Introduction to Design of Experiments

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Outline

1. Confidence Intervals
2. Using Confidence Intervals
3. Design of Experiments: Early Intuition
4. Getting rid of Outliers
5. Issues when studying something else than the mean

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Continuous random variable

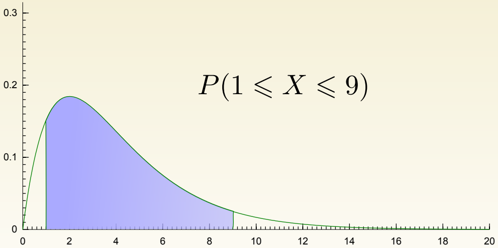
- A random variable (or stochastic variable) is, roughly speaking, a variable whose value results from a measurement.
  Such a variable enables to model uncertainty that may result of *incomplete information* or *imprecise measurements*.
  Formally $(\Omega, \mathcal{F}, P)$ is a probability space where:
  - Ω, the sample space, is the set of all possible outcomes (e.g., $\{1, 2, 3, 4, 5, 6\}$)
  - $\mathcal{F}$ if the set of events where an event is a set containing zero or more outcomes (e.g., the event of having an odd number $\{1, 3, 5\}$)
  - The probability measure $P : \mathcal{F} \rightarrow [0, 1]$ is a function returning an event's probability.
- Since many computer science experiments are based on time measurements, we focus on continuous variables.

$$X : \Omega \rightarrow \mathbb{R}$$

A probability distribution (a.k.a. probability density function or p.d.f.) is used to describe the probabilities of different values occurring.

A random variable X has density f, where f is a non-negative and integrable function, if:

$$P[a \leqslant X \leqslant b] = \int_a^b f(x)\,\mathrm{d}x$$



Expected value

- When one speaks of the "expected price", "expected height", etc. one means the expected value of a random variable that is a price, a height, etc.

$$\begin{aligned}\mathrm{E}[X] &= x_1p_1 + x_2p_2 + \ldots + x_kp_k \\ &= \int_{-\infty}^{\infty} x f(x)\,\mathrm{d}x\end{aligned}$$

  The expected value of X is the "average value" of X.

  It is **not** the most probable value. The mean is one aspect of the distribution of X. The median or the mode are other interesting aspects.

- The variance is a measure of how far the values of a random variable are spread out from each other.
  If a random variable X has the expected value (mean) $\mu = \mathrm{E}[X]$, then the variance of X is given by:

$$\mathrm{Var}(X) = \mathrm{E}\left[(X-\mu)^2\right] = \int_{-\infty}^{\infty} (x-\mu)^2 f(x)\,\mathrm{d}x$$

How to estimate Expected value ?

To empirically estimate the expected value of a random variable, one repeatedly measures observations of the variable and computes the arithmetic mean of the results.

Unfortunately, if you repeat the estimation, you may get a different value since X is a random variable ...

Central Limit Theorem

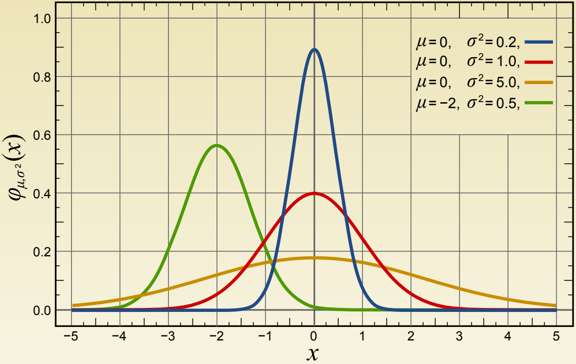
- Let $\{X_1, X_2, \dots, X_n\}$ be a random sample of size n (i.e., a sequence of **independent** and **identically distributed** random variables with expected values μ and variances σ^2).
- The sample average of these random variables is:

$$S_n = \frac{1}{n}(X_1 + \cdots + X_n)$$

  S_n is a random variable too.
- For large n's, the distribution of S_n is approximately normal with mean μ and variance $\frac{\sigma^2}{n}$.

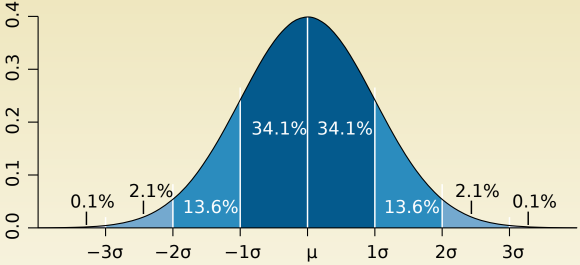
$$S_n \xrightarrow[n\to\infty]{} \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right)$$

The Normal Distribution



The smaller the variance the more “spiky” the distribution.

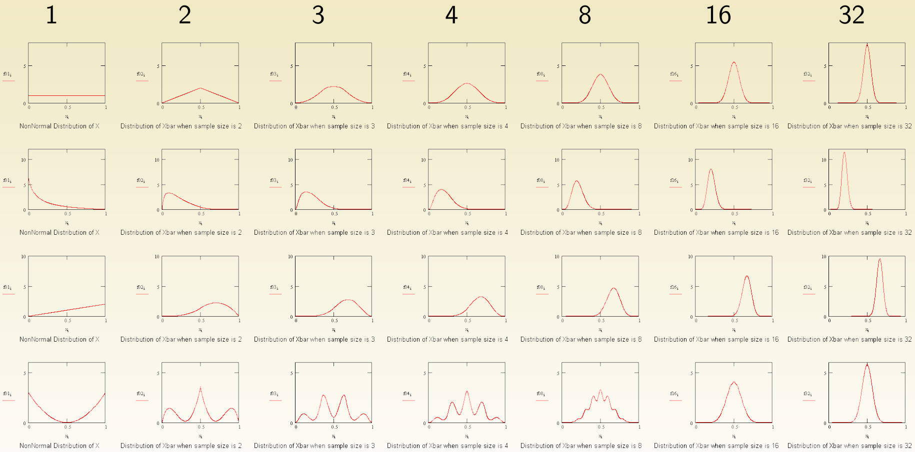
The Normal Distribution



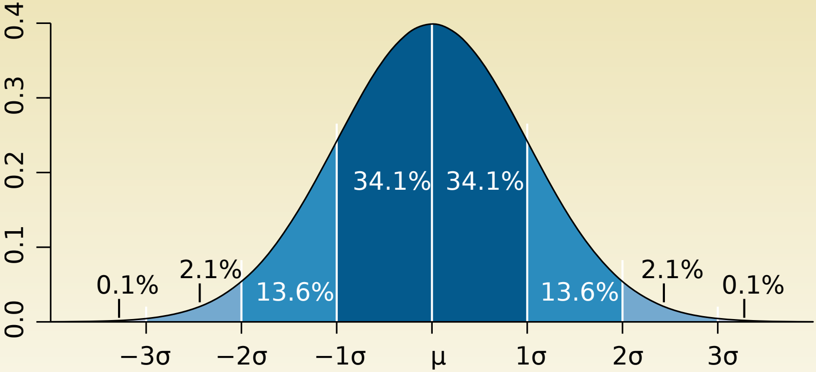
The smaller the variance the more "spiky" the distribution.

- Dark blue is less than one standard deviation from the mean. For the normal distribution, this accounts for about 68% of the set.
- Two standard deviations from the mean (medium and dark blue) account for about 95%
- Three standard deviations (light, medium, and dark blue) account for about 99.7%

Start with an arbitrary distribution and compute the distribution of S_n for increasing values of n.



CLT consequence: confidence interval



When n is large:

$$\mathrm{P}\left(\mu \in \left[S_n - 2\frac{\sigma}{\sqrt{n}}, S_n + 2\frac{\sigma}{\sqrt{n}}\right]\right) = \mathrm{P}\left(S_n \in \left[\mu - 2\frac{\sigma}{\sqrt{n}}, \mu + 2\frac{\sigma}{\sqrt{n}}\right]\right) \approx 95\%$$

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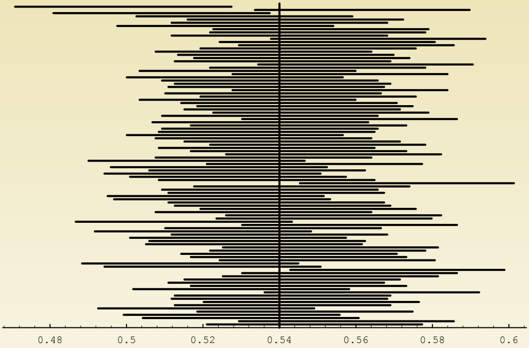

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There is 95% of chance that the true mean lies within $2\frac{\sigma}{\sqrt{n}}$ of the sample mean.

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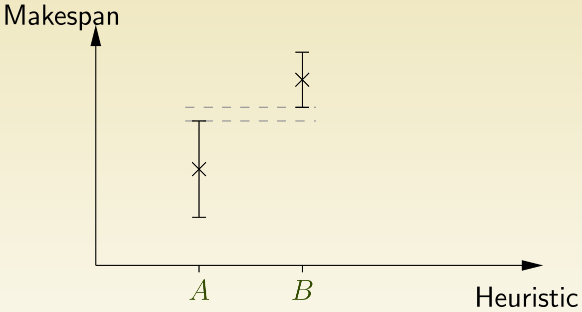
Comparing Two Alternatives

Assume, you have evaluated two scheduling heuristics A and B on n different DAGs.



The two 95% confidence intervals do not overlap $\leadsto \mathrm{P}(\mu_A < \mu_B) > 90\%$.

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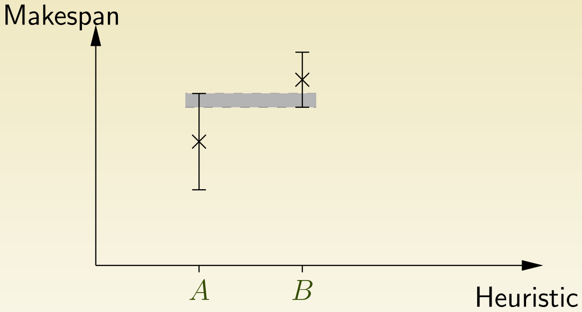

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Reduce C.I ?

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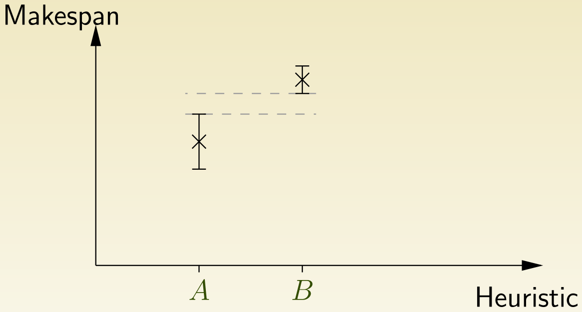

The two 70% confidence intervals do not overlap $\rightsquigarrow \mathrm{P}(\mu_A < \mu_B) > 49\%$.

Let's do more experiments instead.

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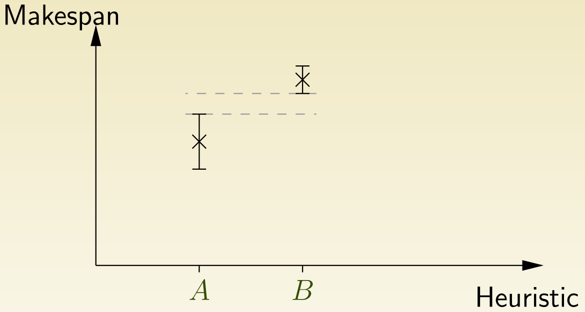


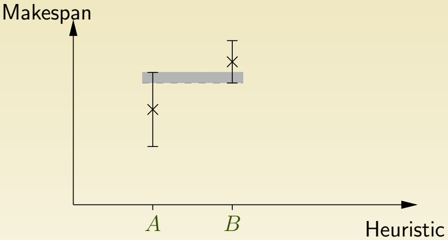
The width of the confidence interval is proportionnal to $\frac{\sigma}{\sqrt{n}}$.

Halving C.I. requires 4 times more experiments!

Try to reduce variance if you can...

Comparing Two Alternatives with Blocking

- C.I.s overlap because variance is large. Some DAGS have an intrinsically longer makespan than others, hence a large $\mathrm{Var}(A)$ and $\mathrm{Var}(B)$



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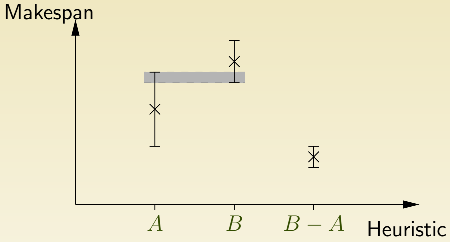

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  $\mathrm{E}[A] < \mathrm{E}[B] \Leftrightarrow \mathrm{E}[B-A] < 0$.
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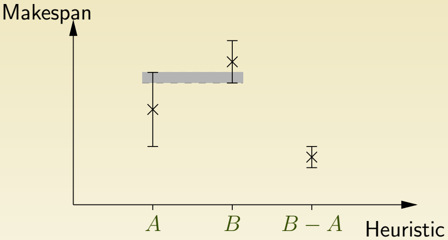

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- Relying on such common points is called blocking and enable to reduce variance.

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  The CLT uses $\sigma = \sqrt{\text{Var}(X)}$ but we only have the sample variance, not the true variance.

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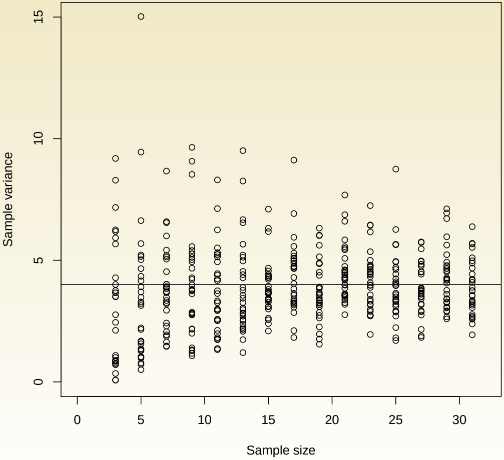

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- **Running the right number of experiments enables to get to conclusions more quickly and hence to test other hypothesis.**

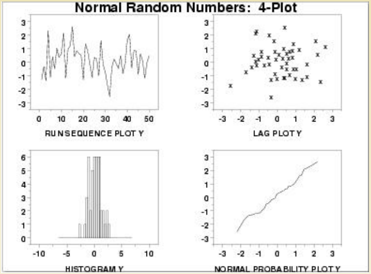
Key Hypothesis

The hypothesis of CLT are very weak. Yet, to qualify as replicates, the repeated measurements:

- must be independent (take care of warm-up)
- must not be part of a time series (the system behavior may temporary change)
- must not come from the same place (the machine may have a problem)
- must be of appropriate spatial scale

Perform graphical checks

Simple Graphical Check



Fixed Location: If the fixed location assumption holds, then the run sequence plot will be flat and non-drifting.

Fixed Variation: If the fixed variation assumption holds, then the vertical spread in the run sequence plot will be the approximately the same over the entire horizontal axis.

Independence: If the randomness assumption holds, then the lag plot will be structureless and random.

Fixed Distribution : If the fixed distribution assumption holds, in particular if the fixed normal distribution holds, then

- the histogram will be bell-shaped, and
- the normal probability plot will be linear.

If you see several modes, you may want to investigate further is there is not another hidden parameter you should take into account.

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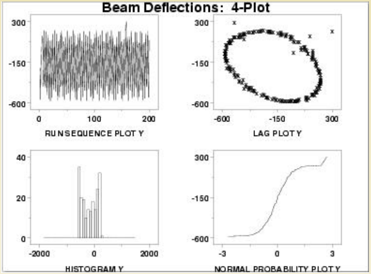

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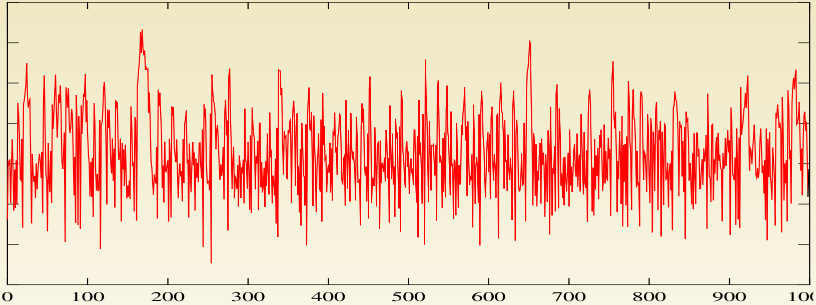

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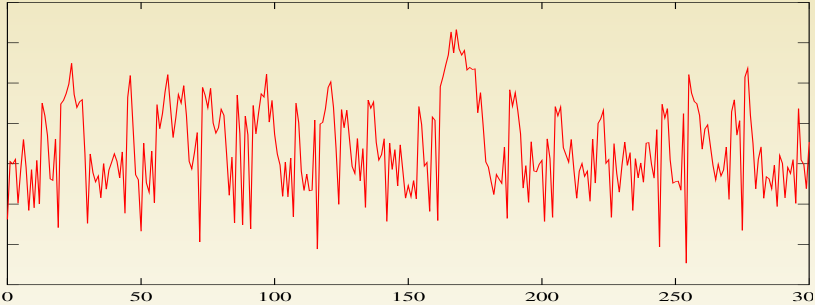
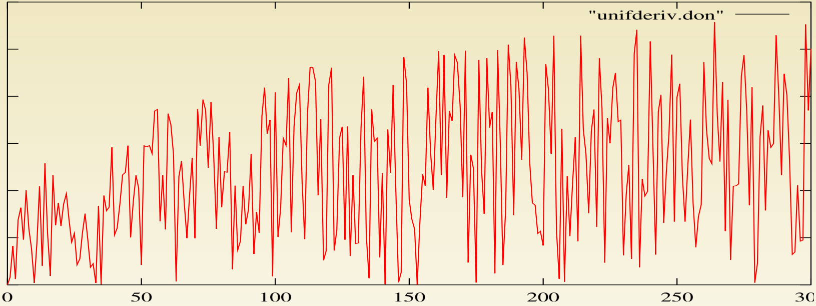


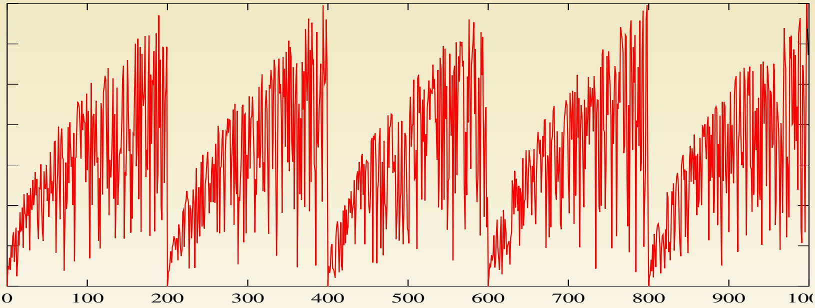
- Looks independant and statistically identical
- Danger: temporal correlation $\rightsquigarrow$ study stationnarity.

Detect Trends



- Model the trend: here increase then saturates
- Possibly remove the trend by compensating it (multiplicative factor here)

Detect Periodicity



May depend on sampling frequency or on horloge resolution.

- Study the period (Fourier)
- Use time series

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- You should better do $A, B, \quad A, B, \quad A, B, \quad A, B, \ldots$.
- Even better, randomize your run order. You should flip a coin for each configuration and start with A on head and with B on tail...

  $$A, B, \quad B, A, \quad B, A, \quad A, B, \ldots.$$

  With such design, you will even be able to check whether being the first alternative to run changes something or not.

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  With such design, you will even be able to check whether being the first alternative to run changes something or not.
- Each configuration you test should be run on different machines. You should record as much information as you can on how the experiments was performed (http://expo.gforge.inria.fr/).

Experimental Design

There are two key concepts:

replication and randomization

You replicate to increase reliability. You randomize to reduce bias.

**If you replicate thoroughly and randomize properly,
you will not go far wrong.**

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you will not go far wrong.

> It doesn't matter if you cannot do your own advanced statistical analysis. If you designed your experiments properly, you may be able to find somebody to help you with the statistics.
>
> If your experiments is not properly designed, then no matter how good you are at statistics, you experimental effort will have been wasted.

No amount of high-powered statistical analysis can turn a bad experiment into a good one.

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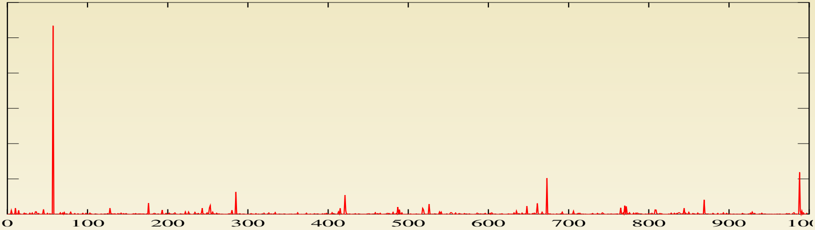
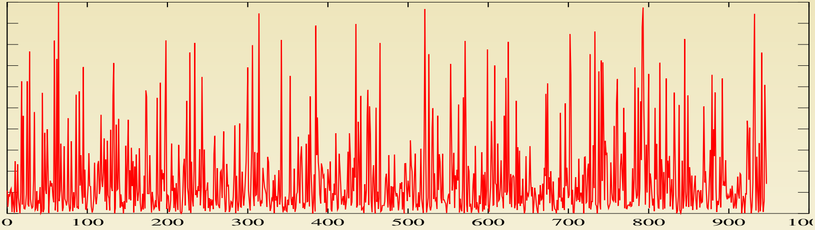
Abnormal measurements



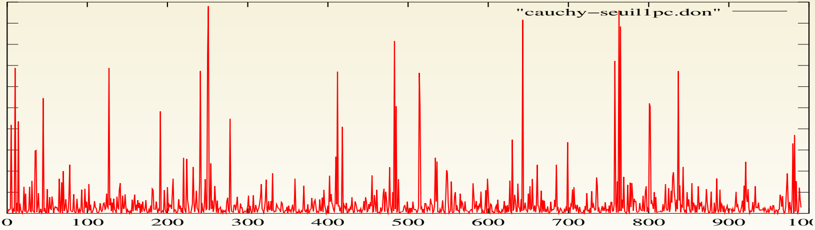
- Rare events: interpretation
- Get rid of it using:
  - a threshold value: what is the right threshold ?
  - quantiles: what is the good rejection rate ?

Thresholds:

Reject values larger than 10 $\rightsquigarrow$ 5% of rejection



Reject values larger than 50 $\rightsquigarrow$ 1% of rejection



Actually, here, the samples are generated using the Cauchy distribution, which is pathological for most ideas you may come up with. :)

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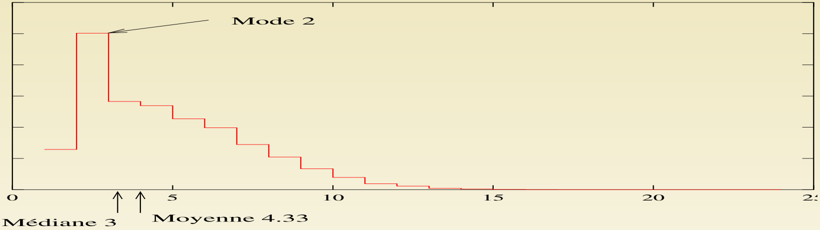
Summarizing the distribution

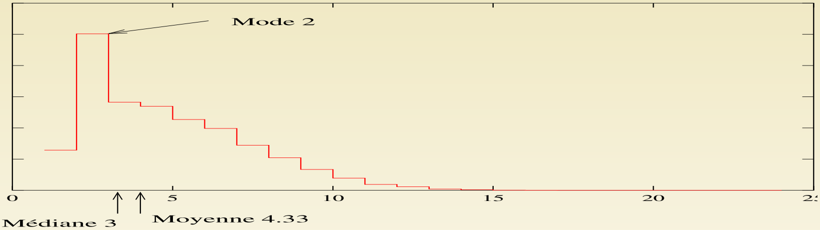


What is the shape of the histogram:

- uni/multi-modal
- symmetrical or not ($\leadsto$ skewness)
- Flat of not ($\leadsto$ kurtosis)

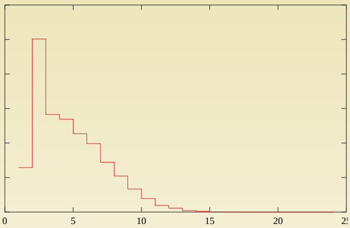
Summarize with central tendancy

Summarizing the distribution



- Mode: the most probable value (higly depends on the bin size)
- Median: splits the samples in half (rather unstable)
- Mean: average "cost" (can simply estimate confidence intervals)

Mode value
histogram



Mode

- **Categorical data**
- Most frequent value
- highly unstable value
- for continuous value distribution depends on the histogram step
- interpretation depends on the flatness of the histogram

$\Longrightarrow$ **Use it carefully**
$\Longrightarrow$ **Predictor function**

Median

- **Ordered data**
- Split the sample in two equal parts

$$\sum_{i \leqslant Median} f_i \leqslant \frac{1}{2} \leqslant \sum_{i \leqslant Median+1} f_i.$$

- more stable value
- does not depends on the histogram step
- difficult to combine (two samples)

$\Longrightarrow$ **Randomized algorithms**

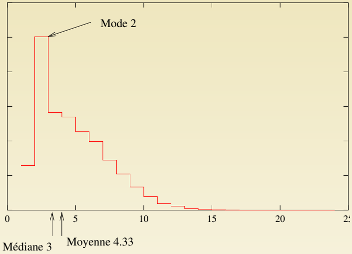
Mean

- **Vector space**
- Average of values

$$Mean = \frac{1}{Sample\_Size} \sum x_i = \sum_x x.f_x.$$

- stable value
- does not depends on the histogram step
- easy to combine (two samples $\Rightarrow$ weighted mean)

$\Longrightarrow$ **Additive problems (cost, durations, length,...)**



Complementarity

- Valid if the sample is "Well-formed"
- **Semantic of the observation**
- Goal of analysis

$\Longrightarrow$ **Additive problems (cost, durations, length,...)**

Central tendency (2)

Summary of Means

- Avoid means if possible
  Loses information
- Arithmetic mean
  When sum of raw values has physical meaning
  Use for summarizing times (not rates)
- Harmonic mean
  Use for summarizing rates (not times)
- Geometric mean
  Not useful when time is best measure of perf
  Useful when multiplicative effects are in play

Computational aspects

- Mode : computation of the histogram steps, then computation of max $O(n)$ “off-line”
- Median : sort the sample $O(nlog(n))$ or $O(n)$ (subtile algorithm) “off-line”
- Mean : sum values $O(n)$ “on-line” computation

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- Mode : computation of the histogram steps, then computation of max $O(n)$ “off-line”
- Median : sort the sample $O(nlog(n))$ or $O(n)$ (subtile algorithm) “off-line”
- Mean : sum values $O(n)$ “on-line” computation

Is the central tendency significant ?
$\Rightarrow$ Explain variability.

Variability

Categorical data (finite set)

f_i : empirical frequency of element i

Empirical entropy

$$H(f) = \sum_i f_i \log f_i.$$

Measure the empirical distance with the uniform distribution

- $H(f) \geqslant 0$
- $H(f) = 0$ iff the observations are reduced to a unique value
- $H(f)$ is maximal for the uniform distribution

Variability (2)

Ordered data

Quantiles : quartiles, deciles, etc
Sort the sample :

$$(x_1, x_2, \cdots, x_n) \longrightarrow (x_{(1)}, x_{(2)}, \cdots, x_{(n)});$$

$$Q_1 = x_{(n/4)};\ Q_2 = x_{(n/2)} = Median;\ Q_3 = x_{(3n/4)}.$$

For deciles

$$d_i = argmax_i\{\sum_{j \leqslant i} f_j \leqslant \frac{i}{10}\}.$$

Utilization as quantile/quantile plots to compare distributions

Variability (3)

Vectorial data

Quadratic error for the mean

$$Var(X) = \frac{1}{n}\sum_{1}^{n}(x_i - \bar{x}_n)^2.$$

Properties:

$$\begin{aligned}
Var(X) &\geqslant 0; \\
Var(X) &= \overline{x^2} - (\bar{x})^2, \text{ où } \overline{x^2} = \frac{1}{n}\sum_{i=1}^{n} x_i^2. \\
Var(X + cste) &= Var(X); \\
Var(\lambda X) &= \lambda^2 Var(X).
\end{aligned}$$

Roadmap for a good data analysis

1. Plot the sample (various representations)
2. Describe the results (data analysis)
3. Preliminary processing : remove or flag outliers, estimate or flag missing values
4. Propose a stochastic model : establish the hypothesis : independence (time correlation, auto-correlation), stationarity, same probability law
5. Summarize data by a histogram
6. Comment the shape (modal/skewness/flatness/...)
7. Estimate the central tendency of the sample : choose the central index
8. Estimate the accuracy of the result (confidence intervals)
9. Propose a visualization

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