the RTD at some time $t < t''$.

Example of an empirical RTD of an SLS algorithm on a problem instance for which static restarting is effective:



'ed[18]' is the CDF of an exponential distribution with median 18; the arrows mark the optimal cutoff-time for static restarting.

Performance improvements based on static restarts (2)

- ▶ To determine the optimal cutoff-time t_{opt} for static restarts, consider the left-most exponential distribution that touches the given empirical RTD and choose t_{opt} to be the smallest t value at which the two respective distribution curves meet.

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- ▶ Optimal cutoff-times for static restarting typically vary considerably between problem instances; for optimisation algorithms, they also depend on the desired solution quality.

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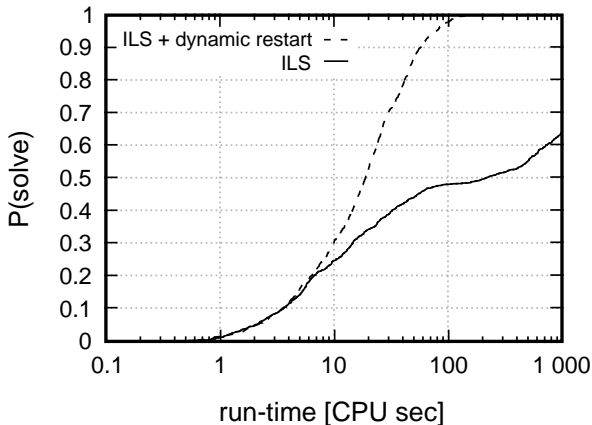
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Example: Effect of simple dynamic restart strategy



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 - ▶ *random walk extensions* that render a given SLS algorithm provably PAC;
 - ▶ adaptive modification of parameters controlling the amount of search diversification, such as temperature in SA or tabu tenure in TS.
- ▶ Effective techniques for overcoming search stagnation are crucial components of high-performance SLS methods.

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Optimal parallelisation speedup of p is achieved for an exponential RTD.

- ▶ The RTDs of many high-performance SLS algorithms are well approximated by exponential distributions; however, deviations for short run-times (due to the effects of search initialisation) limit the maximal number of processors for which optimal speedup can be achieved in practice.

Speedup achieved by multiple independent runs parallelisation of a high-performance SLS algorithm for SAT:

