DM841

Discrete Optimization - Heuristics

Experimental Analysis

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Outline

Outline

Contents and Goals

Provide a view of issues in Experimental Algorithmics

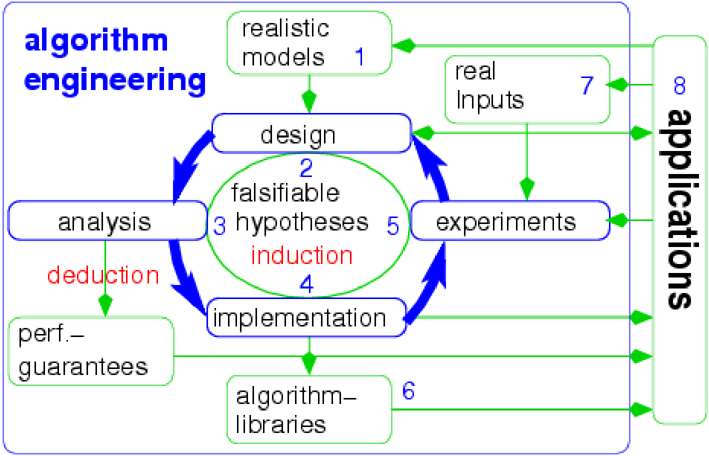
- Exploratory data analysis
- Presenting results in a concise way with graphs and tables
- Organizational issues and Experimental Design

- Basics of inferential statistics
- Sequential statistical testing: race, 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.

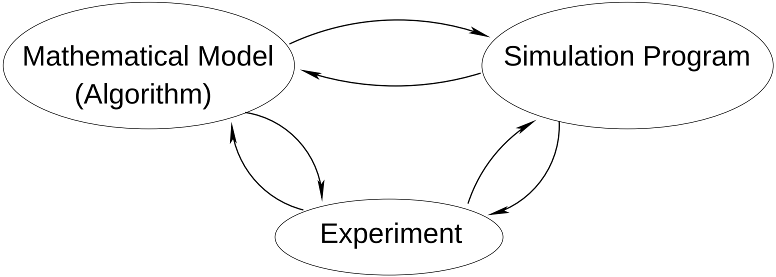
Experimental Algorithmics is an important part in the algorithm production cycle, which is referred to as Algorithm Engineering

The Engineering Cycle



from `http://www.algorithm-engineering.de/`

Experimental Algorithmics



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

[McGeoch, 1996]

Experimental Algorithmics

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 Hoos [2012]
- Providing well documented libraries of efficient algorithm implementations

Fairness Principle

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)

Definitions

The most typical scenario considered in analysis of search heuristics

Asymptotic heuristics with time/quality limit decided *a priori*

The algorithm $\mathcal{A}^\infty$ is halted when time expires or a solution of a given quality is found.

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

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

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

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

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

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

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

Variance

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

Generalization

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

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

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

It is often more interesting to generalize the performance on a class of instances Π, that is,

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

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 π we run the algorithm r times then we have r replicates of the performance measure Y, denoted $Y_1, \ldots, Y_r$, which are independent and identically distributed (i.i.d.), i.e.

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

$$Pr(y_1, \ldots, y_r) = \sum_{\pi \in \Pi} Pr(y_1, \ldots, y_r \mid \pi) Pr(\pi).$$

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 $p(\pi) = c$

Statistical Methods

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

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

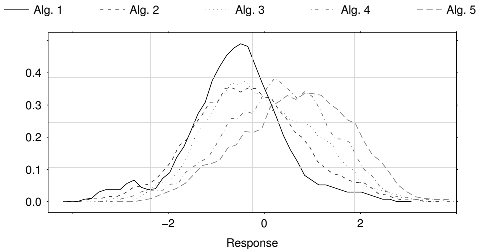
Statistics helps to

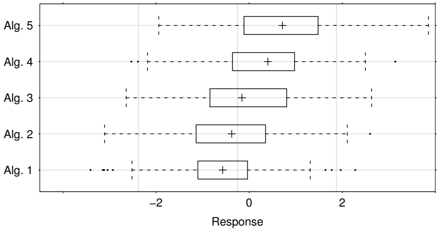
- guarantee reproducibility
- make results reliable
  (are the observed results enough to justify the claims?)
- extract relevant results from large amount of data

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

Objectives of the Experiments

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

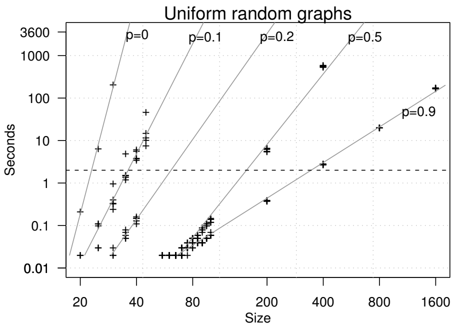




Objectives of the Experiments

- **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



Measures and Transformations

On a single instance

Design: Several runs on an instance

	Algorithm 1	Algorithm 2	...	Algorithm k
Instance 1	X_{11}	X_{21}		X_{k1}
$\vdots$	$\vdots$	$\vdots$		$\vdots$
Instance 1	X_{1r}	X_{2r}		X_{kr}

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
- (optimality) gap $\frac{UB-LB}{LB+\epsilon}$ (if max $\frac{UB-LB}{UB+\epsilon}$)
  ϵ is an infinitesimal for the case $LB = 0$ but $UB - LB \neq 0$
- ranks

Measures and Transformations

On a class of instances

Design A: One run on various instances

	Algorithm 1	Algorithm 2	...	Algorithm k
Instance 1	X_{11}	X_{12}		X_{1k}
$\vdots$	$\vdots$	$\vdots$		$\vdots$
Instance b	X_{b1}	X_{b2}		X_{bk}

Design B: Several runs on various instances

	Algorithm 1	Algorithm 2	...	Algorithm k
Instance 1	$X_{111}, \ldots, X_{11r}$	$X_{121}, \ldots, X_{12r}$		$X_{1k1}, \ldots, X_{1kr}$
Instance 2	$X_{211}, \ldots, X_{21r}$	$X_{221}, \ldots, X_{22r}$		$X_{2k1}, \ldots, X_{2kr}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$
Instance b	$X_{b11}, \ldots, X_{b1r}$	$X_{b21}, \ldots, X_{b2r}$		$X_{bk1}, \ldots, X_{bkr}$

Measures and Transformations

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 imply different scales ⇒ need for an invariant measure

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

On a class of instances (cont.)

Solution quality indicators

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

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

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

$$e_3(x, \pi) = \frac{x(\pi) - x^{opt}(\pi)}{x^{worst}(\pi) - x^{opt}(\pi)} \qquad \text{invariant}$$

[Zemel, 1981]

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

Sampling

- We work with samples (instances, solution quality) drawn from populations

Population		Random Sample
$P(x, \theta)$	———	X^n
Parameter θ		Statistical Estimator $\widehat{\theta}$

Summary Measures

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)

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

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

  - q-quantile

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

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

Measure of dispersion

- Sample range

$$R = x_{(n)} - x_{(1)}$$

- Sample variance

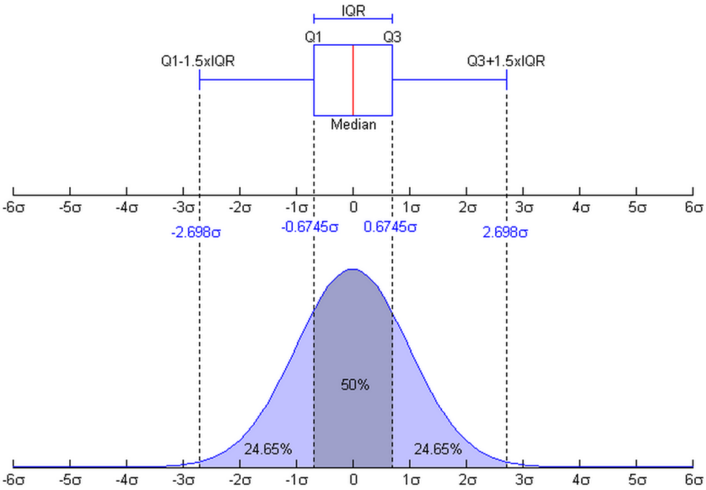
$$s^2 = \frac{1}{n-1} \sum (x_i - \bar{X})^2$$

- Standard deviation

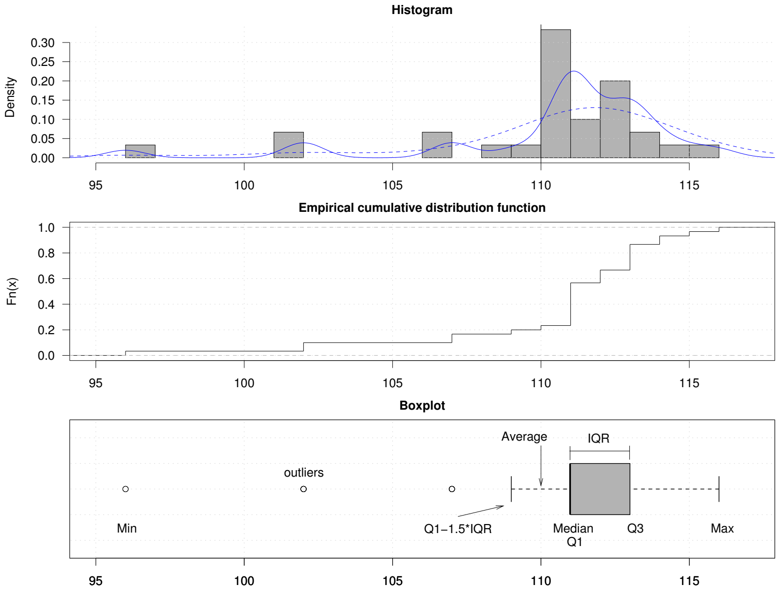
$$s = \sqrt{s^2}$$

- Inter-quartile range

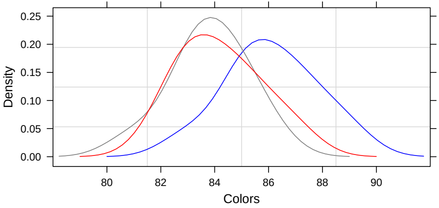
$$IQR = Q_3 - Q_1$$



Boxplot and a probability density function (pdf) of a Normal $N(0, 1)$ Population. (source: Wikipedia)
[see also: http://informationandvisualization.de/blog/box-plot]



Histogram
Density
0.30
0.25
0.20
0.15
0.10
0.05
0.00
95
100
105
110
115
Empirical cumulative distribution function
Fn(x)
1.0
0.8
0.6
0.4
0.2
0.0
95
100
105
110
115
Boxplot
Average
IQR
outliers
Min
Q1−1.5*IQR
Median
Q1
Q3
Max
95
100
105
110
115


Density
0.25
0.20
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0.10
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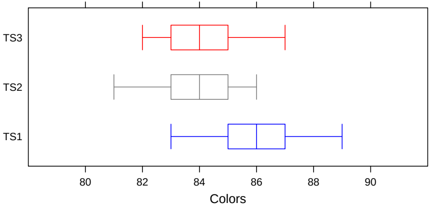
80
82
84
86
88
90
Colors


TS3
TS2
TS1
80
82
84
86
88
90
Colors

In R

```
> 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)
```

Scenarios

A. Single-pass heuristics

B. Asymptotic heuristics
(can be run indefinitely with a chance of continuing to make progress):

Two approaches:

1. Univariate
   1.a Time as an external parameter decided *a priori*
   1.b Solution quality as an external parameter decided *a priori*
2. Cost dependent on running time:

Scenario A

Single-pass heuristics

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

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

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

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

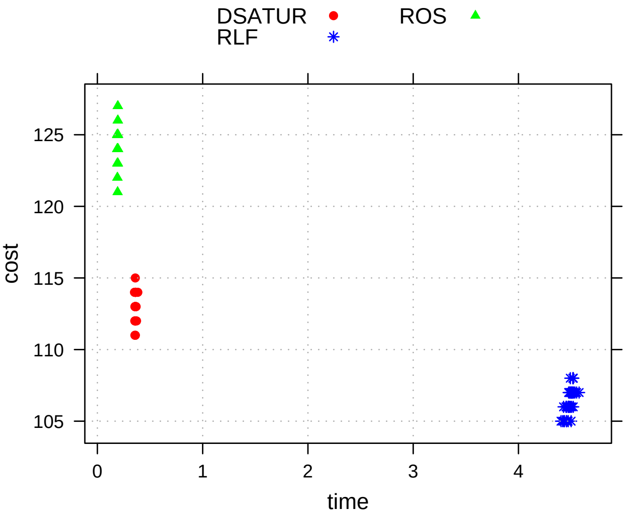
Example

Scenario:

- ▷ 3 heuristics $\mathcal{A}_1^{\dashv}$, $\mathcal{A}_2^{\dashv}$, $\mathcal{A}_3^{\dashv}$ on class Π.
- ▷ 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


DSATUR
ROS
RLF
125
120
115
110
105
cost
0
1
2
3
4
time

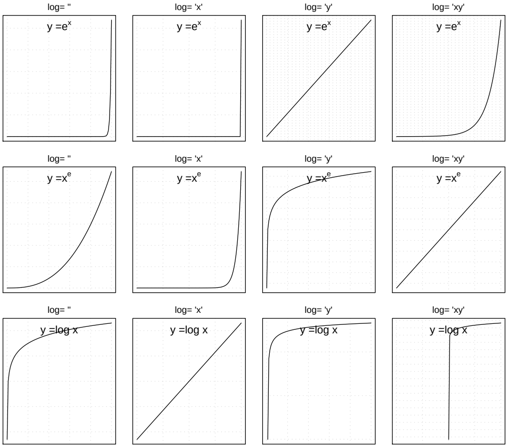
Multi-Criteria Decision Making

Needed some definitions on dominance relations

In Pareto sense, for points in $\mathbb{R}^2$

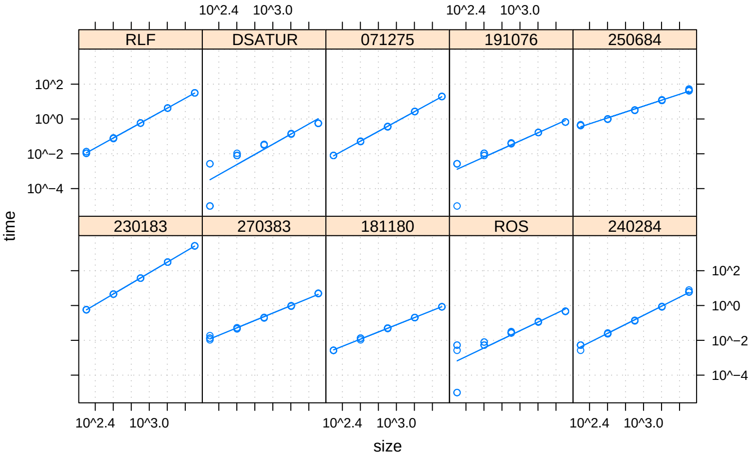
$\vec{x}^1 \preceq \vec{x}^2$	weakly dominates	$x_i^1 \leq x_i^2$ for all $i = 1, \ldots, n$
$\vec{x}^1 \parallel \vec{x}^2$	incomparable	neither $\vec{x}^1 \preceq \vec{x}^2$ nor $\vec{x}^2 \preceq \vec{x}^1$

Scaling Analysis

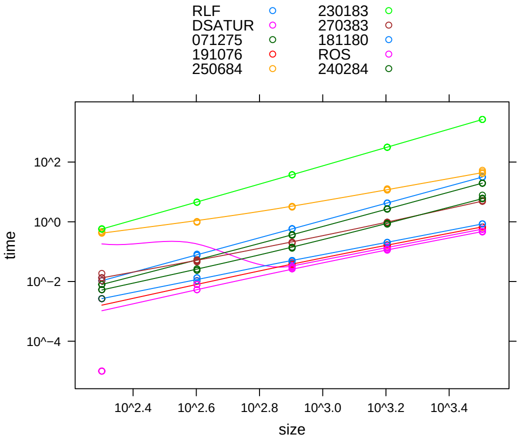


Linear regression in log-log plots $\Rightarrow$ polynomial growth

Linear regression in log-log plots ⇒ polynomial growth



Comparative visualization



Scenarios

A. Single-pass heuristics

B. Asymptotic heuristics
(can be run indefinitely with a chance of continuing to make progress):

Two approaches:

1. Univariate
   1.a Time as an external parameter decided *a priori*
   1.b Solution quality as an external parameter decided *a priori*
2. Cost dependent on running time:

Scenario B

Asymptotic heuristics

There are two approaches:

1.a. Time as an external parameter decided *a priori*.
The algorithm is halted when time expires.

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

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

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

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

Example

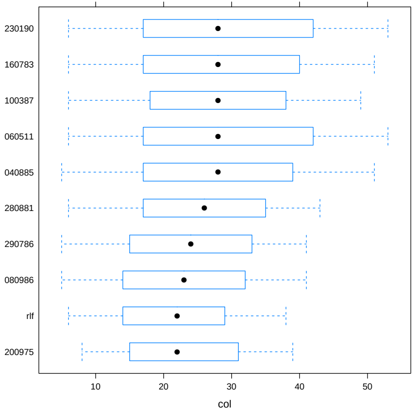
Scenario:

- 3 heuristics $\mathcal{A}_1^\infty$, $\mathcal{A}_2^\infty$, $\mathcal{A}_3^\infty$ on class Π.
  (Or 3 heuristics $\mathcal{A}_1^\infty$, $\mathcal{A}_2^\infty$, $\mathcal{A}_3^\infty$ on class Π 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

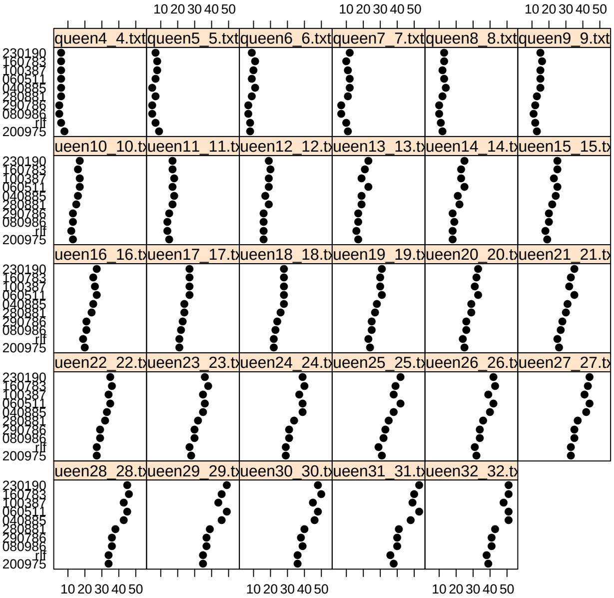
Tools:

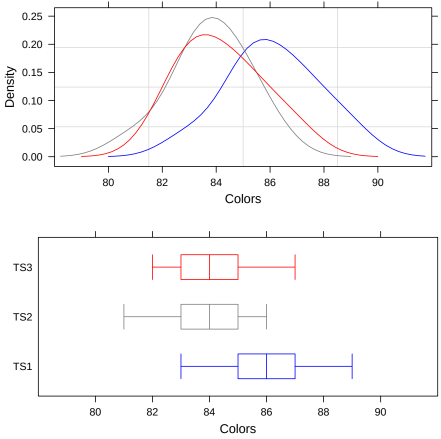
- Histograms (summary measures: mean or median or mode?)
- Boxplots
- Empirical cumulative distribution functions (ECDFs)

```
## load the data
> load("results.rda")
> levels(DATA$instance)
 [1] "queen4_4.txt"   "queen5_5.txt"   "queen6_6.txt"   "queen7_7.txt"
 [5] "queen8_8.txt"   "queen9_9.txt"   "queen10_10.txt" "queen11_11.txt"
 [9] "queen12_12.txt" "queen13_13.txt" "queen14_14.txt" "queen15_15.txt"
[13] "queen16_16.txt" "queen17_17.txt" "queen18_18.txt" "queen19_19.txt"
[17] "queen20_20.txt" "queen21_21.txt" "queen22_22.txt" "queen23_23.txt"
[21] "queen24_24.txt" "queen25_25.txt" "queen26_26.txt" "queen27_27.txt"
[25] "queen28_28.txt" "queen29_29.txt" "queen30_30.txt" "queen31_31.txt"
[29] "queen32_32.txt"
> bwplot(reorder(alg, col, median)~col, data=DATA)
```



```
> bwplot(reorder(alg, col, median)~col|instance,data=DATA,as.table=TRUE)
```




0.25
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0.00
Density
80
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88
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Colors
TS3
TS2
TS1
80
82
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86
88
90
Colors

R Pointers

- R for Data Science.
  Tidyverse tools: https://www.tidyverse.org/.
  Book: https://r4ds.hadley.nz/

- rstudio cheatsheets (you find them from the Help menu) or at https://posit.co/resources/cheatsheets/
  - Data Import Cheat Sheet
  - Data Transformation Cheat Sheet
  - Data Wrangling
  - Data Visualization Cheat Sheet

- ggplot2: Elegant Graphics for Data Analysis. Wickham, Hadley https://www.springer.com/gp/book/9783319242750 http://ggplot2.org/book/
  based on grammar:
  - Wickham H (2010) A layered grammar of graphics. J Comput Graph Stat 19(1):3–28
  - Wilkinson L (2005) The grammar of graphics. Statistics and computing, 2nd edn. Autumner, New York

R Notions

- data are stored in `data.frame` type (see `class(data)`)

```
> head(DATA)
      alg      instance hard soft     eval   time    cost
1 3702445     ns1696083 1492   54 14920100  27.65 1492054
2 3702445 neos-1440225  107   46  1070050   1.22  107046
3 3702445    macrophage    0  800      800   0.22     800
4 3702445 iis-pima-cov    0   77       77   0.47      77
5 3702445           ex9  477 2188  4772190 116.34  479188
6 3702445          ex10  974 6591  9746590 120.15  980591
```

- columns of a data.frame can be of different types, use `str()` to check this
- an important type for a data frame column is `factor`. A factor is made by `levels`

```
> str(DATA)
'data.frame':   60 obs. of  7 variables:
 $ alg     : Factor w/ 7 levels "3702445","5248915",..: 1 1 1 1 1 1 1 1 1 ...
 $ instance: Factor w/ 9 levels "acc-tight6","bnatt350",..: 9 8 7 6 5 4 3 ...
 $ hard    : int  1492 107 0 0 477 974 1201 152 88 7 ...
 $ soft    : num  54 46 800 77 2188 ...
 $ eval    : num  14920100 1070050 800 77 4772190 ...
 $ time    : num  27.65 1.22 0.22 0.47 116.34 ...
 $ cost    : num  1492054 107046 800 77 479188 ...
```

R Notions

- the libraries `tidyverse` make available another type: the tibble (`tbl_df`). Try `glimpse(data)`.
- the library `dplyr` can be helpful to organize data. See the cheatsheet.
- data frames can be in wide or long format. You can transform between them with `pivot_longer()` and `pivot_wider()` from `tidyr`.

```
> require(dplyr)
> require(tidyr)
> spread(select(DATA,instance,alg,hard),alg,hard)
      instance 3702445 5248915 5286294 5506044 5736304 6190028 6240996
1   acc-tight6      88      NA      33     468      33      12    1286
2     bnatt350     152      NA     161     183     150     174    1564
3       co-100    1201      NA     162     162     162     808    1193
4         ex10     974      77     200     200     306     107    1731
5          ex9     477      70     162     162     217      75    1474
6 iis-pima-cov       0       0       0    7201       0       0       0
7   macrophage       0       0       0     609       0       0     424
8 neos-1440225     107      22      80     330      75      35     329
9    ns1696083    1492       7    1381     139    3306      46    3211
```

R Notions

Rank transformation in dplyr:

```
HARD_LONG <- HARD_LONG |> group_by(instance) |>
                          mutate(rank=rank(hard,na.last = TRUE))
```

here `group_by` does the same job as `split`

```
> head(HARD_LONG)
# A tibble: 6 x 4
      instance     alg  hard  rank
        <fctr>   <chr> <int> <dbl>
1   acc-tight6 3702445    88   4.0
2     bnatt350 3702445   152   2.0
3       co-100 3702445  1201   6.0
4         ex10 3702445   974   6.0
5          ex9 3702445   477   6.0
6 iis-pima-cov 3702445     0   3.5
```

R: graphics with ggplot2

A grammar for graphics:

- Data that you want to visualise and a set of aesthetic mappings describing how variables in the data are mapped to aesthetic attributes that you can perceive (eg, the x and y axis and the colors).

```
library(ggplot2)
p <- ggplot(HARD_LONG,aes(x=reorder(alg, rank, median), y=rank))
```

- Layers made up of geometric elements and statistical transformation.
  – Geometric objects, geoms for short, represent what you actually see on the plot: points, lines, polygons, etc.
  – Statistical transformations, stats for short, summarise data in many useful ways. For example, binning and counting observations to create a histogram, or summarising a 2d relationship with a linear model.

```
p <- p + geom_boxplot(aes(fill=alg),width=0.8,stat = "boxplot",
                  position = position_dodge(width = 0),
                  colour = I("#3366FF"),outlier.colour = I("#3366FF"))
```

- The scales map values in the data space to values in an aesthetic space, whether it be colour, or size, or shape. Scales draw a legend or axes, which provide an inverse mapping to make it possible to read the original data values from the plot.

```
p <- p + scale_y_continuous(breaks=seq(1, nlevels(HARD_LONG$alg), 1))
```

- A coordinate system, coord for short, describes how data coordinates are mapped to the plane of the graphic. It also provides axes and gridlines to make it possible to read the graph. We normally use a Cartesian coordinate system, but a number of others are available, including polar coordinates and map projections.

```
p <- p + coord_cartesian(ylim=c(1,nlevels(HARD_LONG$alg)))
```

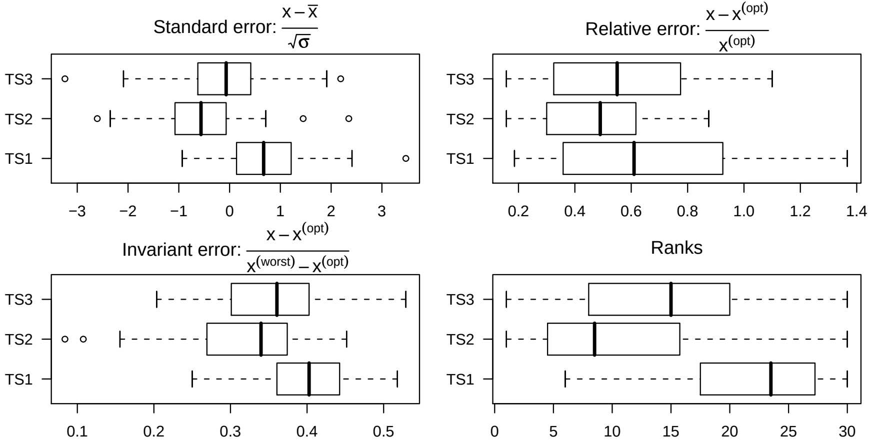
- A faceting specification describes how to break up the data into subsets and how to display those subsets as small multiples. This is also known as conditioning or latticing/trellising.

```
p <- p + facet_grid(.~class) # faceting
```

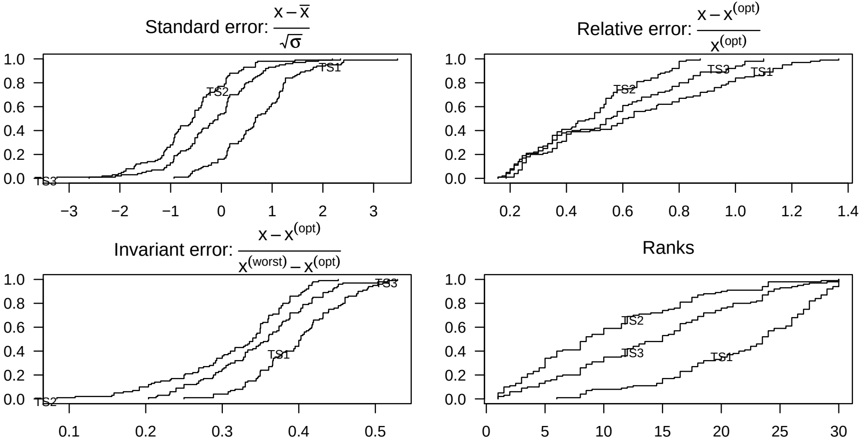
- A theme which controls the finer points of display, like the font size and background colour. But trust the defaults.

```
print(p)
```

On a class of instances



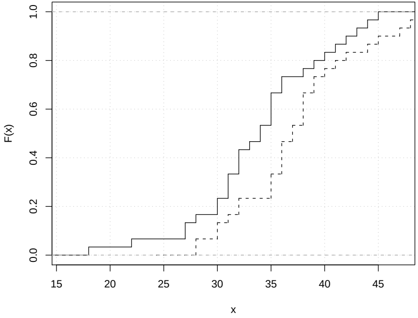
On a class of instances

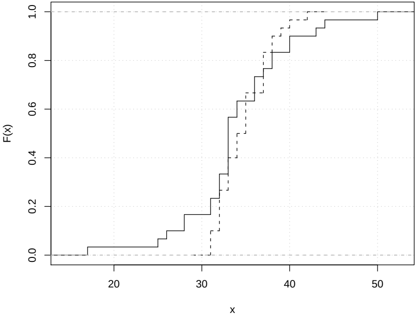


Stochastic Dominance

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.*:

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





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.it parz.it exit.it exit.time opt
1 TS1 G-1000-0.5-30-1   1  59      9.900619   5955     442    5955  10.02463  30
2 TS1 G-1000-0.5-30-1   2  64      9.736608   3880     130    3958  10.00062  30
3 TS1 G-1000-0.5-30-1   3  64      9.908618   4877      49    4877  10.03263  30
4 TS1 G-1000-0.5-30-1   4  68      9.948622   6996     409    6996  10.07663  30
5 TS1 G-1000-0.5-30-1   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.

Maintain the raw data

```
> 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")
```

Transform data in standard error

```
> #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: "
> library(latticeExtra)
> ecdfplot(~values,group=ind,data=T5,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)
```

Transform the data in relative error

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

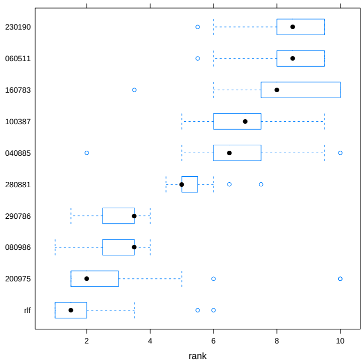
Transform the data in an invariant error
We use as surrogate of x^{worst} the median solution returned by the simplest algorithm for the graph coloring, that is, the ROS heuristic.

```
> #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$opt)
> boxplot(err3~alg,data=G,horizontal=TRUE,main=expression(paste("Invariant error: ",fr
> ecdfplot(G$err3,group=G$alg,main=expression(paste("Invariant error: ",frac(x-x^(opt)
```

Transform the data in ranks

```
> #rank
> G$rank <- G$sol
> split(G$rank, G$inst) <- lapply(split(G$sol, D$inst), rank)
> bwplot(rank~reorder(alg,rank,median),data=G,horizontal=TRUE,main="Ranks")
> ecdfplot(rank,group=alg,data=G,main="Ranks")
```

```r
> ## Let's make the ranks of the colors
> T1 <- split(DATA["col"], DATA["instance"])
> T2 <- lapply(T1, rank, na.last = "keep")
> T3 <- unsplit(T2, DATA["instance"])
> DATA$rank <- T3
>
> ## we plot the ranks for an aggregate analysis
> ## reoder sort the factor algorithm by median values
> bwplot(reorder(alg, rank, median) ~ rank, data = DATA)
```



A modern example of analysis

- https://imada.sdu.dk/u/march/DM841/assignments/pb_benchmarks.html
- https://imada.sdu.dk/u/march/DM841/assets/analysis.html

Scenarios

A. Single-pass heuristics

B. Asymptotic heuristics
(can be run indefinitely with a chance of continuing to make progress):

Two approaches:

1. Univariate
   - 1.a Time as an external parameter decided *a priori*
   - 1.b Solution quality as an external parameter decided *a priori*
2. Cost dependent on running time:

Scenario B

Asymptotic heuristics

There are two approaches:

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

Deterministic case: $\mathcal{A}^\infty$ on class Π finds a solution in running time t.

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

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

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

Dealing with Censored Data

Asymptotic heuristics, Approach 1.b

- Heuristic $\mathcal{A}^{\dashv}$ 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

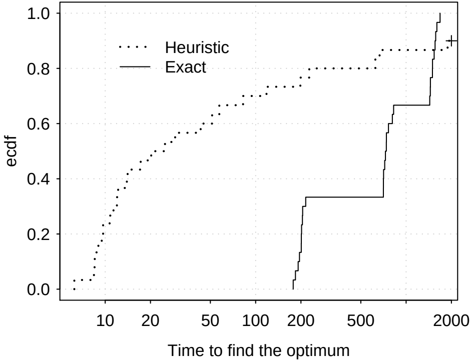
- T_i if $T_i \leq L_i$
- or $T_i \geq L_i$.

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

Example

Asymptotic heuristics, Approach 1.b: 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:

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

Scenarios

A. Single-pass heuristics

B. Asymptotic heuristics
(can be run indefinitely with a chance of continuing to make progress):

Two approaches:

1. Univariate
   - 1.a Time as an external parameter decided *a priori*
   - 1.b Solution quality as an external parameter decided *a priori*
2. Cost dependent on running time:

Scenario B

Asymptotic heuristics

There are two approaches:

2. Cost dependent on running time:

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

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

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

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

Example

Scenario:

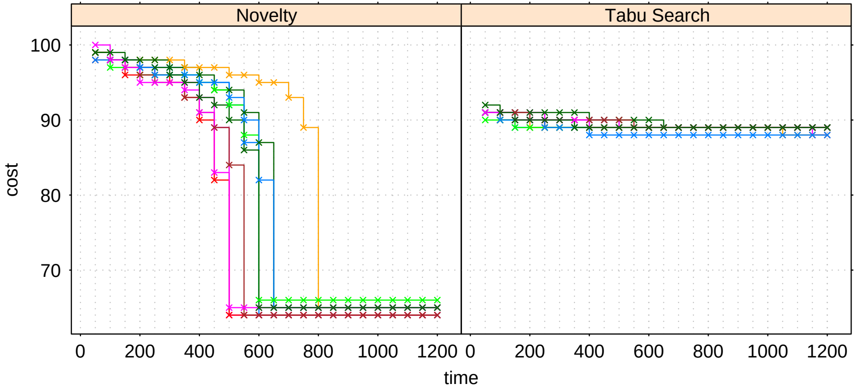
- ▷ 3 heuristics $\mathcal{A}_1^\infty$, $\mathcal{A}_2^\infty$, $\mathcal{A}_3^\infty$ on instance π.
- ▷ single instance hence no data transformation.
- ▷ r runs
- ▶ Interest: inspecting solution cost over running time to determine whether the comparison varies over time intervals

Tools:

- Quality profiles

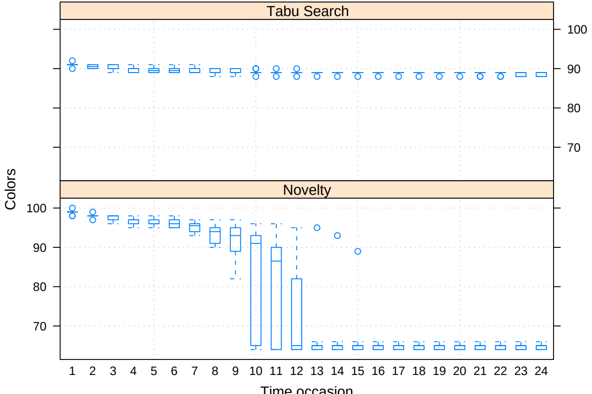
The performance is described by multivariate random variables of the kind $\vec{Y} = \{Y(t_1), Y(t_2), \ldots, Y(l_k)\}$.

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



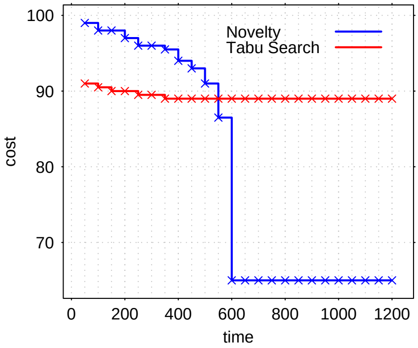
The performance is described by multivariate random variables of the kind $\vec{Y} = \{Y(t_1), Y(t_2), \ldots, Y(l_k)\}$.

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



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

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



The median behavior of the two algorithms

Summary

Visualize your data for your analysis and for communication to others

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.

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?

- 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^o?
- 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.

- 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

Outline

Reproducibility

Artifact: a digital object that was either created by the authors to be used as part of the study or generated by the study itself. ACM distinguishes (see also **?**):

Optimization as an Empirical Science

Scientific Method

1. Observe a phenomenon
2. Construct a hypothesis
3. Conduct an experiment
4. Draw conclusion about hypothesis:
   either provisionally accepted or falsified
   (with some statistical confidence)

What is Reproducibility?

- Repeat your own experiment
  and confirm your previous conclusion?

- Repeat someone else's experiment using their software and data and confirm their conclusion?

- Repeat someone else's experiment using your own re-implementation and confirm their conclusion?

What is Reproducibility?

- ✘ No consensus in terminology [Claerbout & Karrenbach, 1992] [Plesser, 2018]
- ACM distinguishes between:
  Repeatability, Reproducibility and Replicability
- López-Ibáñez, Branke, and Paquete [2021] define the terms more precisely and distinguish between: Repeatability, Reproducibility, Replicability and Generalisability

Terminology

Artifact [ACM, 2020]

"A digital object that was either created by the authors to be used as part of the study or generated by the experiment itself"

- algorithm implementations, benchmark instances, data pre/post-processing scripts, . . .

Measurement [López-Ibáñez, Branke, and Paquete, 2021]

"data that results from an experiment"

- measures of quality, computational effort, etc.
- NOT summary statistics

ACM's Terminology

Repeatability (Same team, same experimental setup)

The measurement can be obtained with stated precision by the same team using the same measurement procedure, the same measuring system, under the same operating conditions, in the same location on multiple trials.

Reproducibility (Different team, same experimental setup)

The measurement can be obtained with stated precision by a different team using the same measurement procedure, the same measuring system, under the same operating conditions, in the same or a different location on multiple trials. [. . .] [A]n independent group can obtain the same result using the author's own artifacts.

Replicability (Different team, different experimental setup)

The measurement can be obtained with stated precision by a different team, a different measuring system, in a different location on multiple trials.[. . .] [A]n independent group can obtain the same result using artifacts which they develop completely independently.

Dimensions of reproducibility

- Artifacts: Re-use of the original artifacts should allow to repeat the exact same experiment described in the original publication
- Random factor:
  - The experiment evaluates a random sample
  - The experimental claim applies to a range or probability distribution
  - Random seeds
- Fixed factor:
  - The experiment evaluates specific chosen values
  - The experimental claim is supported only for those specific values
  - Parameter settings, benchmark problems, computational budget
    . . . unless randomized

Terminology [López-Ibáñez, Branke, and Paquete, 2021]

Label	Artifacts	Random factors	Fixed factors	Purpose of the study
Repeatability	Original	Original	Original	Exactly repeat the original experiment, generating precisely the same results.
Reproducibility	Original	New	Original	Test whether the original results were dependent on specific values of random factors and, hence, only a statistical anomaly.
Replicability	New	New	Original	Test whether it is possible to independently reach the same conclusion without relying on original artifacts.
Generalisability	Original or New	New	New	Test whether the conclusion extends beyond the experimental setup of the original paper. When new artifacts are used, generalisability should come after a replicability study.

References

Birattari M., Stützle T., Paquete L., and Varrentrapp K. (2002). **A racing algorithm for configuring metaheuristics**. In *Proceedings of the Genetic and Evolutionary Computation Conference (GECCO-2002)*, edited by L. et al., pp. 11–18. Morgan Kaufmann Publishers, New York.

Hoos H.H. (2012). **Programming by optimization**. *Commun. ACM*, 55(2), pp. 70–80.

López-ibá nez M., Branke J., and Paquete L. (2021). **Reproducibility in evolutionary computation**. *ACM Trans. Evol. Learn. Optim.*, 1(4).

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.