# Automated Machine Learning
## (AutoML)

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# Lecture 3:
# Evaluation and Visualization

# Where are we? The big picture

- Introduction
- → Background
  - Design spaces in ML
  - → Evaluation and visualization
- Hyperparameter optimization (HPO)
  - Bayesian optimization
  - Other black-box techniques
  - Speeding up HPO with multi-fidelity optimization
- Pentecost (Holiday) – no lecture
- Architecture search I + II
- Meta-Learning
- Learning to learn & optimize
- Beyond AutoML: algorithm configuration and control
- Project announcement and closing

# Learning Goals

After this lecture, you will be able to . . .

- explain the role of outliers in CS/ML
- compare and visualize the performance of different configurations
- compare and visualize the performance of AutoML systems
- explain and correctly apply statistical hypothesis tests

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  - compare e.g., experimental physics: 1 week of beam time per year
- We can conduct and analyze experiments fully automatically
  - we can gather large amounts of data quickly (e.g., 100 repetitions)
  - but: don't confuse statistical significance and relevance

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  - **Environment:** Outliers can indicate a problem with the environment (e.g., file system or network issues)
  - **Datasets:** When characterizing cost across a distribution of datasets, outliers with small values can indicate trivial datasets.

# Lecture Overview

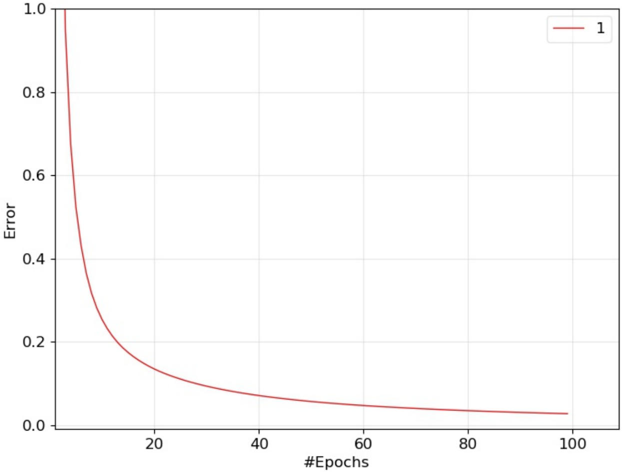
1. Visualization of Configuration Performance
2. Visualization of AutoML Performance
3. Statistical Hypothesis Testing

# Setup

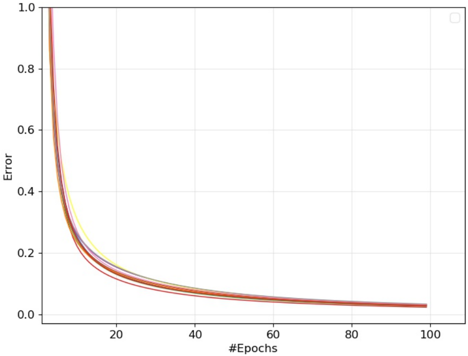
For the following slides, we have used the following setup:

- Model: simple MLP (from sklearn)
  with 2 layers with 128 neurons and 64 neurons, resp.
- Dataset: Digits
- Setting 1: learning rate of $0.001$
- Setting 2: learning rate of $0.01$

# A Single Learning Curve (Setting 1)

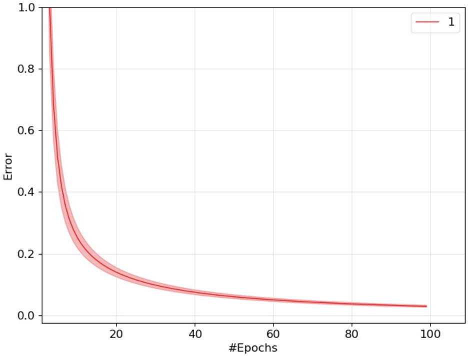


# 10 Learning Curves (Setting 1)



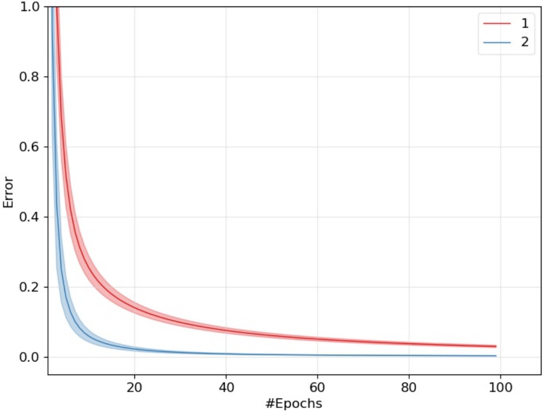

- ⇝ Deep learning (and most other ML algorithms) are non-deterministc
- ⇝ Measure performance more than once and estimate noise-level

# Aggregated Learning Curves (Setting 1)




- Plot mean and stdev (shaded area) across $n$ (here $100$) random seeds
- Only use mean and stdevarcSepA=[0pt] if noise is somehow normal distributed
- alternatives are the mean+standard error or median+25/75-percentiles

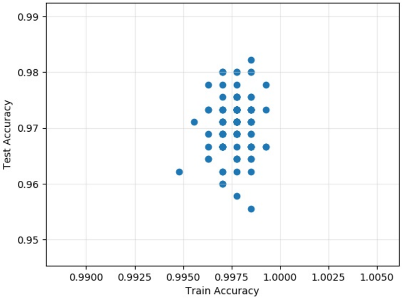
# Comparing Learning Curves




- If uncertainties (shaded area) overlap, results might not be statistically significant but due to noise

# Scatter Plot: Train vs. Test

Setting 1

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- here at least not anti-correlated

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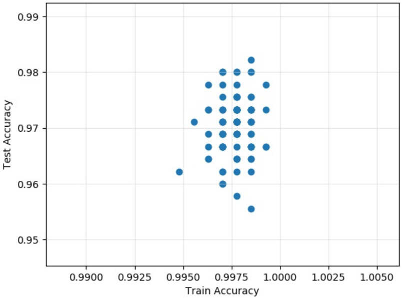


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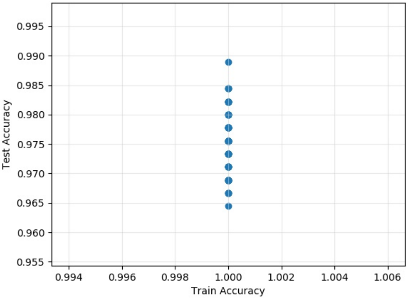
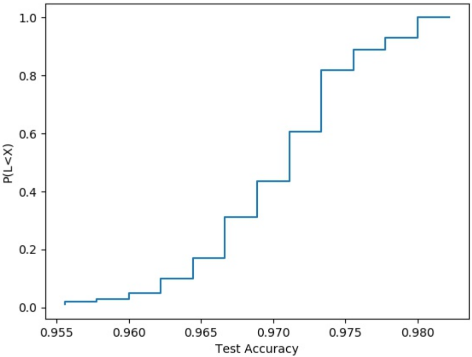



- already perfect training score
- generalization nevertheless noisy

# eCDF: Distribution of Performance (Setting 1)




How to compute an empirical CDF:

1. X: sorted error scores
2. Y: $[1 \dots \#\text{points}]/\#\text{points}$
3. step_function(X,Y)

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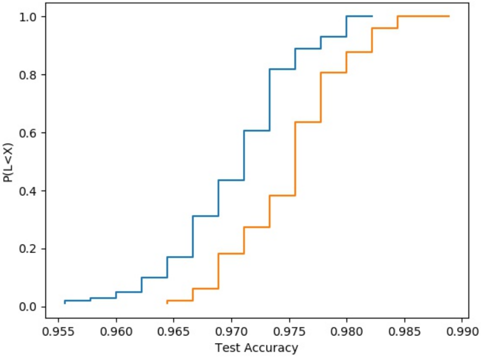
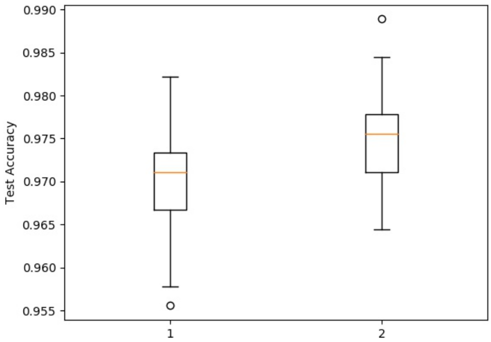



Which curve corresponds to which setting?

# Box Plot: Comparing Two Configurations

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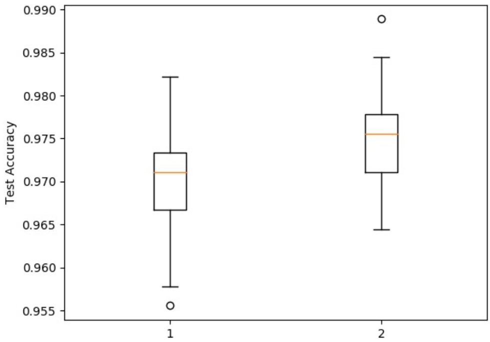


- alternative: violin plots
- if you have paired populations (e.g., configurations evaluated on different datasets), you should generate boxplots with $\mathcal{L}/\mathcal{L}_{\text{baseline}}$

$\rightsquigarrow$ insight on how many datasets one of the two performed better

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# AutoML Systems over Time

- Don't only measure the performance of AutoML systems for a fixed budget because:
  1. A priori, it is unknown how long a user will run an AutoML system
  2. Some systems perform well for small budgets and some others need more time before performing well
     - BO-based systems often perform as good as random search in the beginning, but perform very well later on

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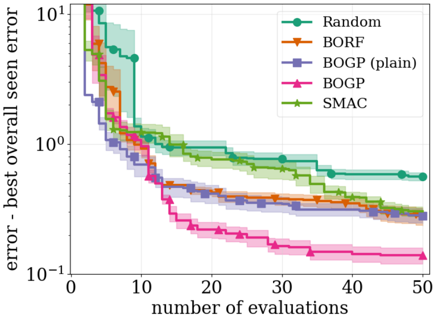
- Recommendation: plot performance (e.g., error) over time
  - Similar to learning curves of DNNs

# Aggregated AutoML Systems over Time




- Different HPO systems minimizing the error of an MLP on MNIST
- How to do it:
  - Run each systems several times and always log its current incumbent
  - Plot mean and stdev for each system after each incumbent update
  - Use step functions, because linear interpolation would be too optimistic

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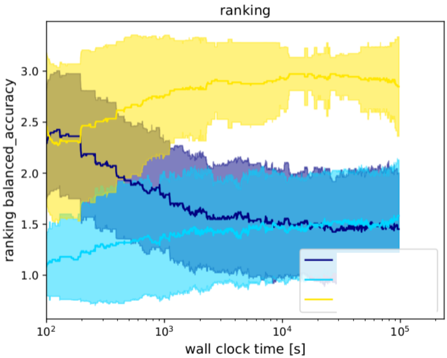
$\rightsquigarrow$ There is no way around that you have some kind of information loss

# Ranked AutoML Systems over Time and Datasets

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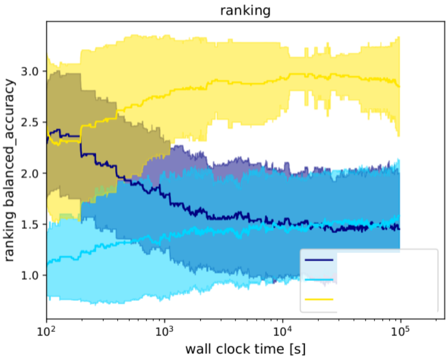


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- Ranks avoid the problem of different scales
- Problem: we don't know whether a better ranking relates to a substantial improvement of the actual cost metric

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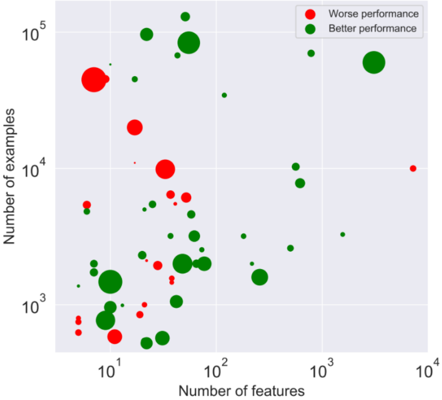
## On a single dataset ($d = 1$)

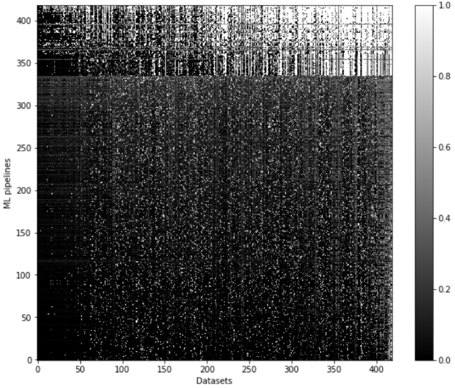
1. for each system, sample a single run out of the $n$ runs
2. compute ranking on these samples
3. repeat 1. and 2. at least $10\,000$ times to obtain many rankings
4. compute mean and stdev across rankings

# Scatter Plot: Meta Features




- Compare two systems (or 1 vs rest)
- each dot is a dataset
- color encoding better or worse
- size indicates performance difference
- meta-features (e.g., #features, #samples) on axes
  - using PCA on a larger set of meta-features leads to algorithm footprints [Smith-Miles et al. 2012]

# Heatmaps: Comparing several Configurations




- compare many configurations on many datasets
- can reveal:
  - homogeneity if smooth transition from hard to easy
  - heterogeneity if stripes exist (here the case)
- Remark: datasets and configurations should be sorted according to their average cost

# Lecture Overview

# Background: statistical hypothesis tests

- When we have a lot of data, we need to summarize it
  - But we already saw that summarization hides a lot of data
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  - Ideally, we want to draw high-level conclusions (e.g., "A outperforms B on datasets of type X")
- Problem: we only have a finite number of observations
  - Can we attribute observed performance differences to chance?
  - Are we reasonably sure that a claim we make is reproducible?
  - $\rightsquigarrow$ Statistical tests can help

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| | Truly not guilty | Truly guilty |
|---|---|---|
| Found not guilty | Acquittal | Type II Error |
| Found guilty | Type I Error | Conviction |

$\rightsquigarrow$ We want to minimize Type I error!

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8. If $p < \alpha$, reject null hypothesis in favor of alternative hypothesis
   - If $p > \alpha$, it doesn't tell you anything about the null hypothesis!

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- IQ values are known to be normally distributed with $X \sim \mathcal{N}(100, 15)$
  - $\rightarrow$ statistical assumption
- Let's say we observed IQ values $x_i$ of 9 students in the class:
  - $\{x_1, \dots, x_9\} = \{116, 128, 125, 119, 89, 99, 105, 116, 118\}$.
  - The sample mean is $\bar{x} = 112.8$
  - Does this data support the claim?

# Example continued

- Distribution of the test statistic
  - Under $H_0$, we know that each $x_i \sim \mathcal{N}(100, 15)$
  - The test statistic that we measure is the sample mean $\bar{x} = \frac{1}{9}\sum_{i=1}^{9} x_i$

# Example continued

- Distribution of the test statistic
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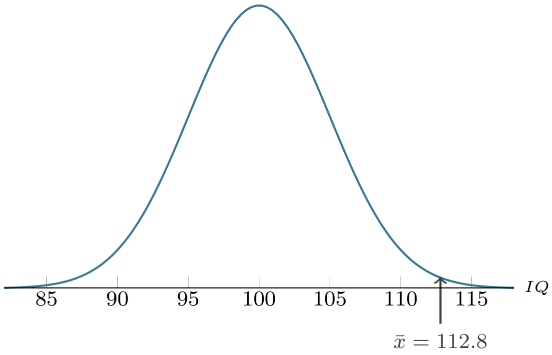
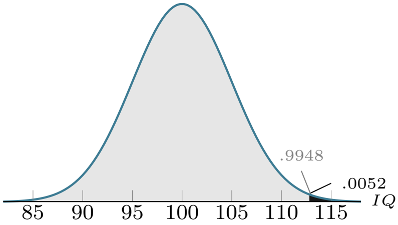
  - The test statistic that we measure is the sample mean $\bar{x} = \frac{1}{9}\sum_{i=1}^{9} x_i$
  - Under $H_0$, the distribution of $\bar{x}$ is $\mathcal{N}(100, 15/\sqrt{9})$
    - Our observation $\bar{x} = 112.8$ is quite extreme under that distribution



# General principle

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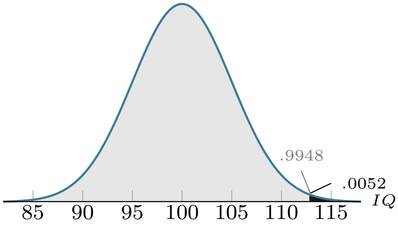


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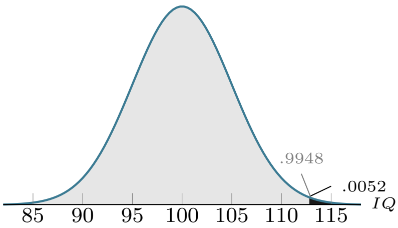


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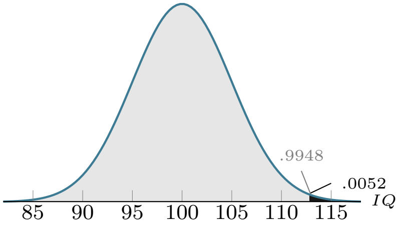


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- Compare $p$ to pre-defined confidence level $\alpha$ (usually $\alpha = 0.05$); if $p < \alpha$, reject $H_0$
- With $\alpha = 0.01$, would we reject $H_0$ in this case?

# Summary of example

- We just used a so-called $Z$-test
- $H_0$: $\mu = \mu_0$, $H_1$: $\mu > \mu_0$
- Assumptions: $X \sim \mathcal{N}(\mu, \sigma^2)$ , with known $\mu$ and $\sigma^2$

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- Assumptions: $X \sim \mathcal{N}(\mu, \sigma^2)$ , with known $\mu$ and $\sigma^2$
- Test statistic: sample mean $\bar{x}$; evaluate under $\mathcal{N}(\mu = \mu_0, s = \sigma^2/\sqrt{n})$

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- Test statistic: sample mean $\bar{x}$; evaluate under $\mathcal{N}(\mu = \mu_0, s = \sigma^2/\sqrt{n})$
- Equivalent: compute the Z-statistic: $Z = (\bar{x} - \mu_0)/s$ and evaluate cumulative distribution $\Phi(Z)$ of $Z$ under $\mathcal{N}(0, 1)$

# Summary of example

- We just used a so-called $Z$-test
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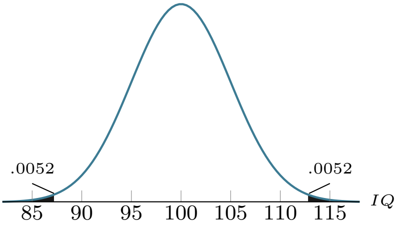
- Equivalent: compute the Z-statistic: $Z = (\bar{x} - \mu_0)/s$ and evaluate cumulative distribution $\Phi(Z)$ of $Z$ under $\mathcal{N}(0, 1)$
  - There are standard tables to look up $\Phi(Z)$ for different values of $Z$
  - Nowadays, there are standard libraries to compute $\Phi(Z)$

# Two-sided tests

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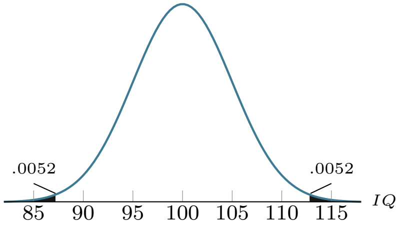


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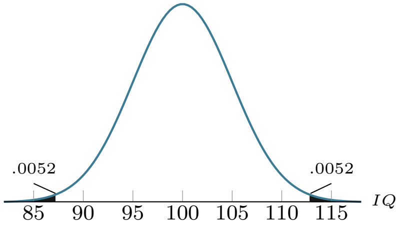


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- With $\alpha = 0.01$, would we reject $H_0$ in this case?

# General points about statistical hypothesis tests

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  - Our data is often far from normally-distributed
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- Beware (ii): if you use cross-validation, observations are not independent (you cannot apply statistical tests that assume independence)

# The Wilcoxon rank-sum test for non-normal data

- Compare the distributions of random variables $X$ and $Y$
  - based on samples $x_1, \ldots, x_n$ and $y_1, \ldots, y_m$
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  - Compute the sum of ranks of $x_i$ and of $y_j$
- Under $H_0$, the distribution of that test statistic is known
  $\rightsquigarrow$ can evaluate how extreme the observed test statistic is

# The permutation test: another test for non-normal data

- Framework for testing several types of claims
- E.g., $H_0$: $X$ and $Y$ have equal means
- Test statistic: $t = \frac{1}{n}\sum_{i=1}^{n} x_i - \frac{1}{m}\sum_{j=1}^{m} y_j$

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- The sampling distribution to compare $t$ against:
  - Put $\{x_1, \ldots, x_n\}$ and $\{y_1, \ldots, y_m\}$ into a single pool
  - $S = []$; repeat, e.g., 10 000 times
    - draw a random permutation & permute pool with it
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- $p$-value: percentile of $s$ in $S$:
  fraction of samples $s$ in $S$ with $s < t$

# Paired vs. unpaired tests

- if you have two unsorted populations (e.g., repeated measurements with different random seeds), you use an unpaired test (as discussed above)
- if you can attribute a measurement to concrete objects (e.g., measurements on different datasets), you use a paired test
  - paired test are more powerful
    (i.e., higher confidence for the same amount of data)
- Examples for paired permutation tests
  - Wilcoxon signed rank test
  - paired permutation test
    - permutation of measurement pairs (e.g., same dataset)

# Paired Permutation Test

Given:

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- ordered observations $[x_1, ...x_n]$ in $X$ (resp. in $Y$) where each observation is attributed to concrete objects
- S = []; repeat, e.g., 10 000 times
  1. $X' = []$ and $Y' = []$
  2. for each pair of observations $\langle x_i, y_i \rangle$ sample whether (i) you put $x_i$ into $X'$ and $y_i$ into $Y'$ or (ii) $x_i$ into $Y'$ and $y_i$ into $X'$.
  3. add test statistic based on $X'$ and $Y'$ to $S$

# Multiple Testing Correction

- To compare many systems, we apply statistical tests several time (once for each pair of systems)
- Each test induces some error (bounded by $\alpha$)

$\leadsto$ the error probability for $k$ tests is bounded by $1 - (1 - \alpha)^k$

| $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
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$\leadsto$ multiple testing correction

- Bonferronie testing correction: $\alpha_{\text{local}} = \alpha_{\text{global}}/k$
  - very conservative approach
  - there exist other, less conservative approaches

# Checklist for good scientific practices

Incomplete list of good scientific practices (specifically for students):

1. keep track of your code and design decisions (on all levels)
2. measure performance of randomized algorithms multiple times and show uncertainty of results
3. apply suitable statistical tests to check for significance
4. choose a metric that is relevant for the application
5. always add legends, axis labels and so on in plots
6. be aware of other research results
7. avoid peeking at your test data
    - no cherry-picking!

# Learning Goals

Now, you should be able to . . .

- explain the role of outliers in CS/ML
- compare and visualize the performance of different configurations
- compare and visualize the performance of AutoML systems
- explain and correctly apply statistical hypothesis tests

# Literature [These are links]

- [P. Langley 1988. Machine Learning as an Experimental Science]
- [C. Drummod 2006. Machine Learning as an Experimental Science (Revisited)]
- [J. Demsar 2006. Statistical Comparisons of Classifiers over Multiple Data Sets]
- [Wilson et al. 2014. Best Practices for Scientific Computing]
- [Wilson et al. 2017. Good enough practices in scientific computing]