# Sequential Benchmarking

Manuel J. A. Eugster

Institut für Statistik Ludwig-Maximiliams-Universität München

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## **Benchmark experiments**

### Data generating process:

Given a data generating process DGP, we draw B independent and indentically distributed learning samples:

$$\mathfrak{L}^{1} = \{z_{1}^{1}, \dots, z_{n}^{1}\} \sim DGP$$
$$\vdots$$
$$\mathfrak{L}^{B} = \{z_{1}^{B}, \dots, z_{n}^{B}\} \sim DGP$$

(\*) Following Hothorn, Leisch, Zeileis, and Hornik (2005).

#### Candidate algorithms:

There are K > 1 algorithms  $a_k$  (k = 1, ..., K) with the function  $a_k(\cdot | \mathfrak{L}^b)$  the fitted model on the learning sample  $\mathfrak{L}^b$ :

$$\mathsf{a}_k(\cdot \mid \mathfrak{L}^b) \sim \mathcal{A}_k(\mathsf{DGP})$$

#### Performance measure:

Performance of algorithm  $a_k$  when provied with the learning sample  $\mathfrak{L}^b$  is measured by a scalar function p:

$$p_{kb} = p(a_k, \mathfrak{L}^b) \sim \mathcal{P}_k = \mathcal{P}_k(DGP)$$

### Inference:

Given the K different random samples  $\{p_{k1}, \ldots, p_{kB}\}$  with B iid samples drawn from the distributions  $\mathcal{P}_k(DGP)$  the null hypothesis of interest for most problems is:

$$H_0$$
 :  $\mathcal{P}_1 = \cdots = \mathcal{P}_K$ 

#### Test procedure:

An algorithm  $a_i$  is better than an algorithm  $a_j$  with respect to a performance measure p and a functional  $\phi$  iff  $\phi(\mathcal{P}_i) < \phi(\mathcal{P}_j)$  $(i, j \in \{1, \dots, K\}).$ 

$$T \begin{cases} H_0: & \phi(\mathcal{P}_1) = \dots = \phi(\mathcal{P}_K) \\ H_1: & \exists i, j: \phi(\mathcal{P}_i) \neq \phi(\mathcal{P}_j) \end{cases}$$

- In most benchmark experiments *B* is a **freely chosen** number (often specified depending on the algorithms' runtime).
- Benchmark experiments are considered as **fixed-sample** experiments; hypotheses of interests are tested using a test *T* at the end.
- The nature of benchmark experiments is sequential.



### Sequential benchmarking:

Execute test T successively on the accumulating data.

This enables

- (1) to monitor the benchmark experiment, and
- (2) to make a decision to stop or to go on.

Sequen	
Execute	Do
This su	<b>1.</b> Draw learning sample $\mathfrak{L}^b$ .
i nis ena	<b>2.</b> Measure performance $p_{kb}$ of the
(1) to	$k=1,\ldots,K$ candidate algorithms.
<b>(2)</b> to	<b>3.</b> Execute test procedure $T$ on the $K$
	performance estimations $\{p_{k1},\ldots,p_{kb}\}$ .
	While no decision for a given $\alpha$ (and $b \leq B$ ).

# Exemplar benchmark experiment

(1) Pima Indians Diabetes database; (2) Linear discriminant analysis, Support vector machines (not tuned!); (3) Misclassification; (4) B = 100; (5) Friedman test procedure,  $\alpha = 0.05$ ;



# Monitoring

Scenario 1 – Clear situation:



(\*) LDA versus SVM.

### Scenario 2 – Not so clear situation:



<sup>(\*)</sup> SVM versus Random forest.

### Scenario 2 – Not so clear situation:



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### Scenario 3 – Undecidable situation:



<sup>(\*)</sup> SVM versus SVM.

### Scenario 3 – Undecidable situation:



<sup>(\*)</sup> SVM versus SVM.

## Interpretation

### Point of consecutively significance:

$$\Pi_{\text{Scenario 1}} = 13, \ \Pi_{\text{Scenario 2}} = 165, \ \Pi_{\text{Scenario 3}} = \infty$$

Measure of "how big is the difference" - indicator for relevance?

# **Decision making**

**Goal:** Execute the benchmark experiment as long as needed – either to reject  $H_o$  or to "accept" (fail to reject)  $H_0$ .

**Requirement:** Decision for an arbitrary hypothesis of interest, on the basis of an arbitrarily corresponding test procedure T and for a given significance level  $\alpha$ .



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# Analyses on accumulating data

**Sequential:** Sample observations one by one; the test is executed after each new observation – the experiment can be stopped at any point.

**Group sequential:** Sample groups of observations; the test is executed after each group – the experiment can be stopped after each group.

Adaptive: Group sequential with more flexibility, e.g., to change hypothesis, group sample size, etc.

(\*) Following Vandemeulebroecke (2008).

### Repeated significance testing:

Testing not once but multiple times causes the inflation of the probability for the error of the first kind, i.e., the probability of rejecting the global null hypothesis when in fact this hypothesis is true; known as **alpha inflation**.

(\*) First addressed by Armitage, McPherson, and Rowe (1969).

## **Recursive combination tests**

Adaptive test procedure based on the recursive application of two-stage combination tests; and a p-value function to combine p-values from two separate stages.

(\*) Defined by Brannath, Posch, and Bauer (2002).

#### Two-stage combination tests:

Test a one-sided null hypothesis  $H_0$  at level  $\alpha$  using two stages.

Stage 1: Sample size  $n_1$ , early decision boundaries  $a_0$  and  $a_1$  $(0 \le \alpha_1 < \alpha < \alpha_0 \le 1)$ , *p*-value  $p_1$ .

$$\mathsf{Decision} = \begin{cases} p_1 \leq \alpha_1, & \text{reject } H_0 \\ p_1 > \alpha_0, & \text{accept } H_0 \\ \alpha_1 < p_1 \leq \alpha_0, & \text{perform Stage 2} \end{cases}$$

Stage 2: Sample size  $n_2$ , combination function  $C(\cdot, \cdot)$  with corresponding  $c(\cdot, \cdot, \cdot)$ , *p*-value  $p_2$ .

$$\mathsf{Decision} = \begin{cases} C(p_1, p_2) \leq c(\alpha, \alpha_1, \alpha_0), & \mathsf{reject} \ H_0 \\ \mathsf{otherwise}, & \mathsf{undecidable} \end{cases}$$

Overall p-value:

$$q(p_1, p_2) = \begin{cases} p_1, & \text{if } p_1 \leq \alpha_1 \text{ or } p_1 > \alpha_0 \\ \alpha_1 + \int_{\alpha_1}^{\alpha_0} \int_0^1 \mathbb{1}_{[C(x,y) \leq C(p_1, p_2)]} dy dx, & \text{otherwise} \end{cases}$$

### **Recursive combination tests:**



#### Example – Fisher's weighted product test:

$$C(p_1, p_2) = p_1^w \cdot p_2, w > 0$$

For 
$$w = 1$$
:  

$$c(\alpha, \alpha_1, \alpha_0) = \frac{\alpha - \alpha_1}{\ln \alpha_0 - \ln \alpha_1}$$

$$q(p_1, p_2) = \begin{cases} p_1, & \text{if } p_1 \le \alpha_1 \text{ or } p_1 > \alpha_0 \\ \alpha_1 + p_1 \cdot p_2 \cdot (\ln \alpha_0 - \ln \alpha_1), & \text{if } p_1 \in (\alpha_1, \alpha_0] \text{ and } p_1 \cdot p_2 \le \alpha_1 \\ p_1 \cdot p_2 + p_1 \cdot p_2 \cdot (\ln \alpha_0 - \ln p_1 \cdot p_2), & \text{if } p_1 \in (\alpha_1, \alpha_0] \text{ and } p_1 \cdot p_2 \ge \alpha_1 \end{cases}$$

Recursive stopping boundaries:

$$\alpha_{1,t} < \alpha_t(p_1,\ldots,p_{t-1}) \le \alpha_{0,t}$$
$$\alpha_t(p_1,\ldots,p_{t-1}) = c_{t-1}/p_{t-1}$$

#### Scenario 2 – Not so clear situation:





# So ...

### Monitoring:

• Point of consecutively significance.

### Decision making:

- "Interactive" interim phase or sound automatization?
- Advantage in real-world benchmark experiments?
- Green Benchmarking!

http://CRAN.R-project.org/package=benchmark

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