The Design and Analysis of Benchmark Experiments – Part II: Analysis

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Benchmark Experiments

A comparison of algorithms with respect to certain performance measures is of special interest in the following problems

- select the best out of a set of candidates,
- identify groups of algorithms with the same performance,
- test whether any useful structure is inherent in the data or
- demonstrate equivalence of two algorithms.

Illustrating Example

Stabilization of a Linear Discriminant Analysis (LDA) by using low-dimensional Principal Component (PC-q) scores (Läuter, 1992; Läuter et al., 1998; Kropf, 2000) for Glaucoma diagnosis (Hothorn et al., 2003; Mardin et al., 2003).

Laser-scanning images from 98 patients and 98 controls ($n = 196$), $p = 62$ numeric input variables.

Data generating process: The empirical distribution function $\hat{Z}_n$.

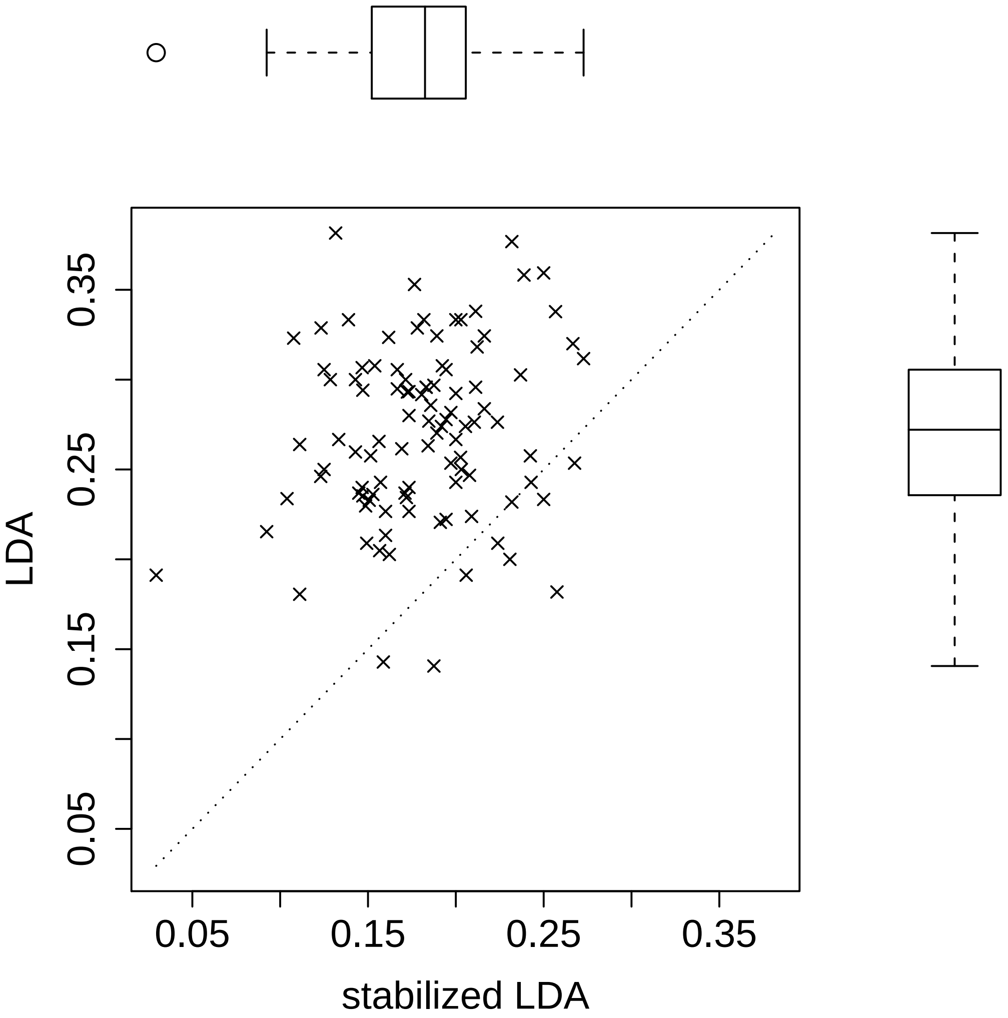
Performance measure: Out-of-bootstrap misclassification error.

Experiment

Question: Does the performance distribution $\hat{P}_{\mathsf{LDA}}(\hat{Z}_n)$ of a LDA using the original p input variables differ from the performance distribution $\hat{P}_{\mathsf{sLDA}}(\hat{Z}_n)$ of a stabilized LDA?

Experiment: Draw B samples $\mathcal{L}^b$ from the data generating process $\hat{Z}_n$ and compute $\hat{p}_{\mathsf{LDA},b}$ and $\hat{p}_{\mathsf{sLDA},b}$, the misclassification errors evaluated on the out-of-bootstrap observations.

Benchmark Experiments



Inference

$$H_0 : \hat{P}_{\mathsf{LDA}}(\hat{Z}_n) = \hat{P}_{\mathsf{sLDA}}(\hat{Z}_n)$$

Problem: We do not know anything about the performances, except that parametric assumptions are surely not appropriate.

Solution: Dispose the performance distributions by conditioning on all permutations of the labels for each bootstrap sample.

Inference

$$T = \sum_{b=1}^{B} \hat{p}_{\textsf{LDA},b} - \hat{p}_{\textsf{sLDA},b} = B(\bar{p}_{\textsf{LDA},\cdot} - \bar{p}_{\textsf{sLDA},\cdot})$$

The conditional distribution of the test statistic T under the conditions described by H_0 can be used to construct a permutation test.

In our case, the P-value based on the asymptotic conditional distribution is $p < 0.001$ and therefore H_0 can be rejected.

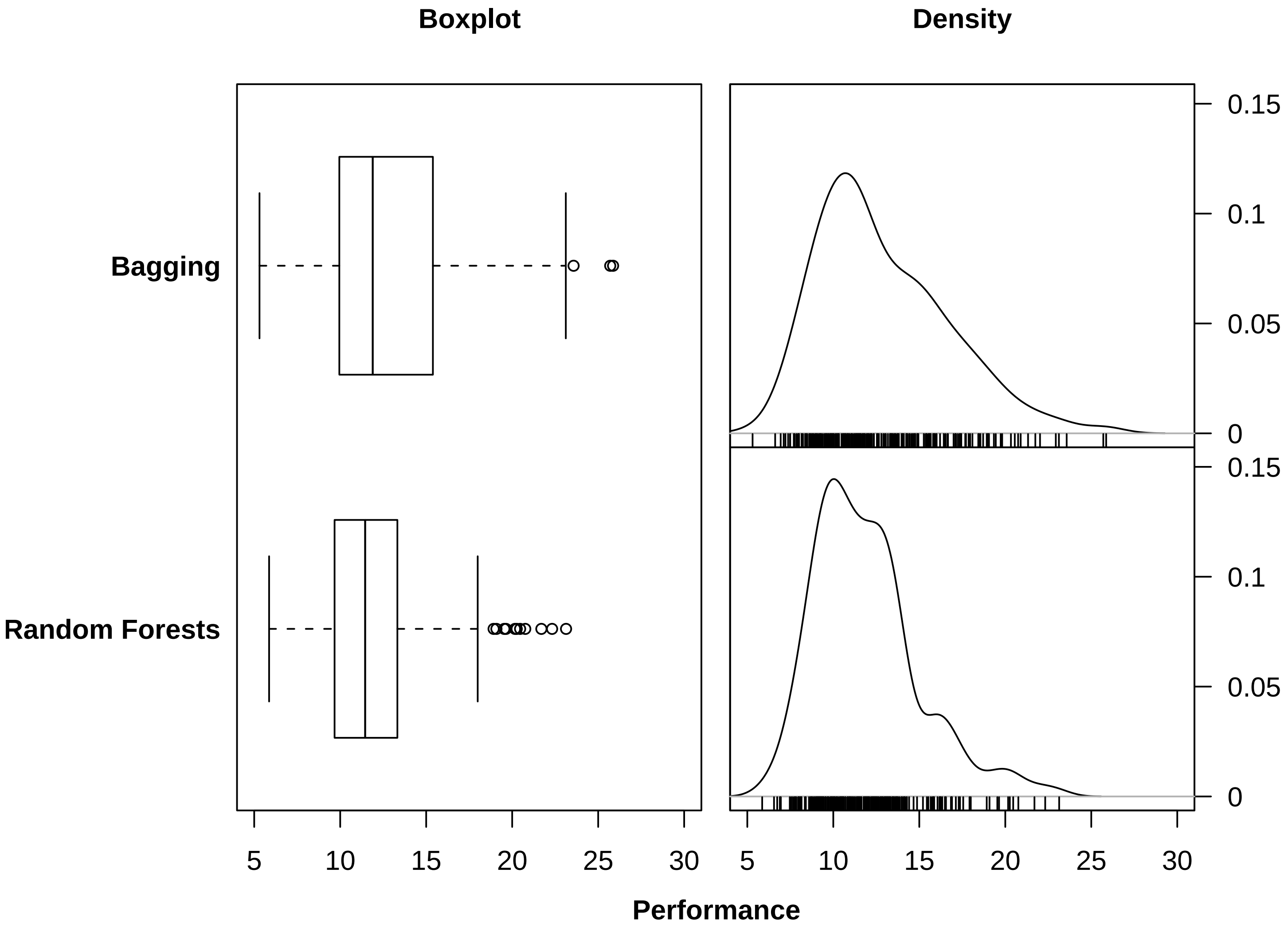
A Regression Example

Exactly the same methodology can be applied to regression problems with univariate numeric responses. Example: Can additional randomness via Random Forests improve Bagging for the Boston Housing data?

House prices for $n = 506$ houses near Boston, $p = 13$ input variables.

Data generating process: The empirical distribution function $\hat{Z}_n$.

Performance measure: Out-of-bootstrap mean squared error.


Boxplot
Density
Bagging
Random Forests
5
10
15
20
25
30
0.15
0.1
0.05
0
Performance

Inference

The null-hypothesis of equal performance distributions can be rejected (P-value < 0.001).

The estimated difference of the mean square error of Bagging compared to Random Forests is 0.969 with confidence limits $(0.633, 1.305)$.

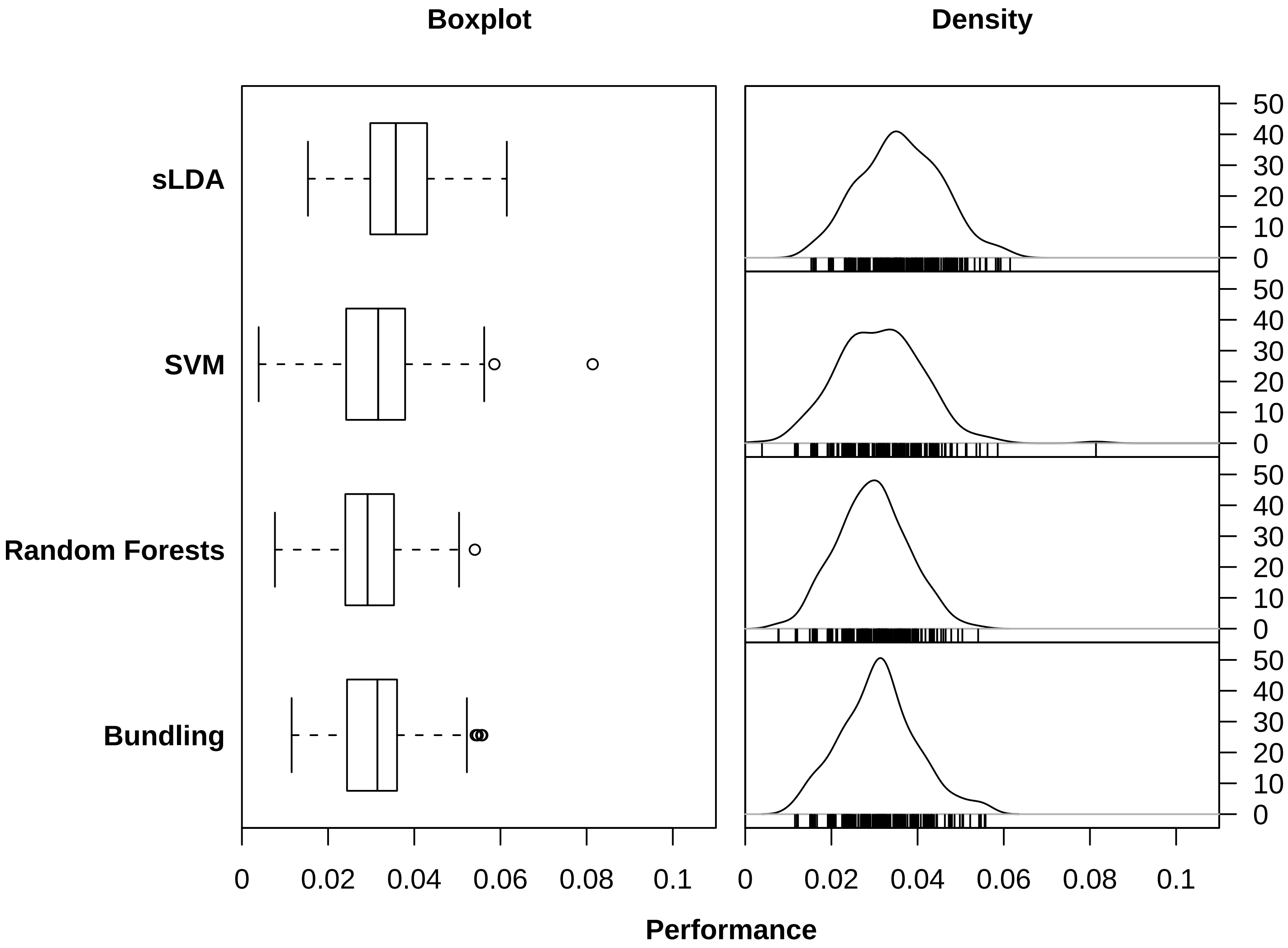
Comparison of Multiple Algorithms

When multiple algorithms are under test, we are interested in both a global test and a multiple test procedure showing where the differences, if any, come from. Example: Breast Cancer data with tumor classification from $n = 699$ observations with $p = 9$ inputs.

Comparison of sLDA, Support Vector Machine, Random Forests and Bundling (Hothorn and Lausen, 2003).

Data generating process: The empirical distribution function $\hat{Z}_n$.

Performance measure: Out-of-bootstrap misclassification error.


Boxplot
Density
sLDA
SVM
Random Forests
Bundling
0
0.02
0.04
0.06
0.08
0.1
0
10
20
30
40
50
Performance

Inference

Again, the global hypothesis

$$H_0 : \hat{P}_1(\hat{Z}_n) = \ldots = \hat{P}_K(\hat{Z}_n)$$

can be rejected (P-value < 0.001).

Problem: Which differences 'cause' the rejection of H_0?

Solution: One can avoid complicated closed testing procedures by computing confidence intervals after mapping the B-block design into a K-sample problem via alignment (Hájek et al., 1999).

Alignment

When we look at the performance measure of algorithm k in the bth sample drawn from the data generating process, we might want to write

$$p_{kb} = \mu + \beta_b + \gamma_k + \varepsilon_{kb}$$

where μ corresponds to the performance of the Bayes-rule, β_b is the error induced by the b sample and γ_k is the error of the kth algorithm, the quantity we are primarily interested in, ε indicates an error term.

Alignment (cont'd)

The aligned performance measures $p^\star_{kb}$ cover the difference of the performance of the kth algorithm from the average performance of all K algorithms:

$$p^\star_{kb} = p_{kb} - \bar{p}_{\cdot b} = (\gamma_k + \varepsilon_{kb}) - \frac{1}{K}\sum_{k=1}^{K}(\gamma_k + \varepsilon_{kb})$$

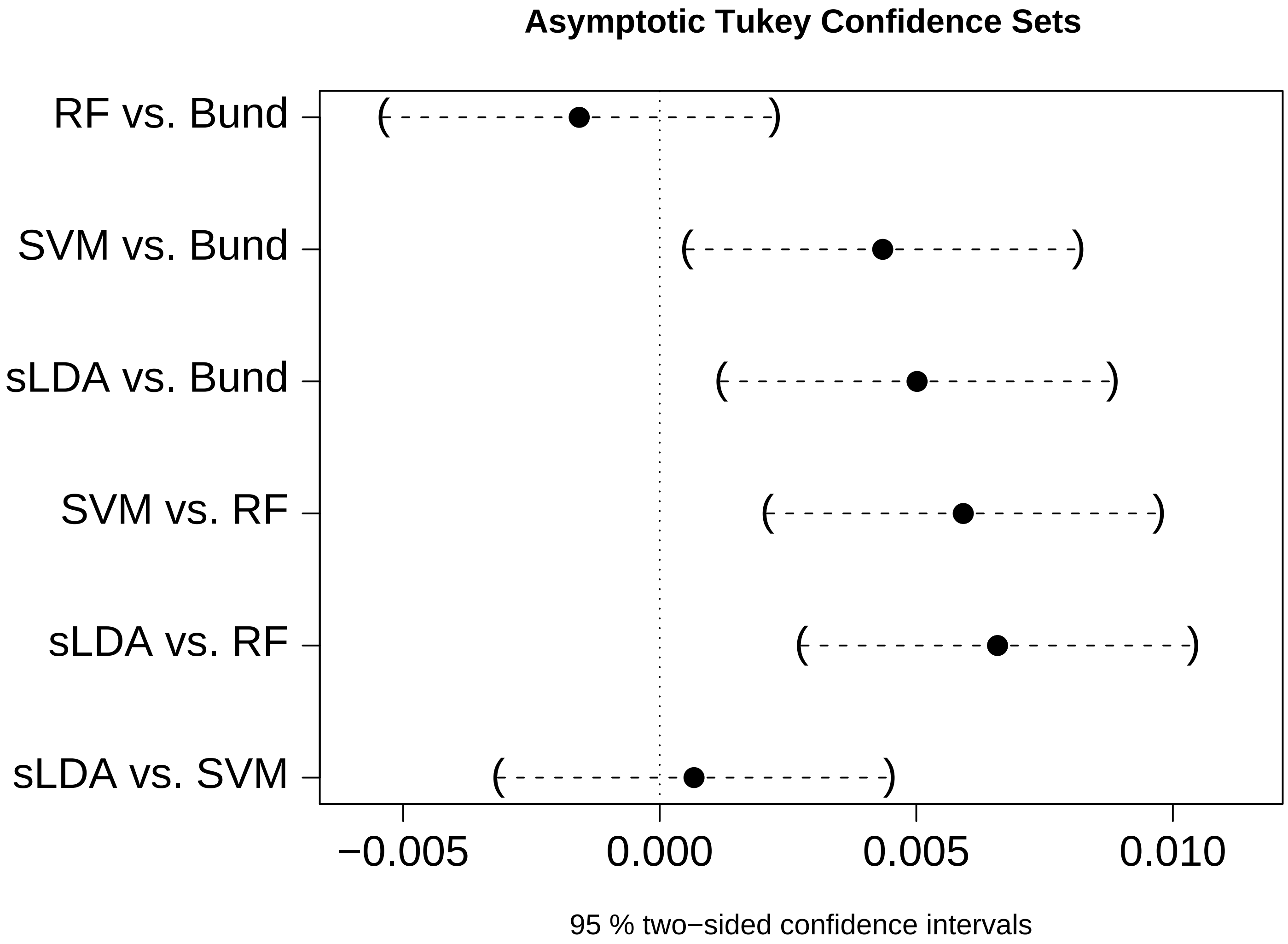
For classification problems, $p^\star_{k_1 b} - p^\star_{k_2 b}$ is the difference of the misclassification error.

Alignment (cont'd)

The aligned random variables are not independent but exchangeable for each of the b samples and are independent between samples.

Therefore, (asymptotic) permutation test procedures can be used to assess the deviations from the global null-hypothesis.

For example, asymptotic simultaneous confidence intervals for Tukey-contrasts can be used for an all-pair comparison of the K algorithms under test.


Asymptotic Tukey Confidence Sets
RF vs. Bund
SVM vs. Bund
sLDA vs. Bund
SVM vs. RF
sLDA vs. RF
sLDA vs. SVM
−0.005
0.000
0.005
0.010
95 % two−sided confidence intervals

Classical Tests?

We advocate usage of permutation tests, but what about more classical tests?

Consider a paired comparison of sLDA vs. SVM for the Breast Cancer data:

- Permutation test: $T = 1.488, \quad p = 0.776$
- t test: $t = 0.284, \quad p = 0.777$
- Wilcoxon signed rank test: $W = 18216, \quad p < 0.001$

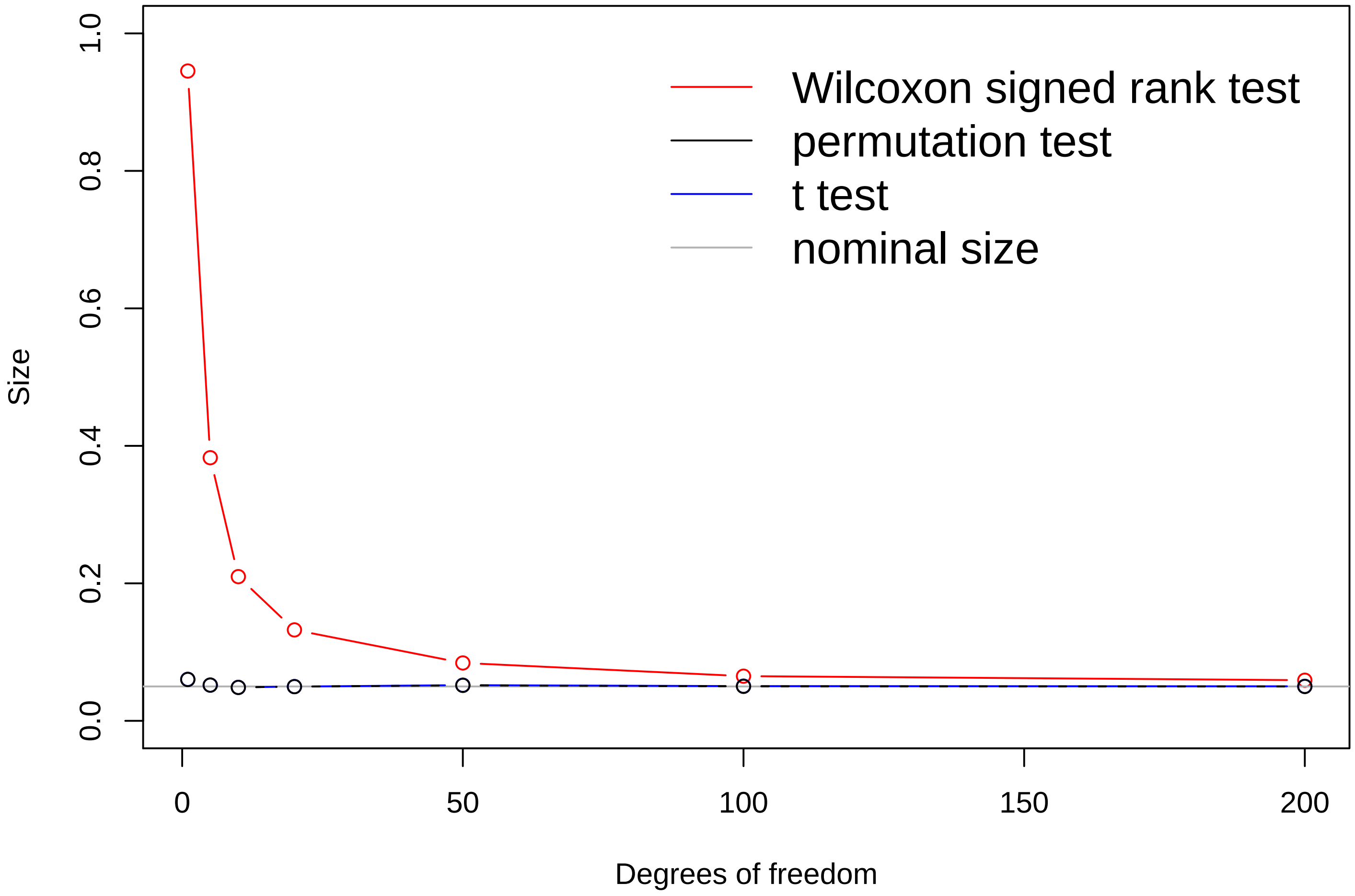
Rank Tests: A Warning

Tests like the Wilcoxon signed rank test are constructed for the null-hypothesis ‘the difference of the performance measures is **symmetrically** distributed around zero’. For non-symmetric distributions this leads to a complete desaster.

Look at $n = 500$ realizations of a skewed random variable

$$\frac{X - d}{\sqrt{2d}}$$

with expectation zero and unit variance with $X \sim \chi^2_d$.

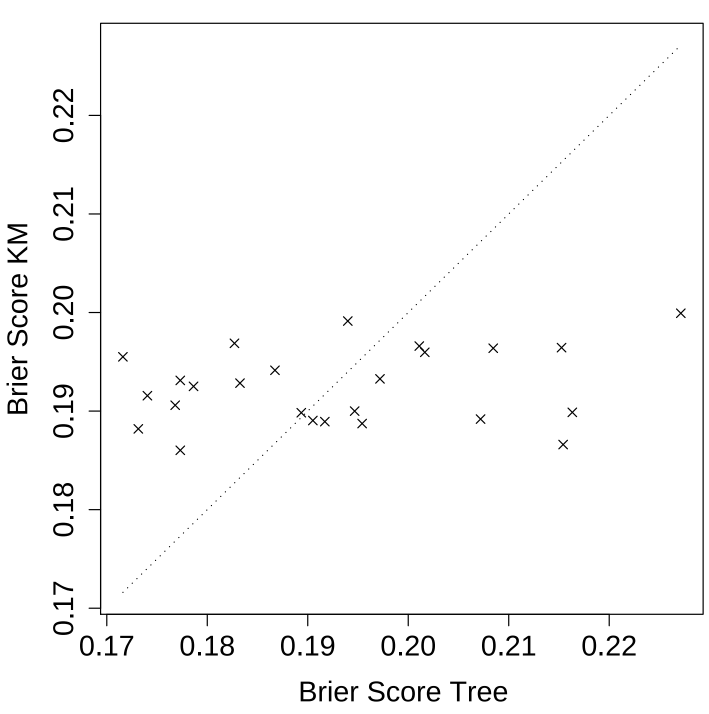

Wilcoxon signed rank test
permutation test
t test
nominal size
Size
0.0
0.2
0.4
0.6
0.8
1.0
Degrees of freedom
0
50
100
150
200

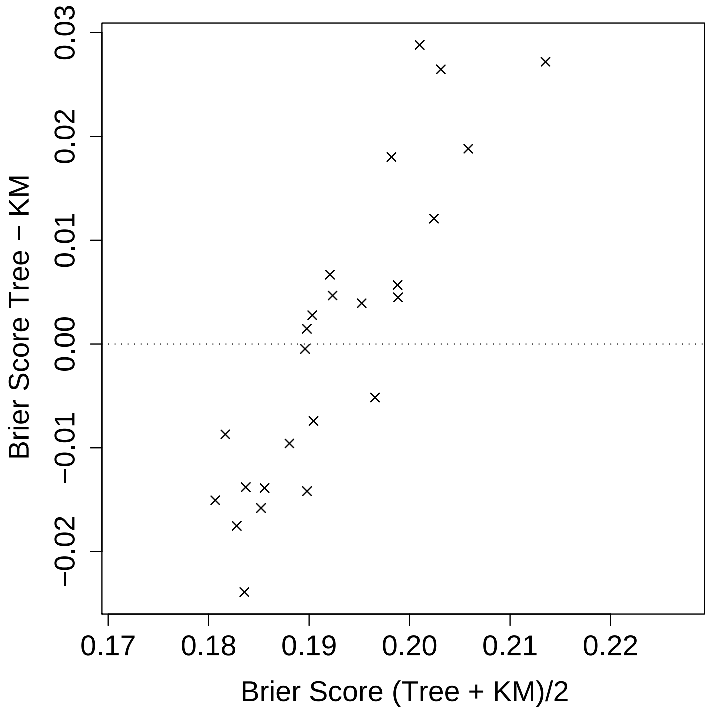
Lifetime Analysis Problems

Appropriate performance measures for censored responses are by no means obvious and still a matter of debate (Henderson, 1995; Graf et al., 1999; Molinaro et al., 2004). We use the Brier score for censored data suggested by Graf et al. (1999).

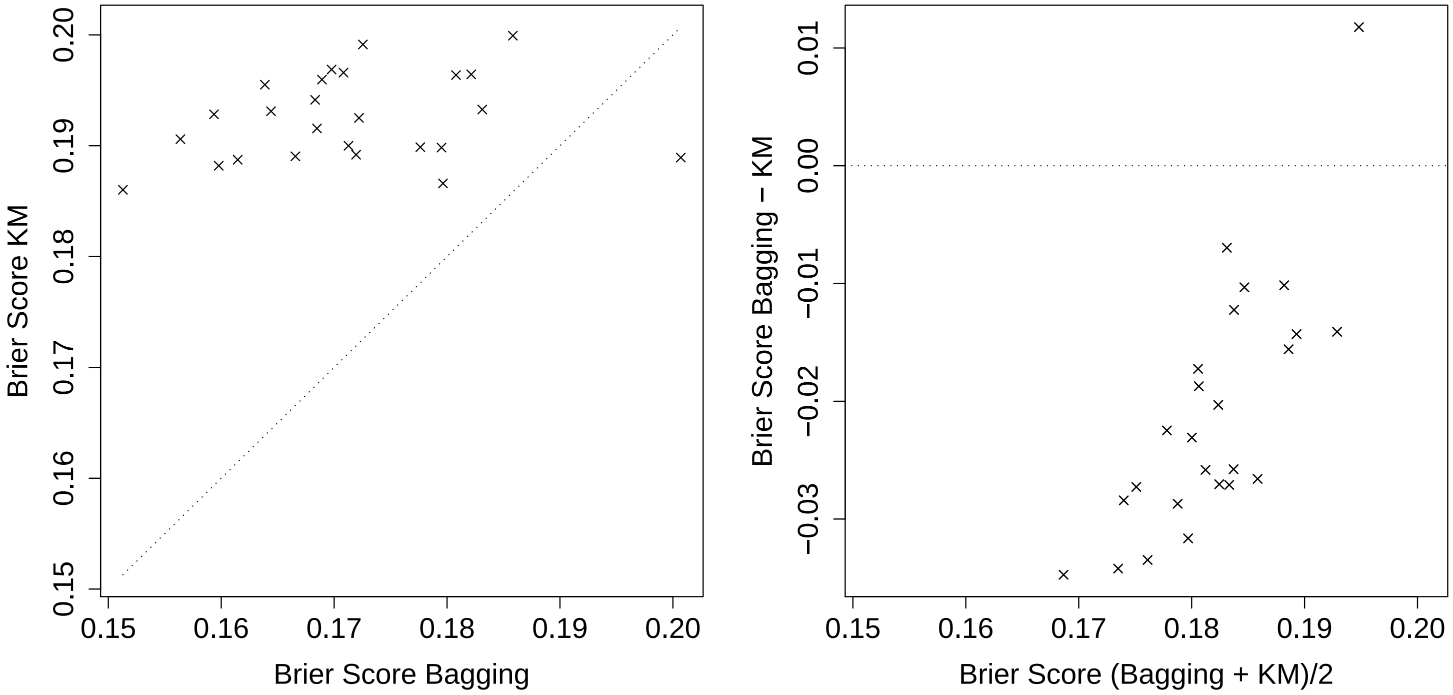
Example: Predictive performance of the Kaplan-Meier estimator, a single survival tree and Bagging of survival trees (Hothorn et al., 2004) measured for $n = 686$ women enrolled in the German Breast Cancer Study (Group 2).

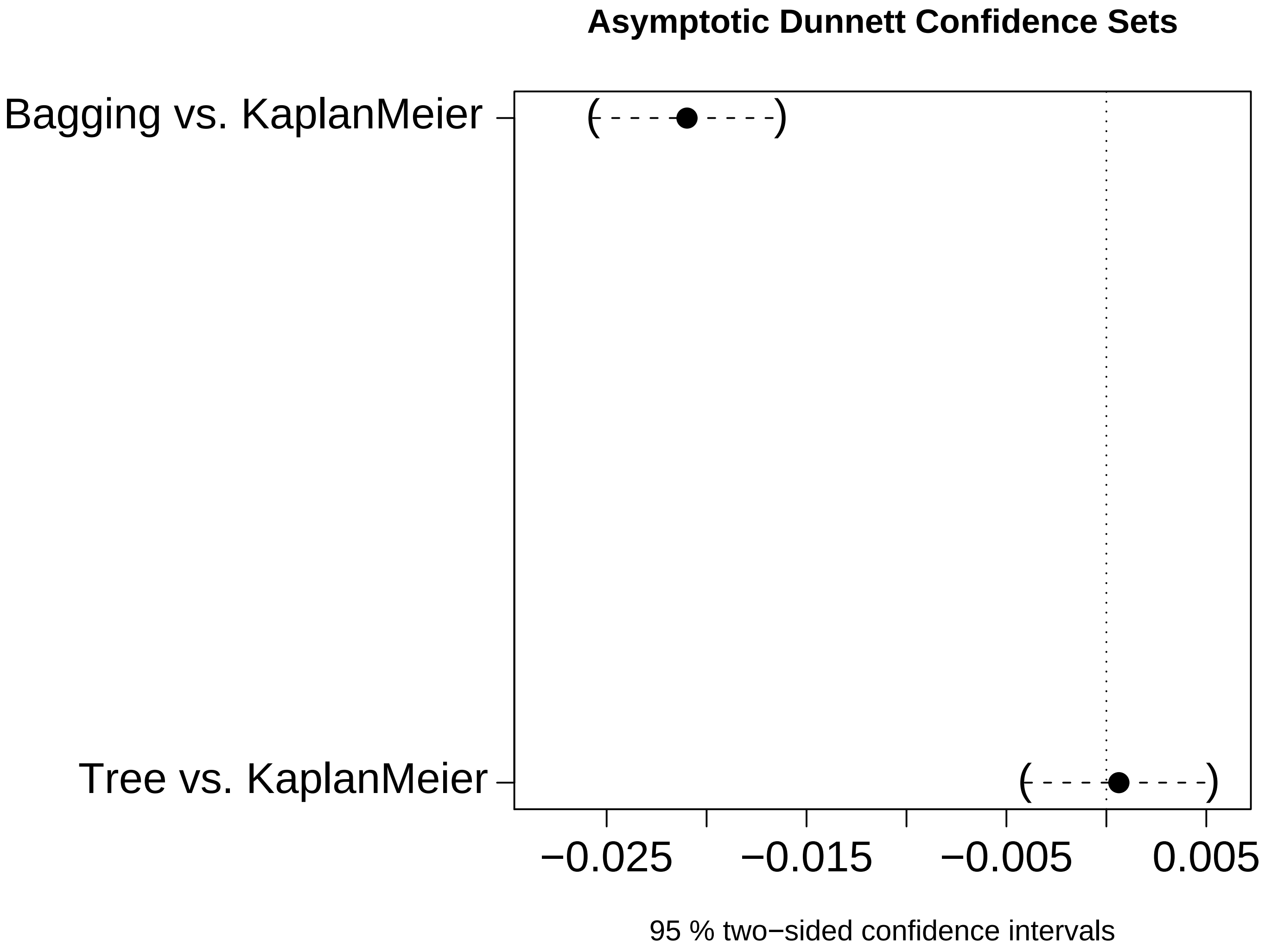
Kaplan-Meier vs. Single Tree





Kaplan-Meier vs. Bagging




Asymptotic Dunnett Confidence Sets
Bagging vs. KaplanMeier
Tree vs. KaplanMeier
−0.025
−0.015
−0.005
0.005
95 % two−sided confidence intervals

Interpretation

Predictions derived from the estimated Kaplan-Meier curve don't take any information covered by the input variables into account. A test for the hypothesis

> *there is no (detectable) relationship between the input variables and the response*

can therefore be performed by comparing the performance of the simple Kaplan-Meier curve with the performance of the best tools available for predicting survival times.

Conclusion

When comparing the performance of K algorithms it is appropriate to treat the B samples from the data generating process as blocks.

Standard statistical test procedures can be used to compare arbitrary performance measures for multiple algorithms.

Some classical parametric and non-parametric procedures are only sub-optimal, we advocate procedures based on the conditional distribution of test statistics for inference.

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