

DM811  
HEURISTICS AND LOCAL SEARCH ALGORITHMS  
FOR COMBINATORIAL OPTIMIZATION

Lecture 13  
**Experimental Analysis**

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## Outline

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1. **Experimental Algorithmics**
  - Definitions
  - Performance Measures
2. **Exploratory Data Analysis**
  - Sample Statistics
  - Scenarios of Analysis
  - Guidelines for Presenting Data
3. **Examples**
  - Results Task 1
  - Results Task 2
4. **Organizational Issues**

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  - Performance Measures
2. **Exploratory Data Analysis**
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  - Results Task 2
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## Contents and Goals

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Goals of this part of the course (to be continued in DM812):  
Provide a view of issues in **Experimental Algorithmics**

- ▶ **Exploratory data analysis**
- ▶ Presenting results in a concise way with graphs and tables
- ▶ Organizational issues and Experimental Design
- ▶ Basics of **inferential statistics**
- ▶ Sequential statistical testing: a methodology for tuning

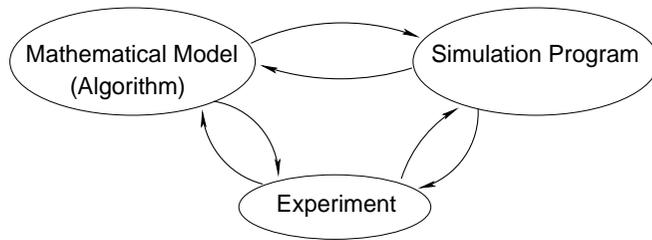
The goal of Experimental Algorithmics is not only producing a sound **analysis** but also adding an important tool to the development of a good solver for a given problem.

Experimental Algorithmics is an important part in the algorithm production cycle, which is referred to as **Algorithm Engineering**

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## Experimental Algorithmics

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In empirical studies we consider simulation programs which are the implementation of a mathematical model (the algorithm)

[McGeoch, 1996]

Algorithmic models of programs can vary according to their level of **instantiation**:

- ▶ **minimally instantiated** (algorithmic framework), e.g., simulated annealing
- ▶ **mildly instantiated**: includes implementation strategies (data structures)
- ▶ **highly instantiated**: includes details specific to a particular programming language or computer architecture

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## Experimental Algorithmics

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### Goals

- ▶ Defining standard methodologies
- ▶ Comparing relative performance of algorithms so as to identify the best ones for a given application
- ▶ Characterizing the behavior of algorithms
- ▶ Identifying algorithm separators, *i.e.*, families of problem instances for which the performance differ
- ▶ Providing new insights in algorithm design

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**Fairness principle**: being completely fair is perhaps impossible but try to remove any possible bias

- ▶ possibly all algorithms must be implemented with the same style, with the same language and sharing common subprocedures and data structures
- ▶ the code must be optimized, e.g., using the best possible data structures
- ▶ running times must be comparable, e.g., by running experiments on the same computational environment (or redistributing them randomly)

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## Definitions

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For each general problem  $\Pi$  (e.g., TSP, GCP) we denote by  $C_\Pi$  a **set (or class) of instances** and by  $\pi \in C_\Pi$  a **single instance**.

The object of analysis are **SLS algorithms**, *i.e.*, randomized search heuristics (with no guarantee of optimality).

- ▶ **single-pass heuristics** (denoted  $\mathcal{A}^1$ ): have an embedded termination, for example, upon reaching a certain state

Eg. Construction heuristics, iterative improvement

- ▶ **asymptotic heuristics** (denoted  $\mathcal{A}^\infty$ ): do not have an embedded termination and they might improve their solution asymptotically

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## Definitions

The most typical scenario considered

**Asymptotic heuristics with time (or iteration) limit decided *a priori***

The algorithm  $\mathcal{A}^\infty$  is halted when time expires.

**Deterministic case:**  $\mathcal{A}^\infty$  on  $\pi$  returns a solution of cost  $x$ .

The performance of  $\mathcal{A}^\infty$  on  $\pi$  is a scalar  $y = x$ .

**Randomized case:**  $\mathcal{A}^\infty$  on  $\pi$  returns a solution of cost  $X$ , where  $X$  is a **random variable**.

The performance of  $\mathcal{A}^\infty$  on  $\pi$  is the univariate  $Y = X$ .

[This is not the only relevant scenario: to be refined later]

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## Random Variables and Probability

Statistics deals with **random (or stochastic) variables**.

A variable is called random if, prior to observation, its outcome cannot be predicted with certainty.

The uncertainty is described by a **probability distribution**.

*Discrete variables*

Probability distribution:

$$p_i = P[x = v_i]$$

Cumulative Distribution Function (CDF)

$$F(v) = P[x \leq v] = \sum_i p_i$$

Mean

$$\mu = E[X] = \sum x_i p_i$$

Variance

$$\sigma^2 = E[(X - \mu)^2] = \sum (x_i - \mu)^2 p_i$$

*Continuous variables*

Probability density function (pdf):

$$f(v) = \frac{dF(v)}{dv}$$

Cumulative Distribution Function (CDF):

$$F(v) = \int_{-\infty}^v f(v) dv$$

Mean

$$\mu = E[X] = \int x f(x) dx$$

Variance

$$\sigma^2 = E[(X - \mu)^2] = \int (x - \mu)^2 f(x) dx$$

## Generalization

**On a specific instance**, the random variable  $Y$  that defines the performance measure of an algorithm is described by its probability distribution/density function

$$\Pr(Y = y | \pi)$$

It is often more interesting to generalize the performance **on a class of instances**  $C_\Pi$ , that is,

$$\Pr(Y = y, C_\Pi) = \sum_{\pi \in \Pi} \Pr(Y = y | \pi) \Pr(\pi)$$

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## Sampling

In experiments,

1. **we sample the population of instances** and
2. **we sample the performance of the algorithm** on each sampled instance

If on an instance  $\pi$  we run the algorithm  $r$  times then we have  $r$  replicates of the performance measure  $Y$ , denoted  $Y_1, \dots, Y_r$ , which are independent and identically distributed (i.i.d.), i.e.

$$\Pr(y_1, \dots, y_r | \pi) = \prod_{j=1}^r \Pr(y_j | \pi)$$

$$\Pr(y_1, \dots, y_r) = \sum_{\pi \in C_\Pi} \Pr(y_1, \dots, y_r | \pi) \Pr(\pi).$$

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## Instance Selection

In **real-life applications** a simulation of  $p(\pi)$  can be obtained by historical data.

In **simulation studies** instances may be:

- ▶ real world instances
- ▶ random variants of real world-instances
- ▶ online libraries
- ▶ randomly generated instances

They may be grouped in classes according to some features whose impact may be worth studying:

- ▶ type (for features that might impact performance)
- ▶ size (for scaling studies)
- ▶ hardness (focus on hard instances)
- ▶ application (e.g., CSP encodings of scheduling problems), ...

Within the class, instances are drawn with uniform probability  $p(\pi) = c$

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## Statistical Methods

The analysis of performance is based on finite-sized sampled data. Statistics provides the methods and the mathematical basis to

- ▶ describe, summarizing, the data (descriptive statistics)
- ▶ make inference on those data (inferential statistics)

Statistics helps to

- ▶ guarantee reproducibility
- ▶ make results reliable  
(are the observed results enough to justify the claims?)
- ▶ extract relevant results from large amount of data

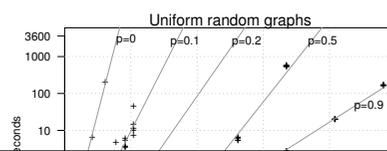
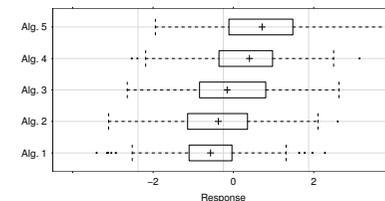
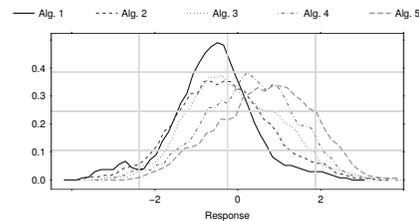
In the **practical context** of heuristic design and implementation (i.e., **engineering**), statistics helps to take correct design decisions with the **least amount of experimentation**

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## Objectives of the Experiments

- ▶ **Comparison:**  
bigger/smaller, same/different, Algorithm Configuration, Component-Based Analysis
  - ▶ Standard statistical methods: *experimental designs, test hypothesis and estimation*

- ▶ **Characterization:**  
Interpolation: fitting models to data  
Extrapolation: building models of data, explaining phenomena
  - ▶ Standard statistical methods: *linear and non linear regression model fitting*



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## Measures and Transformations

### On a single instance

#### Computational effort indicators

- ▶ number of elementary operations/algorithmic iterations (e.g., search steps, objective function evaluations, number of visited nodes in the search tree, consistency checks, etc.)
- ▶ total CPU time consumed by the process (sum of *user* and *system* times returned by getrusage)

#### Solution quality indicators

- ▶ value returned by the cost function
- ▶ error from optimum/reference value
- ▶ gap  $\frac{|UB-LB|}{UB}$  or  $\frac{|UB-LB|}{LB}$
- ▶ ranks

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## Measures and Transformations

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### On a class of instances

#### Computational effort indicators

- ▶ no transformation if the interest is in studying scaling
- ▶ standardization if a fixed time limit is used
- ▶ geometric mean (used for a set of numbers whose values are meant to be multiplied together or are exponential in nature),
- ▶ otherwise, better to group homogeneously the instances

#### Solution quality indicators

Different instances implies different scales  $\Rightarrow$  need for an invariant measure

(However, many other measures can be taken both on the algorithms and on the instances [McGeoch, 1996])

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## Measures and Transformations

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### On a class of instances

#### Solution quality indicators

- ▶ Distance or error from a reference value (assume minimization case):

$$e_1(x, \pi) = \frac{x(\pi) - \bar{x}(\pi)}{\sqrt{\hat{\sigma}(\pi)}} \quad \text{standard score}$$

$$e_2(x, \pi) = \frac{x(\pi) - x^{\text{opt}}(\pi)}{x^{\text{opt}}(\pi)} \quad \text{relative error}$$

$$e_3(x, \pi) = \frac{x(\pi) - x^{\text{opt}}(\pi)}{x^{\text{worst}}(\pi) - x^{\text{opt}}(\pi)} \quad \text{invariant [Zemel, 1981]}$$

- ▶ optimal value computed exactly or known by instance construction
- ▶ surrogate value such bounds or best known values
- ▶ Rank (no need for standardization but loss of information)

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### 3. Examples

Results Task 1

Results Task 2

### 4. Organizational Issues

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## Summary Measures for Sampled Data

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Measures to describe or characterize a population

- ▶ Measure of central tendency, location
- ▶ Measure of dispersion

One such a quantity is

- ▶ a **parameter** if it refers to the population (Greek letters)
- ▶ a **statistics** if it is an *estimation* of a population parameter from the sample (Latin letters)

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## Measures of central tendency

- ▶ Arithmetic Average (Sample mean)

$$\bar{X} = \frac{\sum x_i}{n}$$

- ▶ *Quantile*: value above or below which lie a fractional part of the data (used in nonparametric statistics)

- ▶ Median

$$\mathcal{M} = x_{(n+1)/2}$$

- ▶ Quartile

$$Q_1 = x_{(n+1)/4} \quad Q_3 = x_{3(n+1)/4}$$

- ▶ q-quantile

q of data lies below and  $1 - q$  lies above

- ▶ Mode

value of relatively great concentration of data  
(*Unimodal vs Multimodal* distributions)

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## Measure of dispersion

- ▶ Sample range

$$R = x_n - x_1$$

- ▶ Sample variance

$$s^2 = \frac{1}{n-1} \sum (x_i - \bar{X})^2$$

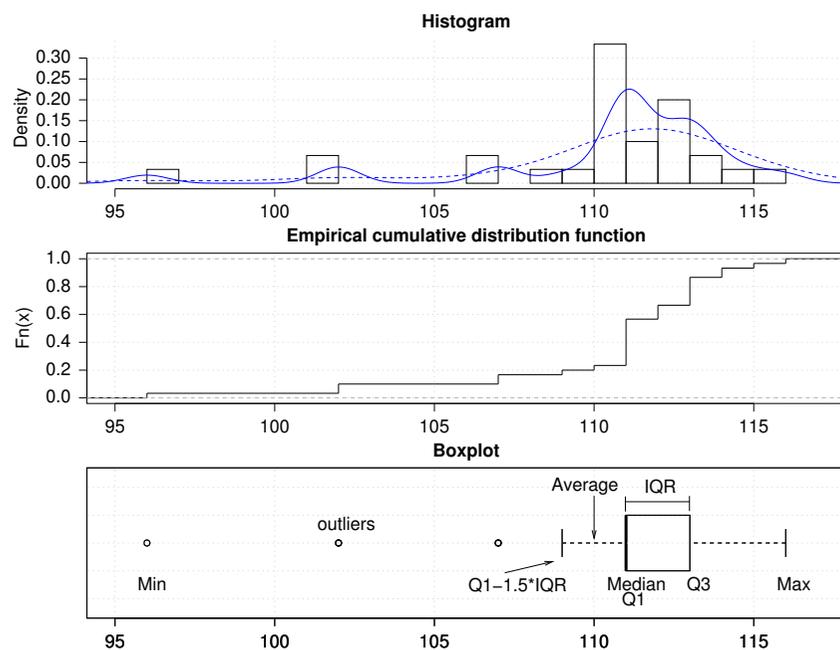
- ▶ Standard deviation

$$s = \sqrt{s^2}$$

- ▶ Inter-quartile range

$$\text{IQR} = Q_3 - Q_1$$

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## R functions:

```
> x<-runif(10,0,1)
> mean(x), median(x), quantile(x), quantile(x,0.25)
> range(x), var(x), sd(x), IQR(x)
> fivenum(x)
#(minimum, lower-hinge, median, upper-hinge, maximum)
[1] 0.18672 0.26682 0.28927 0.69359 0.92343
> summary(x)
> aggregate(x,list(factors),median)
> boxplot(x)
```

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## Scenarios

- A. Single-pass heuristics
- B. Asymptotic heuristics:
  - Two approaches:
    1. Univariate
      - 1.1 Time as an external parameter decided *a priori*
      - 1.2 Solution quality as an external parameter decided *a priori*
    2. Cost dependent on running time:

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## Scenario A

### Single-pass heuristics

**Deterministic case:**  $\mathcal{A}^{-1}$  on class  $C_{\Pi}$  returns a solution of cost  $x$  with computational effort  $t$  (e.g., running time).

**Randomized case:**  $\mathcal{A}^{-1}$  on class  $C_{\Pi}$  returns a solution of cost  $X$  with computational effort  $T$ , where  $X$  and  $T$  are random variables.

The performance of  $\mathcal{A}^{-1}$  on class  $C_{\Pi}$  is the vector  $\vec{y} = (x, t)$ .

The performance of  $\mathcal{A}^{-1}$  on class  $C_{\Pi}$  is the bivariate  $\vec{Y} = (X, T)$ .

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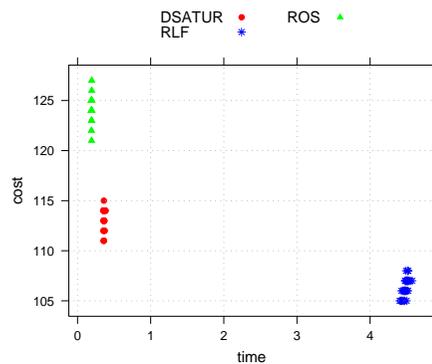
## Example

### Scenario:

- ▷ 3 heuristics  $\mathcal{A}_1^{-1}$ ,  $\mathcal{A}_2^{-1}$ ,  $\mathcal{A}_3^{-1}$  on class  $C_{\Pi}$ .
- ▷ homogeneous instances or need for data transformation.
- ▷ 1 or  $r$  runs per instance
- ▶ **Interest:** inspecting solution cost and running time to observe and compare the level of approximation and the speed.

### Tools:

- ▶ Scatter plots of solution-cost and run-time



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## Multi-Criteria Decision Making

Needed some definitions on [dominance relations](#)

In [Pareto sense](#), for points in  $\mathbf{R}^2$

$$\begin{array}{ll} \vec{x}^1 \preceq \vec{x}^2 & \text{weakly dominates} \\ \vec{x}^1 \parallel \vec{x}^2 & \text{incomparable} \end{array} \quad \begin{array}{l} x_i^1 \leq x_i^2 \text{ for all } i = 1, \dots, n \\ \text{neither } \vec{x}^1 \preceq \vec{x}^2 \text{ nor } \vec{x}^2 \preceq \vec{x}^1 \end{array}$$

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## Scenario B

### Asymptotic heuristics

There are two approaches:

#### 1.1. Time as an external parameter decided *a priori*.

The algorithm is halted when time expires.

**Deterministic case:**  $\mathcal{A}^\infty$  on class  $C_\Pi$  returns a solution of cost  $x$ .

**Randomized case:**  $\mathcal{A}^\infty$  on class  $C_\Pi$  returns a solution of cost  $X$ , where  $X$  is a random variable.

The performance of  $\mathcal{A}^\infty$  on class  $C_\Pi$  is the scalar  $y = x$ .

The performance of  $\mathcal{A}^\infty$  on class  $C_\Pi$  is the **univariate**  $Y = X$ .

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## Example

### Scenario:

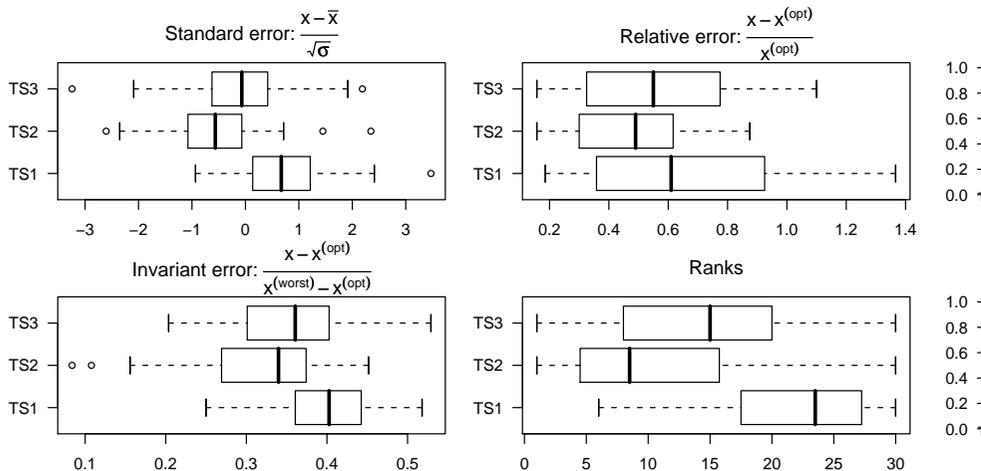
- ▷ 3 heuristics  $\mathcal{A}_1^\infty, \mathcal{A}_2^\infty, \mathcal{A}_3^\infty$  on class  $C_\Pi$ .  
(Or 3 heuristics  $\mathcal{A}_1^\infty, \mathcal{A}_2^\infty, \mathcal{A}_3^\infty$  on class  $C_\Pi$  without interest in computation time because negligible or comparable)
- ▷ homogeneous instances (no data transformation) or heterogeneous (data transformation)
- ▷ 1 or  $r$  runs per instance
- ▷ a priori time limit imposed
- ▶ **Interest:** inspecting solution cost

### Tools:

- ▶ Histograms (summary measures: mean or median or mode?)
- ▶ Boxplots
- ▶ Empirical cumulative distribution functions (ECDFs)

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### On a class of instances

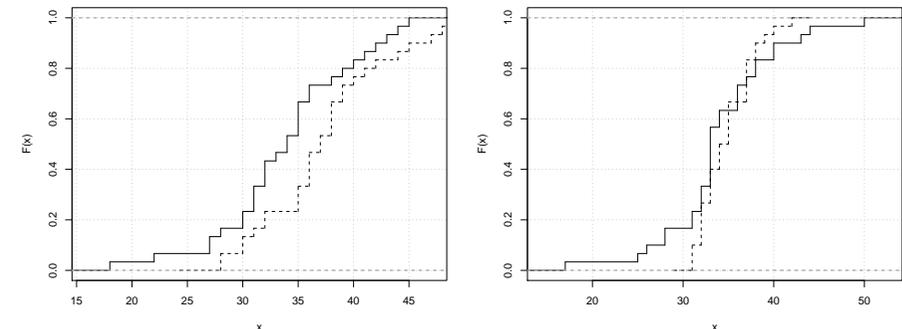


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## Stochastic Dominance

Definition: Algorithm  $\mathcal{A}_1$  probabilistically dominates algorithm  $\mathcal{A}_2$  on a problem instance, iff its CDF is always "below" that of  $\mathcal{A}_2$ , i.e.:

$$F_1(x) \leq F_2(x), \quad \forall x \in X$$



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## R code behind the previous plots

We load the data and plot the comparative boxplot for each instance.

```
> load("TS.class-G.dataR")
> G[1:5,]
  alg inst run sol time.last.imp tot.iter parz.iter exit.iter exit.time opt
1 TS1 G-1000-0.5-30-1.1.col 1 59 9.900619 5955 442 5955 10.02463 30
2 TS1 G-1000-0.5-30-1.1.col 2 64 9.736608 3880 130 3958 10.00062 30
3 TS1 G-1000-0.5-30-1.1.col 3 64 9.908618 4877 49 4877 10.03263 30
4 TS1 G-1000-0.5-30-1.1.col 4 68 9.948622 6996 409 6996 10.07663 30
5 TS1 G-1000-0.5-30-1.1.col 5 63 9.912620 3986 52 3986 10.04063 30
>
> library(lattice)
> bwplot(alg ~ sol | inst,data=G)
```

If we want to make an aggregate analysis we have the following choices:

- ▶ maintain the raw data,
- ▶ transform data in standard error,
- ▶ transform the data in relative error,
- ▶ transform the data in an invariant error,
- ▶ transform the data in ranks.

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Maintain the raw data

R functions:

```
> par(mfrow=c(3,2),las=1,font.main=1,mar=c(2,3,3,1))
> #original data
> boxplot(sol~alg,data=G,horizontal=TRUE,main="Original data")
```

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Transform data in standard error

R functions:

```
> #standard error
> T1 <- split(G$sol,list(G$inst))
> T2 <- lapply(T1,scale,center=TRUE,scale=TRUE)
> T3 <- unsplit(T2,list(G$inst))
> T4 <- split(T3,list(G$alg))
> T5 <- stack(T4)
> boxplot(values~ind,data=T5,horizontal=TRUE,main=expression(paste("Standard
error: ",frac(x-bar(x),sqrt(sigma))))))
> Ecdf(T5$values,group=T5$ind,main=expression(paste("Standard error:
",frac(x-bar(x),sqrt(sigma))))))

> #standard error
> G$scale <- 0
> split(G$scale, G$inst) <- lapply(split(G$sol, G$inst), scale,center=TRUE,
scale=TRUE)
```

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Transform the data in relative error

R functions:

```
> #relative error
> G$err2 <- (G$sol-G$opt)/G$opt
> boxplot(err2~alg,data=G,horizontal=TRUE,main=expression(paste("Relative
error: ",frac(x-x^(opt),x^(opt))))))
> Ecdf(G$err2,group=G$alg,main=expression(paste("Relative error: ",frac(x-x
^(opt),x^(opt))))))
```

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Transform the data in an invariant error

We use as surrogate of  $\chi^{\text{worst}}$  the median solution returned by the simplest algorithm for the graph coloring, that is, the ROS heuristic.

```
> #error 3
> load("ROS.class-G.dataR")
> F1 <- aggregate(F$sol,list(inst=F$inst),median)
> F2 <- split(F1$x,list(F1$inst))
> G$ref <- sapply(G$inst,function(x) F2[[x]])
> G$err3 <- (G$sol-G$opt)/(G$ref-G$opt)
> boxplot(err3~alg,data=G,horizontal=TRUE,main=expression(paste("Invariant
  error: ",frac(x-x^(opt),x^(worst)-x^(opt))))))
> Ecdf(G$err3,group=G$alg,main=expression(paste("Invariant error: ",frac(x-x
  ^ (opt),x^(worst)-x^(opt))))))
```

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Transform the data in ranks

```
> #rank
> T2 <- lapply(T1,rank)
> T3 <- unsplit(T2,list(G$inst))
> T4 <- split(T3,list(G$alg))
> T5b <- stack(T4)
> boxplot(values~ind,data=T5b,horizontal=TRUE,main="Ranks")
> Ecdf(T5b$values,group=T5b$ind,main="Ranks")
```

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## Scenario B

### Asymptotic heuristics

There are two approaches:

1.2. Solution quality as an external parameter decided *a priori*. The algorithm is halted when quality is reached.

**Deterministic case:**  $\mathcal{A}^\infty$  on class  $C_\Pi$  finds a solution in running time  $t$ .  
**Randomized case:**  $\mathcal{A}^\infty$  on class  $C_\Pi$  finds a solution in running time  $T$ , where  $T$  is a random variable.

The performance of  $\mathcal{A}^\infty$  on class  $C_\Pi$  is the scalar  $y = t$ .

The performance of  $\mathcal{A}^\infty$  on class  $C_\Pi$  is the univariate  $Y = T$ .

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## Dealing with Censored Data

- ▶ Heuristics  $\mathcal{A}^\dagger$  stopped before completion or  $\mathcal{A}^\infty$  truncated (always the case)
- ▶ **Interest:** determining whether a prefixed goal (optimal/feasible) has been reached

The computational effort to attain the goal can be specified by a cumulative distribution function  $F(t) = P(T < t)$  with  $T$  in  $[0, \infty)$ .

If in a run  $i$  we stop the algorithm at time  $L_i$  then we have a **Type I right censoring**, that is, we know either

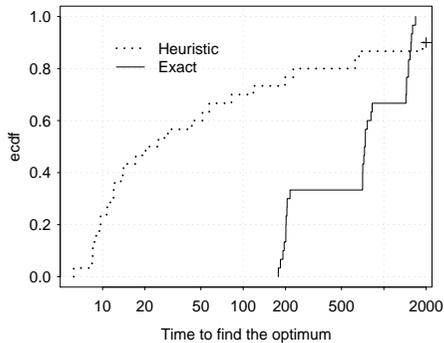
- ▶  $T_i$  if  $T_i \leq L_i$
- ▶ or  $T_i \geq L_i$ .

Hence, for each run  $i$  we need to record  $\min(T_i, L_i)$  and the indicator variable for observed optimal/feasible solution attainment,  $\delta_i = I(T_i \leq L_i)$ .

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## Example

- ▷ An exact vs an heuristic algorithm for the *2-edge-connectivity augmentation problem*.
- ▶ **Interest:** time to find the optimum on different instances.



Uncensored:

$$F(t) = \frac{\# \text{ runs} < t}{n}$$

Censored:

$$F(t) = \frac{\# \text{ runs} < t}{n}$$

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## Scenario B

### Asymptotic heuristics

There are two approaches:

#### 2. Cost dependent on running time:

**Deterministic case:**  $\mathcal{A}^\infty$  on  $\pi$  returns a current best solution  $x$  at each observation in  $t_1, \dots, t_k$ .

The performance of  $\mathcal{A}^\infty$  on  $\pi$  is the **profile** indicated by the vector  $\vec{y} = \{x(t_1), \dots, x(t_k)\}$ .

**Randomized case:**  $\mathcal{A}^\infty$  on  $\pi$  produces a monotone stochastic process in solution cost  $X(\tau)$  with any element dependent on the predecessors.

The performance of  $\mathcal{A}^\infty$  on  $\pi$  is the **multivariate**  $\vec{Y} = (X(t_1), X(t_2), \dots, X(t_k))$ .

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## Example

### Scenario:

- ▷ 3 heuristics  $\mathcal{A}_1^\infty, \mathcal{A}_2^\infty, \mathcal{A}_3^\infty$  on instance  $\pi$ .
- ▷ single instance hence no data transformation.
- ▷  $r$  runs
- ▶ **Interest:** inspecting solution cost over running time to determine whether the comparison varies over time intervals

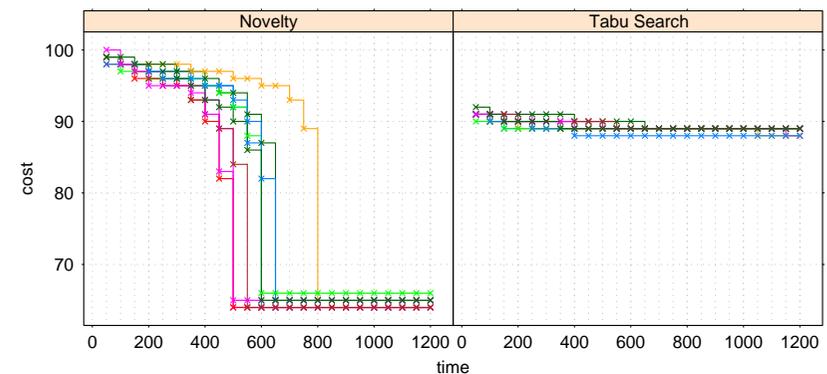
### Tools:

- ▶ Quality profiles

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The performance is described by **multivariate random variables** of the kind  $\vec{Y} = \{Y(t_1), Y(t_2), \dots, Y(t_k)\}$ .

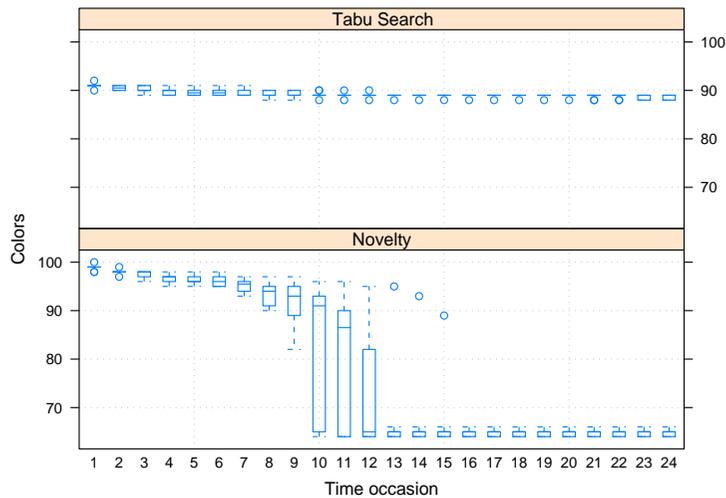
Sampled data are of the form  $\vec{Y}_i = \{Y_i(t_1), Y_i(t_2), \dots, Y_i(t_k)\}$ ,  $i = 1, \dots, 10$  (10 runs per algorithm on one instance)



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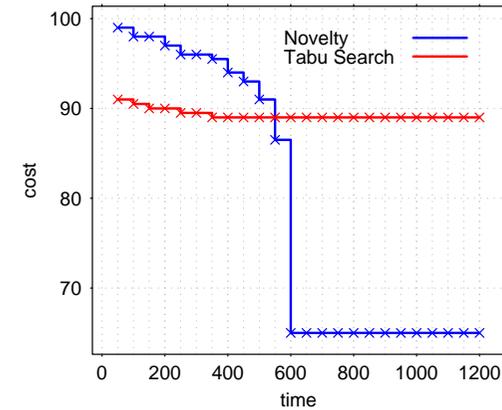
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Sampled data are of the form  $\vec{Y}_i = \{Y_i(t_1), Y_i(t_2), \dots, Y_i(t_k)\}$ ,  $i = 1, \dots, 10$  (10 runs per algorithm on one instance)



The median behavior of the two algorithms

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## Exploratory Data Analysis

**Explore** your data:

- ▶ make plots: histograms, boxplots, empirical cumulative distribution functions, correlation/scatter plots
- ▶ look at the numerical data and interpret them in practical terms: computation times, distance from optimum
- ▶ look for patterns

All the above both at a single instance level and at an aggregate level.

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## Making Plots

<http://algo2.iti.uni-karlsruhe.de/sanders/courses/bergen/bergenPresenting.pdf>  
[Sanders, 2002]

- ▶ Should the experimental setup from the exploratory phase be redesigned to increase conciseness or accuracy?
- ▶ What parameters should be varied? What variables should be measured?
- ▶ How are parameters chosen that cannot be varied?
- ▶ Can tables be converted into curves, bar charts, scatter plots or any other useful graphics?
- ▶ Should tables be added in an appendix?
- ▶ Should a 3D-plot be replaced by collections of 2D-curves?
- ▶ Can we reduce the number of curves to be displayed?
- ▶ How many figures are needed?
- ▶ Should the x-axis be transformed to magnify interesting subranges?

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- ▶ Should the x-axis have a logarithmic scale? If so, do the x-values used for measuring have the same basis as the tick marks?
- ▶ Is the range of x-values adequate?
- ▶ Do we have measurements for the right x-values, i.e., nowhere too dense or too sparse?
- ▶ Should the y-axis be transformed to make the interesting part of the data more visible?
- ▶ Should the y-axis have a logarithmic scale?
- ▶ Is it misleading to start the y-range at the smallest measured value? (if not too much space wasted start from 0)
- ▶ Clip the range of y-values to exclude useless parts of curves?
- ▶ Can we use banking to 45°?
- ▶ Are all curves sufficiently well separated?
- ▶ Can noise be reduced using more accurate measurements?
- ▶ Are error bars needed? If so, what should they indicate? Remember that measurement errors are usually not random variables.

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- ▶ Connect points belonging to the same curve.
- ▶ Only use splines for connecting points if interpolation is sensible.
- ▶ Do not connect points belonging to unrelated problem instances.
- ▶ Use different point and line styles for different curves.
- ▶ Use the same styles for corresponding curves in different graphs.
- ▶ Place labels defining point and line styles in the right order and without concealing the curves.
- ▶ Give axis units
- ▶ Captions should make figures self contained.
- ▶ Give enough information to make experiments reproducible.
- ▶ Golden ratio rule: make the graph wider than higher [Tufte 1983].
- ▶ Rule of 7: show at most 7 curves (omit those clearly irrelevant).
- ▶ Avoid: explaining axes, connecting unrelated points by lines, cryptic abbreviations, microscopic lettering, pie charts

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## Suggested Reading

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- Coffin M. and Saltzman M.J. (2000). **Statistical analysis of computational tests of algorithms and heuristics**. *INFORMS Journal on Computing*, 12(1), pp. 24–44.
- Demetrescu C., Finocchi I., and Italiano G. (2004). **Algorithm engineering**. In *Current Trends in Theoretical Computer Science: the Challenge of the New Century*, edited by A. G.Paun G.Rozemberg, vol. 1: Algorithms and Complexity. World Scientific Publishing.
- Johnson D.S. (2002). **A theoretician's guide to the experimental analysis of algorithms**. In *Data Structures, Near Neighbor Searches, and Methodology: Fifth and Sixth DIMACS Implementation Challenges*, edited by M.H. Goldwasser, D.S. Johnson, and C.C. McGeoch, vol. 59 of **DIMACS Series in Discrete Mathematics and Theoretical Computer Science**, pp. 215–250. American Mathematical Society, Providence, RI, USA.
- McGeoch C.C. (1996). **Toward an experimental method for algorithm simulation**. *INFORMS Journal on Computing*, 8(1), pp. 1–15.
- Sanders P. (2002). **Presenting data from experiments in algorithmics**. In *Experimental Algorithmics – From Algorithm Design to Robust and Efficient Software*, vol. 2547 of **LNCS**, pp. 181–196. Springer.

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## Outline

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1. Experimental Algorithmics
  - Definitions
  - Performance Measures
2. Exploratory Data Analysis
  - Sample Statistics
  - Scenarios of Analysis
  - Guidelines for Presenting Data
3. Examples
  - Results Task 1
  - Results Task 2
4. Organizational Issues

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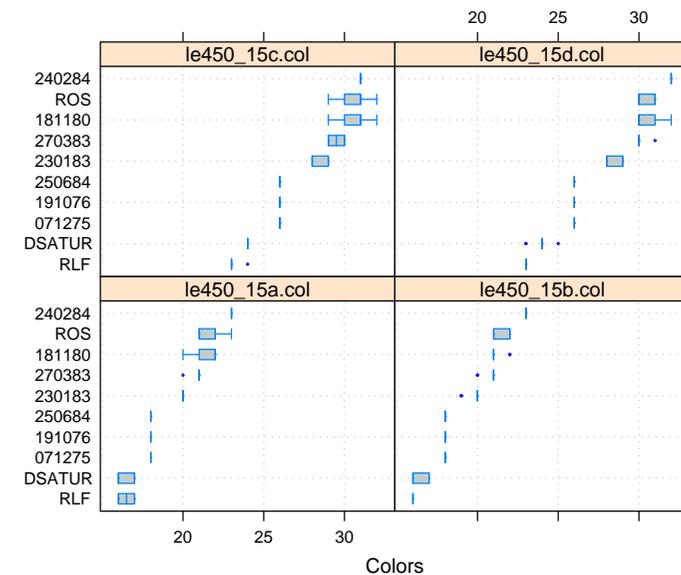
## Last year competition

- ▶ Graph Coloring Problem
- ▶ Task 1: submit a construction heuristic  
Set of instances A: 4 instances
- ▶ Task 2: submit an algorithm derived from the use of a metaheuristic for construction heuristics  
Time limit for each single run: 90 seconds  
Set of instances B: 15 instances
- ▶ Task 3: a peak performance algorithm  
Time limit for each single run: 360 seconds  
Set of instance C: The instances in the set are generated in order to admit different kind of colorings, ranging from equi-partite classes to highly variable classes.

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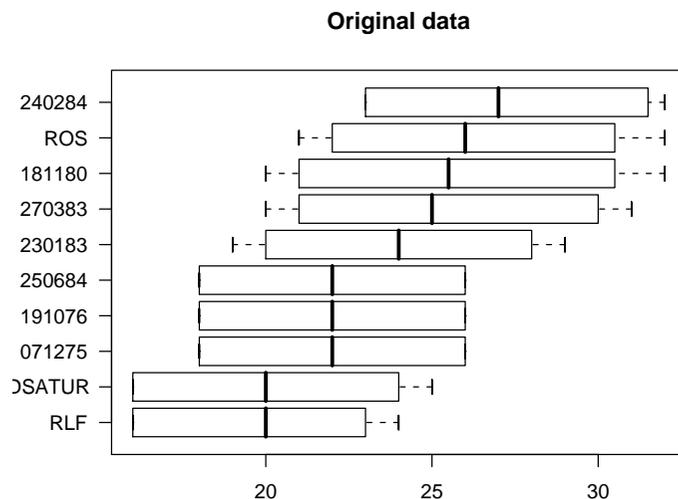
## Comparative Analysis

View of raw data within each instance



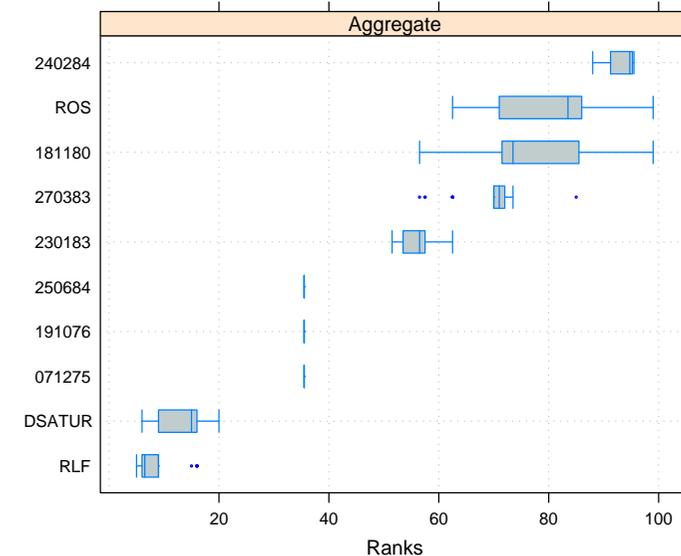
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View of raw data aggregated for the 4 instances



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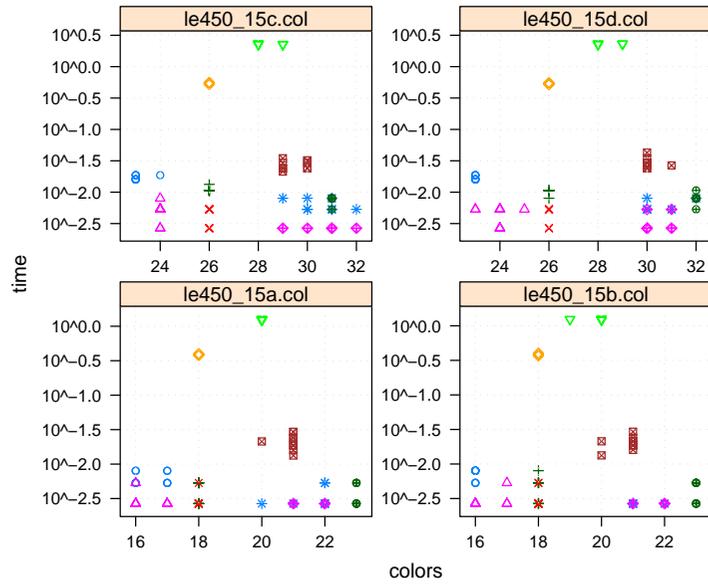
View of raw data **ranked within instances** and aggregated for the 4 instances



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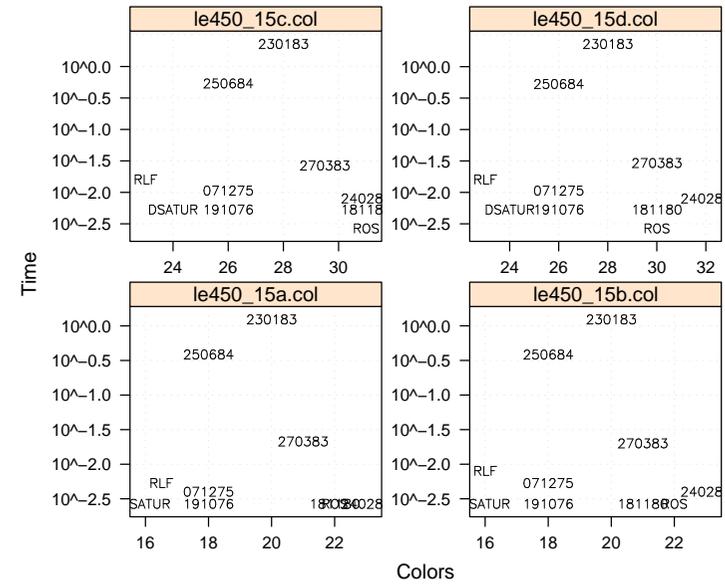
## Trade off Solution-Quality vs Run-Time

The trade off computation time vs sol quality. Raw data.



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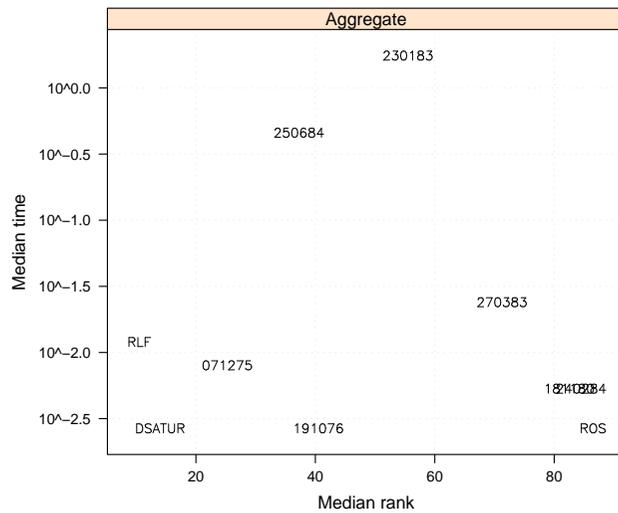
The trade off computation time vs sol quality. Raw data.



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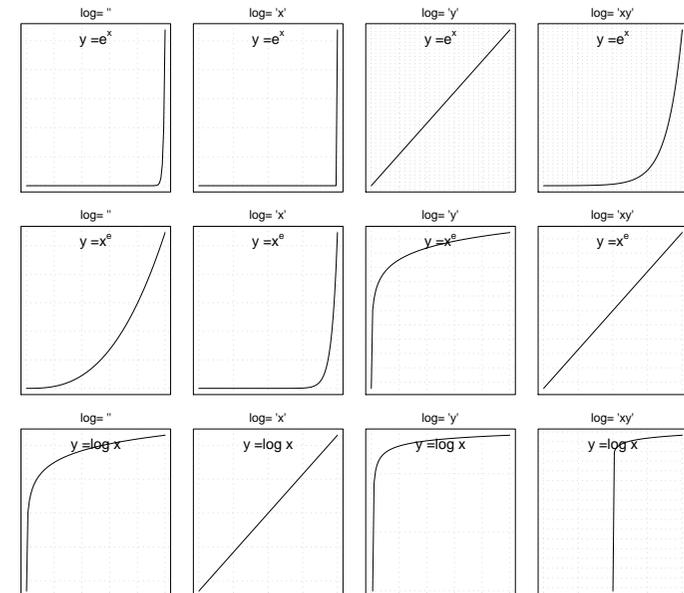
The trade off computation time vs sol quality.

Solution quality ranked within the instances and computation time in raw terms



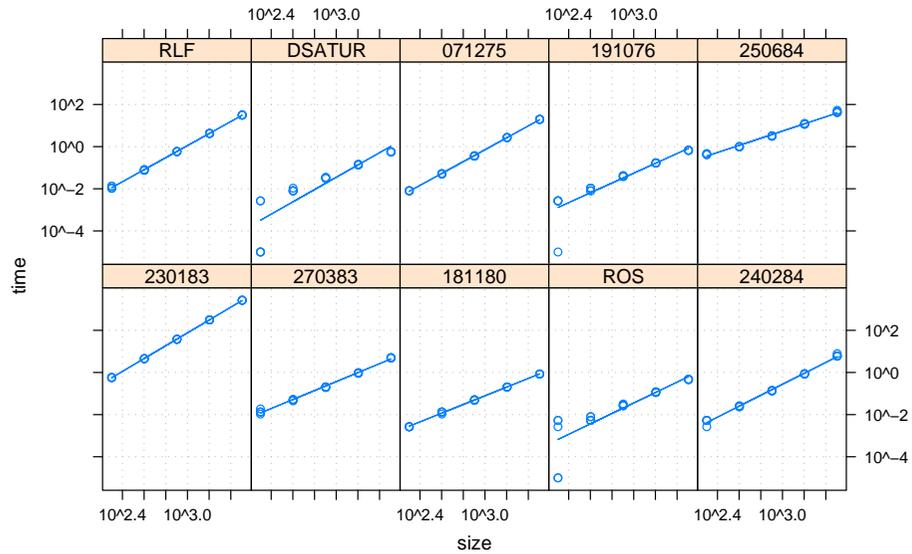
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## Scaling Analysis



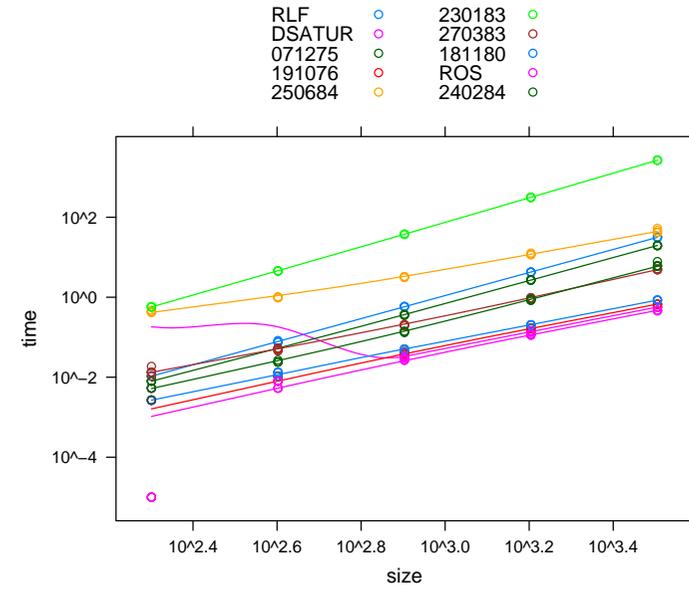
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Linear regression in log-log plots  $\Rightarrow$  polynomial growth



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Comparative visualization



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## Numerical data

Size	071275	181180	191076	230183	240284	250684	270383
200	0.008	0.00267	0.00267	0.5787	0.00533	0.42933	0.01333
400	0.05067	0.01333	0.01067	4.5443	0.024	0.98667	0.05067
800	0.36002	0.05067	0.04	37.68	0.13868	3.2313	0.2
1600	2.7175	0.20268	0.16801	313.27	0.85339	11.709	0.96267
3200	19.711	0.84805	0.66937	2674.8	6.1524	42.287	4.9413

Size	DSATUR	RLF	ROS
200	0	0.01067	0.00267
400	0.008	0.07734	0.00533
800	0.032	0.58404	0.02667
1600	0.13601	4.2563	0.11467
3200	0.5627	31.519	0.46936

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## Experimental Setup

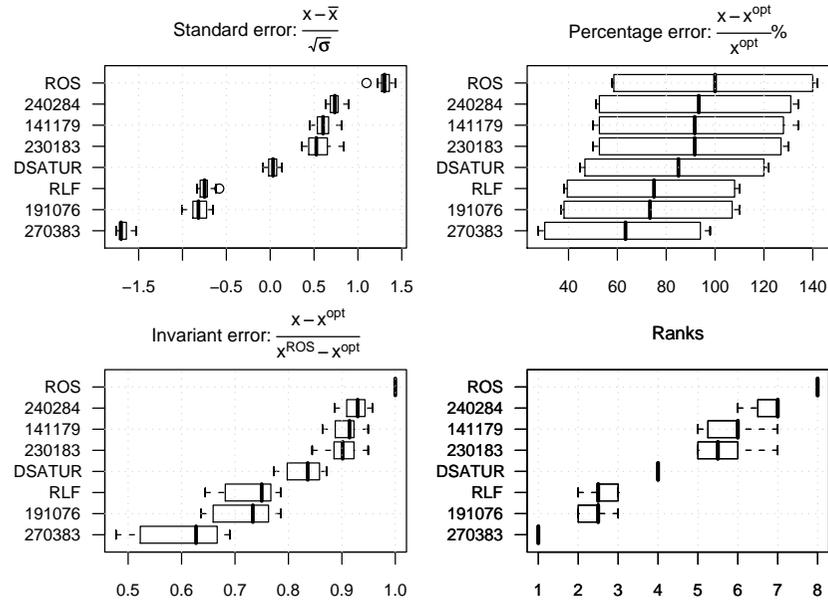
- ▶ 15 new flat instances created

Type	# instances	Upper bound
flat-1000-50-0-?.col	5	50
flat-1000-60-0-?.col	5	60
flat-1000-76-0-?.col	5	76

- ▶ each algorithm run once on each of the 15 new instances
- ▶ fairness principle: same computational resources to all algorithms  
 $\Rightarrow$  90 seconds on Intel(R) Celeron(R) CPU 2.40GHz, 1GB RAM  
 (120 seconds for 230183)
- ▶ restart ROS heuristic used as reference algorithm
- ▶ restart RLF and DSATUR also included

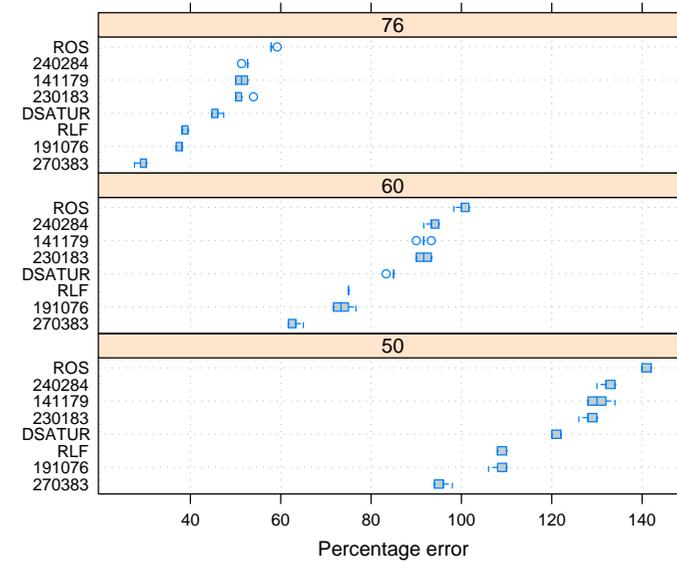
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## Results



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## Results



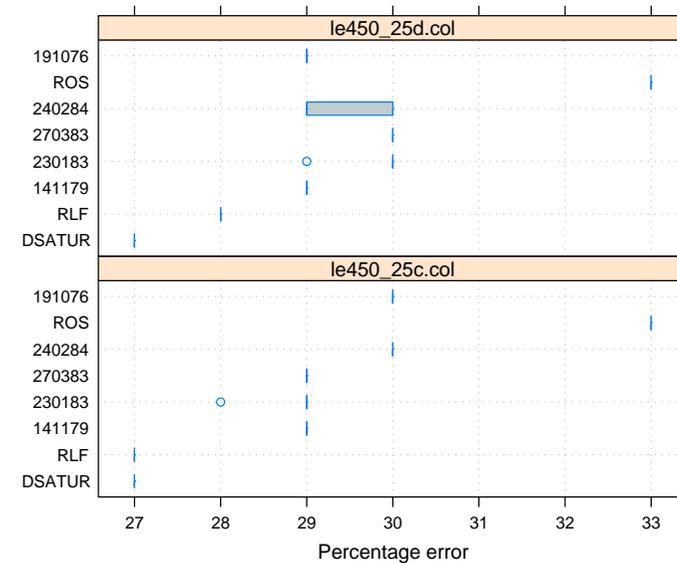
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## Results

Algorithm	flat-1000-50	flat-1000-60	flat-1000-76
270383	98	98	99
191076	105	104	105
RLF	104	105	105
DSATUR	111	111	111
230183	114	115	114
141179	115	115	115
240284	116	116	116
ROS	120	120	120

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## Results



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## Outline

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### 1. Experimental Algorithmics

Definitions

Performance Measures

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Results Task 1

Results Task 2

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## Notes on Experimental Environment

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Some organizational hints:

- ▶ run a script (bash, perl, python, php) that calls different programs, one for each algorithm to test, on different instances.
- ▶ when launched each program writes the search profile in a file (log file or output file).

```
Read instance. Time: 0.016001
begin try 1
best 0 col 22 time 0.004000 iter 0 par_iter 0
best 3 col 21 time 0.004000 iter 0 par_iter 0
best 1 col 21 time 0.004000 iter 0 par_iter 0
best 0 col 21 time 0.004000 iter 1 par_iter 1
best 6 col 20 time 0.004000 iter 3 par_iter 1
best 4 col 20 time 0.004000 iter 4 par_iter 2
best 2 col 20 time 0.004000 iter 6 par_iter 4
exit iter 7 time 1.000062
end try 1
```

- ▶ run a script (bash, perl, python, php) that parses the output files above and put it in a file with the format similar to:

```
alg instance      run sol time
RDS le450_15a.col 3 21 0.00267
RDS le450_15b.col 3 21 0
RDS le450_15d.col 3 31 0.00267
RLF le450_15a.col 3 17 0.00533
RLF le450_15b.col 3 16 0.008
...
```

- ▶ load the data in R and make all kind of analysis.

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## Program Profiling

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- ▶ Check the correctness of your solutions many times
- ▶ Plot the development of
  - ▶ best visited solution quality
  - ▶ current solution qualityover time and compare with other features of the algorithm.
- ▶ Profile time consumption per program components under Linux: gprof
  1. add flag `-pg` in compilation
  2. run the program
  3. `gprof program-file > a.txt`

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