MULTIPLICITY-ADJUSTED BOOTSTRAP TILTING LOWER CONFIDENCE BOUNDS FOR CONDITIONAL PREDICTION PERFORMANCE MEASURES

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ABSTRACT

In machine learning, the selection of a promising model from a potentially large number of competing models and the assessment of its generalization performance are critical tasks that need careful consideration. Typically, model selection and evaluation are strictly separated endeavors, splitting the sample at hand into a training, validation, and evaluation set, and only compute a single confidence interval for the prediction performance of the final selected model. We however propose an algorithm how to compute valid lower confidence bounds for multiple models that have been selected based on their prediction performances in the evaluation set by interpreting the selection problem as a simultaneous inference problem. We use bootstrap tilting and a maxT-type multiplicity correction. The approach is universally applicable for any combination of prediction models, any model selection strategy, and any prediction performance measure that accepts weights. We conducted various simulation experiments which show that our proposed approach yields lower confidence bounds that are at least comparably good as bounds from standard approaches, and that reliably reach the nominal coverage probability. In addition, especially when sample size is small, our proposed approach yields better performing prediction models than the default selection of only one model for evaluation does.

1 Introduction

Many machine learning applications involve both model selection and the assessment of that model’s prediction performance on future observations. This is particularly challenging when only little data is available to perform both tasks. By allocating a greater fraction of the data towards model selection the goodness assessment gets less reliable, and allocation of a greater fraction towards goodness assessment poses the risk of selecting a sub-par prediction model. In such situations it is desirable to have a procedure at hand that resolves this problem reliably.

Recent work by [WB20] showed that it is beneficial in terms of final model performance and statistical power to select multiple models for goodness assessment in spite of the need to correct for multiplicity then. While [WB20] proposed a multiple test in such cases, we here propose a way how to compute valid lower confidence bounds for the conditional prediction performance of the final selected model. Note that reporting a confidence interval here perfectly makes sense since a point estimate for the performance does not incorporate the uncertainty of estimation from an evaluation set at all.

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Figure 1: Default evaluation pipeline, as predominantly recommended in the literature. Only a single model \( \hat{\beta}_s \) is selected for evaluation based on its validation performance \( \hat{\eta}_s \). \( \hat{\eta}_r \) is the lower confidence bound for that model’s evaluation performance.

Figure 2: Proposed evaluation pipeline. Multiple models \( s_1, \ldots, s_m \) are selected for evaluation based on their validation performances \( \hat{\eta}_{s_1}, \ldots, \hat{\eta}_{s_m} \), and a final model \( s \) is selected based on the evaluation performances \( \hat{\theta}_{s_1}, \ldots, \hat{\theta}_{s_m} \). This introduces a multiplicity problem concerning \( \hat{\theta}_{s_1}, \ldots, \hat{\theta}_{s_m} \) and an upward bias in \( \hat{\theta}_s \). We propose a lower confidence bound \( \hat{\theta}_{s,L} \) that compensates for this multiplicity and bias.
We follow the idea of [BBB+13] and interpret this post-selection inference problem as a simultaneous inference problem, controlling for the family-wise error rate

\[ P_{\theta}(\theta_i < \theta_{i,L} \text{ for any } i \in \{1, \ldots, m\}) \leq \alpha, \]

where \( \theta_i \) denotes the performance of prediction model \( i \), \( \theta_{i,L} \) denotes the corresponding lower confidence bound at significance level \( \alpha > 0 \), and \( \theta \) is the true predictive performance. With this type 1 error control, in practice, we are therefore able to answer the question whether there is a model among the competition that has prediction performance \( \theta_i \) at least as large as a reference performance \( \theta_0 \) with high confidence, no matter how and which subset of the initial competition has been selected for evaluation. In particular, since

\[ \alpha \geq P_{\theta}(\cup_{i=1}^{m} \{ \theta_i < \theta_{i,L} \}) \geq P_{\theta}(\theta_s < \theta_{s,L}) \]

for some \( s \in \{1, \ldots, m\} \), this coverage guarantee carries over to a potentially final selected model \( s \).

This might be an overly eager requirement to meet in certain cases and might lead to somewhat conservative decisions. Therefore, in order to increase power, we do not evaluate all of the candidate models, but only a promising selection of them. Or to put it the other way around: we exclude models from evaluation that are likely not going to be the best performing ones. However, in principle, it is also possible to report lower confidence bounds for the prediction performance of all the competing models that remain universally valid in the sense that they work with any measure of prediction performance (as long as it accepts weights), with any combination of prediction models even from different model classes, any model selection strategy, and are computationally undemanding as no additional model training is involved. While [BBB+13] proposed universally valid post-selection confidence bounds for regression coefficients, we are interested in a post-selection lower confidence bound for the conditional prediction performance of a model selected based on its evaluation performance.

### Conditional vs unconditional performance

We are particularly interested in the conditional prediction performance, i.e. the generalization performance of the model trained on the present sample. For that, in a model selection and performance estimation regime, the prevailing recommendation in the literature is to split the sample at hand into three parts, a training, validation, and evaluation set, cf. [GBC16], [HTF09], [JS11], [Mur12], [Ras18], and Figure 1. Depending on the specific selection rule, the training and validation set can sometimes be combined to form a learning set. For instance, this is true when cross-validation is used to identify promising models from a competition of models, based on their cross-validated prediction performance. Cross-validation using the entire sample at hand however is not a solution to our problem since it actually estimates the unconditional prediction performance, i.e. the average prediction performance of a model fit on other training data from the same distribution as the original data, cf. [BHT21], [HTF09]. There are examples in the literature how to correct for this unwanted behavior and report an estimate of the conditional performance, for instance [BHT21] and [TGB18]. Yet, we choose an approach that directly and inherently estimates the conditional performance.

### Bootstrap tilting confidence intervals

Our proposed confidence bounds are obtained using bootstrap resampling. In particular, we use bootstrap tilting, introduced by [Efr81], which is a general approach to estimate confidence intervals for some statistic \( \theta = \theta(F) \) using an i.i.d. sample \( (y_1, y_2, \ldots, y_n) \) from an unknown distribution \( F \). This statistic \( \theta \) will later be our performance estimate of choice. Different than many other bootstrap confidence intervals, bootstrap tilting estimates the distribution of \( \hat{\theta} - \theta_0 \) for some test value \( \theta_0 \). The lower confidence bound is then formed consisting of those values of \( \theta_0 \) that could not be rejected in a test of the null hypothesis \( H_0: \theta \leq \theta_0 \). This way the distribution to sample from is consistent with the null distribution. In particular, this is achieved by reducing the problem to one-parametric family \( (F_\tau)_\tau \) of distributions, where \( \tau \) is called the tilting parameter and \( F_\tau \) has support on the observed data \( \{y_1, y_2, \ldots, y_n\} \). A specific value of \( \tau \) induces nonnegative sampling weights \( p_\tau = (p_1(\tau), p_2(\tau), \ldots, p_n(\tau)) \) such that \( \sum_{i=1}^{n} p_i(\tau) = 1 \). The tilting parameter \( \tau \) is monotonically related to \( \theta \) such that a specific value of \( \tau \) corresponds to a specific value of \( \theta_0 \).

In order to find a lower confidence bound \( \theta_L \), we find the largest value of \( \tau < 0 \) such that the corresponding level \( \alpha \) test still rejects \( H_0; i.e. \theta_L \) is the largest value of \( \theta_0 \) such that, if the sample came from a distribution with parameter \( \theta_0 \), the probability of observing \( \hat{\theta} \) or an ever larger value is \( \alpha \).

\[ P_{F_\tau}(\theta \geq \hat{\theta}) = \alpha. \]  

Conceptually, for any given value of \( \tau \), we need to sample from \( F_\tau \) and check whether equation (3) holds true. This is both expensive and exposed to the randomness of repeated sampling. What we actually do is to employ an importance sampling reweighting approach as proposed by [Efr81]. This allows us to find the lower bound \( \theta_L \) using only bootstrap resamples from the observed empirical distribution \( \hat{F} \). We reweight each resample \( b = 1, \ldots, B \)
Figure 3: Bootstrap tilting confidence bound estimation. The blue distribution represents $\hat{F}$, the yellow one $\hat{F}_\tau$. Bootstrap tilting finds a value for $\tau$ such that the probability under $\hat{F}_\tau$ to observe at least $\hat{\theta}$ is $\alpha$. The associated value $\hat{\theta}_L$ of $\theta$ under $\hat{F}_\tau$ is the desired lower confidence bound.

with the relative likelihood $W_b(\tau) = \prod_{i=1}^{n} p_i(\tau) / \prod_{i=1}^{n} n^{-1}$ of the resample under $p_\tau$-weighted sampling relative to ordinary sampling with equal weights $n^{-1}$, and calibrate the tilting parameter $\tau < 0$ such that the estimated probability of observing at least $\hat{\theta}$ under the tilted distribution $F_\tau$ is $\alpha$,

$$\alpha = P_{F_\tau}(\theta(\hat{F}^*) \geq \hat{\theta}) = B^{-1} \sum_{b=1}^{B} W_b(\tau) I\{\hat{\theta}^*_b \geq \hat{\theta}\},$$

where $\hat{F}^*$ is the resampling empirical distribution. Then the value of the statistic $\theta$ that corresponds to that calibrated value of $\tau$ and the respective sampling weights $p_\tau$ is the desired lower confidence bound $\hat{\theta}_L = \theta(p_\tau)$. Figure 3 illustrates this idea.

The tilting approach does not work if $y_1 = \ldots = y_n$ because then $p_1(\tau) = \ldots = p_n(\tau)$ for any $\tau$ and the empirical distribution cannot be tilted. This can especially be an issue in binary classification, when the model always predicts one of the classes. There are options to deal with this that render the approach only more conservative. For instance, we could randomly disturb one of the $y_i$ or, in a classification setting, alter the class prediction of that $y_i$ that has the smallest probability to fall into the specific class.

Bootstrap tilting is known to be second-order correct and to work well for a single model, when no model selection is involved, cf. [DR90] and [Hes99], respectively. However, in our proposed pipeline, multiple models are being evaluated, cf. Figure 2. Thus, we modify the bootstrap tilting routine and incorporate a maxT-type multiplicity control, which is a well-known standard approach in simultaneous inference, cf. for example [Dic14]. To the best of our knowledge, this is the first time that bootstrap tilting is extended to simultaneous inference and applied in a machine learning evaluation setup. Our approach enables us to simultaneously evaluate the conditional performances of multiple models and provide valid confidence bounds for them and in particular one for the final selected model.

In the following, we consider a binary classification problem where a potentially large number $r$ of candidate models have already been trained and a number of promising models $s_1, \ldots, s_m$ have already been selected for evaluation, based on their validation performances $\hat{\eta}_{s_1}, \ldots, \hat{\eta}_{s_m}$ and following some selection rule. We call this multitude of models selected for evaluation to be the set of preselected models. In addition, we suppose that retraining of the preselected models on the entire learning data has already been performed, yielding models $\hat{\beta}_{s_1}, \ldots, \hat{\beta}_{s_m}$. Also, suppose that the associated performance estimates $\hat{\theta}_{s_1}, \ldots, \hat{\theta}_{s_m}$ have been obtained based on the predictions from the hold-out evaluation set, and a final model $s \in \{s_1, \ldots, s_m\}$ has been selected due to its evaluation performance $\hat{\theta}_s$ following some (other) selection rule.

Section 2 has all the details to our proposed method. In Section 3 we show a selection of results from our simulation experiments and a complete presentation can be found in the Supplement Document. We apply our proposed approach on a real data set in Section 4. Our presentation ends with a discussion in Section 5.
2 Method

2.1 Setup, model training, and selection

For brevity, let \( j = 1, \ldots, m \) denote the preselected models instead of \( s_1, \ldots, s_m \) and let \( s \in \{1, \ldots, m\} \) denote the final selected model, i.e. the model with the most promising evaluation performance \( \hat{\theta}_s \), which is a function of that model’s evaluation predictions \( \hat{y}_{1s}, \hat{y}_{2s}, \ldots, \hat{y}_{ns} \), where \( n \) is the size of the evaluation set at hand. Note that this estimate \( \hat{\theta}_s \) of generalizing prediction performance is subject to selection bias and therefore overly optimistic. To compute our proposed multiplicity-adjusted bootstrap tilting lower confidence bound we only need these predictions \( \hat{y}_{ij} \) from all of the competing preselected models \( j = 1, \ldots, m \) in the evaluation set and the associated true class labels \( y_{is}, i = 1, \ldots, n \). For instance, in case the performance measure of interest is prediction accuracy, the predictions are the predicted class labels; in case of the area under the receiver operating characteristic curve (AUC), they may be class probabilities.

2.2 Bootstrap resampling

Our proposed confidence bounds come from bootstrap tilting with a multiplicity adjustment due to the simultaneous evaluation of multiple candidate models. The general idea is to first estimate the tilted distribution under hypothetical values for the performance measure, and then to adjust for multiplicity in order to finally calibrate the tilting parameter \( \tau \) accordingly. Note that no additional model training is needed here, once the models are preselected and retrained, values for the performance measure, and then to adjust for multiplicity in order to finally calibrate the tilting parameter \( \tau \) accordingly. No additional model training is needed here, once the models are preselected and retrained.

2.3 Tilting

The first of these empirical cumulative distribution functions stems from the estimation of conventional bootstrap tilting confidence intervals. From the bootstrap performance estimates \( \hat{\theta}_{bs} \) of the final selected model \( s \), we estimate the empirical tilted cumulative distribution function

\[
\hat{F}_{s, \tau}^*(x) = \frac{1}{B} \sum_{b=1}^{B} W_b(\tau) I\{\hat{\theta}_{bs} \leq x\},
\]

where \( I \) is the indicator function, with importance sampling weights \( W_b(\tau) \), as introduced in Section 1. We plug the observed performance \( \hat{\theta}_s \) of the final selected model \( s \) into \( \hat{F}_{s, \tau}^* \) to get \( \hat{F}_{s, \tau}^*(\hat{\theta}_s) \). Later, we plug this value into another distribution function that we derive next. This will provide the multiplicity correction that we need to account for the evaluation of multiple models.

2.4 Multiplicity correction and calibration

Since the performance estimates \( \hat{\theta}_{bs} \) all come from different and not necessarily comparable models, we need to transform them appropriately to bring them to a comparable scale and compute a multiplicity-adjusted (1 minus) \( p \)-value that can be used later on to calibrate the tilting parameter \( \tau \) and finally obtain the desired lower confidence bound. For each of the models \( j \), we estimate the empirical cumulative distribution function

\[
\hat{F}_j^*(x) = \frac{1}{B} \sum_{b=1}^{B} I\{\hat{\theta}_{jb} \leq x\}
\]

from the bootstrap performance estimates \( \hat{\theta}_{jb} \). Plugging these into \( \hat{F}_j^* \) for each \( j \) yields transformed bootstrap performance estimates \( \hat{u}_{bj}^* \) that are now uniformly distributed on the unit interval. Similar to a maxT multiplicity correction, for each bootstrap resample \( b \), among the transformed estimates \( \hat{u}_{bj}^* \), we now identify the maximum estimate \( \hat{u}_{b, \text{max}}^* = \max_{j=1}^{m} \hat{u}_{bj}^* \). From these maximum values, we estimate

\[
\hat{F}_{\text{max}}^*(x) = \frac{1}{B} \sum_{b=1}^{B} I\{\hat{u}_{b, \text{max}}^* \leq x\}
\]

(5)
2.5 Lower confidence bound

In the previous paragraphs, we estimated two empirical cumulative distribution functions, \( \hat{F}_{s,\tau}^* \) and \( \hat{F}^{\text{max}}_\tau \) in equations (4) and (5), respectively. The former estimates the tilted cumulative distribution function while the latter corrects for multiplicity. We next bring those two together and state the calibration task to obtain a conditional lower confidence bound for the performance of the final selected model \( s \) from our proposed multiplicity-adjusted bootstrap tilting approach: Find a value of the tilting parameter \( \tau < 0 \) such that

\[
\hat{F}^{\text{max}}_\tau[\hat{F}_{s,\tau}^*(\hat{\theta}_s)] = 1 - \alpha.
\]  

Once this specific value for \( \tau \) has been found, we finally obtain the desired lower confidence bound via

\[
\hat{\theta}_{s,L} = \theta(\hat{F}_{s,\tau}^*).
\]

We implemented this numerically as a root-finding problem which calibrates the tilting parameter \( \tau \) conservatively, i.e. equation (6) holds with \( \geq \). An R implementation of our proposed confidence bounds can be accessed via a public GitHub repository at https://github.com/pascalrink/mabt. It is able to compute our proposed confidence bounds for the prediction accuracy and the AUC of a prediction model.

Figure 4 illustrates our proposed approach. In summary, we estimate a bootstrap tilting confidence bound using an adjusted significance level due to the maximum distribution \( \hat{F}^{\text{max}}_\tau \) of all the preselected prediction models \( j = 1, \ldots, m \). This yields simultaneous confidence bounds \((\hat{\theta}_{1,L}, \ldots, \hat{\theta}_{m,L})\) for all the preselected models \( j \), i.e. equation (1) holds. This way, due to equation (2), we obtain a valid confidence bound for the prediction performance of any model \( j = 1, \ldots, m \) and hence a valid confidence bound \( \hat{\theta}_{s,L} \) for the selected model \( s \).

3 Simulation experiments

We now investigate the goodness of our proposed confidence bounds in extensive simulation experiments and compare them to existing standard approaches in terms of four aspects: coverage probability, size of lower confidence bound,
true performance of the final selected model, and the distance between the true performance and the lower bound, which we call rightness for brevity. We expect our procedure to produce models with better true predictive performance than standard methods due to the gainful way we select models for evaluation (cf. Figure 2) in comparison to the default pipeline (cf. Figure 1). On the other hand, due to the present multiplicity that we need to account for, the question is if this reflects in larger lower confidence bounds, as this is the main quantity when reporting. In other words, there is no real advantage to have found a better prediction model if we are unable to identify it as such.

The R code used for our simulation experiments and for all the associated figures can be found in a publicly accessible GitHub repository at https://github.com/pascalrink/mabt-experiments.

3.1 Setup

3.1.1 Data generation

Using a standard 50%/25%/25% split for the samples sizes of 200 and 400 observations for prediction accuracy and, because it is a more complex measure, 400 and 600 observations for the AUC, respectively, we sample the training, validation, and evaluation data as well as another larger data set of 20,000 observations all from the same distribution. The latter serves as a ground truth from which we derive the true model performances. We consider two different setups how to generate the features and how to get the true class labels from them. They represent different data complexities in some way. Nonetheless, both setups lead to balanced classes.

Case A In the first, simpler, and somewhat synthetic case, we draw uncorrelated random numbers from the standard normal distribution and put them into the feature matrix \( X = (x_i) \) with columns \( x_i \). We specify a sparse true coefficient vector \( \beta \) with only 1\% non-zero coefficients and obtain the true class labels using the inverse logit function and a vector of uncorrelated observations \( u_i \) that are uniform on the unit interval,

\[
y_i = \mathbb{I}\left\{ \frac{1}{1 + \exp(-x_i \beta)} \geq u_i \right\}.
\]

Specifically, we draw 1000 features and choose \( \beta = c \cdot (1, 1, \ldots, 1, 0, 0, \ldots, 0) \) to have only 10 nonzero entries, with signal strength \( c = 2 \).

Case B Here we use the twoClassSim R function from the caret R package, cf. [Kuh08]. As to the true class labels, this function generates a feature matrix that includes linear effects, non-linear effects, and noise variables, each both uncorrelated and correlated with constant correlation \( \rho = 0.8 \), and 1\% mislabeled data. We try to mimic a more complex case here, which is closer to real-world applications than case A.

3.1.2 Model training

As to model training, we train lasso models with 100 equidistant values for the tuning parameter \( \lambda \) between zero and the maximum regularization value \( \lambda_{\text{max}} = \min\{\lambda > 0: \hat{\beta}_\lambda = 0\} \), which is the smallest tuning parameter value such that none of the features is selected into the model, where \( \hat{\beta}_\lambda \) is the estimate of the true vector \( \beta \) of coefficients from a lasso regression with regularization parameter value \( \lambda \). Note that \( \lambda_{\text{max}} \) depends on the input training data and we leave its computation to the glmnet R function from the glmnet R package, cf. [FHT10].

3.1.3 Performance estimation

In our proposed pipeline (cf. Figure 2), performance estimation happens at two different stages. First, the performances \( \hat{\eta}_1, \ldots, \hat{\eta}_r \) of all of the candidate models is estimated. One way to do this is to train the models using the training data and estimate their performances using the validation data. Another option is to perform ten-fold cross-validation on the entire learning data, i.e., the combination of training and validation data. We expect these estimates to be less dependent on the split of the data into training and validation sets and, thus, to lead to better final selections. For brevity, we only compute the cross-validated estimates in case of the AUC. Note that when using cross-validation the resulting performance estimates are neither conditional on the trained model nor validation performances in the sense of the non-cross-validated estimates; they are averaged unconditional performances over the ten folds. However, we use these performances only to identify promising models to preselect for evaluation later on.

Once models are preselected for evaluation based on their (cross-) validation performances, they are refitted using the entire learning data before their generalization performances are estimated using the evaluation data. This is the second and final round of performance estimation.
3.1.4 Model selection

As with performance estimation, model selection happens at two different stages, too, cf. Figure 2. First, promising models are identified based on their validation performance and preselected for evaluation. Second, a final model \( s \) is selected among them, based on its evaluation performance \( \hat{\theta}_s \). The two selection rules do not necessarily need to be the same. In our simulation experiments, based on their validation performance, we preselect for evaluation either the single best model, or the top 10\% of the models. In case the cross-validation performance is used for selection, in addition to the single best and the top 10\% selection rule, we select all the models with cross-validation performance within one cross-validation standard error of the best model. The preselected models are then refitted using all of the training and validation data. In any case, in the final selection stage, we select the one model \( s \) with the best evaluation performance \( \hat{\theta}_s = \max_{i=1}^m \hat{\theta}_i \) and report a lower confidence bound \( \hat{\theta}_{s,L} \) for it.

3.1.5 Confidence bounds

We compute our proposed multiplicity-adjusted bootstrap tilting confidence bounds (MABT) using 10,000 bootstrap resamples when the performance measure of interest is the prediction accuracy, and 2000 resamples in case of AUC, for computational brevity. We use the R function auc from the R package pROC to estimate the AUC, cf. [RTH+11]. Table 1 provides a summary of the confidence bounds estimated for each configuration. In case of prediction accuracy, we compare our proposed bounds to a number of existing standard approaches: the Wald normal approximation interval, which is known to sometimes struggle to reach the nominal significance level, especially when sample size is small; the Wilson interval, which is an improvement over the Wald interval in many respects as it allows for asymmetric intervals, incorporates a continuity correction, and can also be used when sample size is small; the Clopper-Pearson (CP) exact interval, which uses the binomial and, thus, the correct distribution rather than an approximation to it; and the default bootstrap tilting confidence interval (BT) as presented in Section 1. In case of the AUC, we again take the default bootstrap tilting confidence interval for comparison, as well as DeLong intervals, which are the default choice for an asymptotic interval here, and Hanley-McNeil intervals, which use a simpler variance estimator. To compute the DeLong intervals we use the R function \( \text{ci.auc} \) from the pROC R package, cf. [RTH+11].

In those scenarios where multiple models are evaluated simultaneously, a multiplicity adjustment is necessary. Our proposed confidence bounds control for such multiplicity, whatever the selection rule applied. For the standard methods in the competition however we apply the Šidák-correction and estimate the confidence bound using a reduced and adjusted significance level of \( \alpha_{\text{Sidak}}(m) = 1 - (1 - \alpha)^{1/m} \), where \( m \) is the number of preselected models. We can safely assume that the predictions from the various candidate models are not negatively dependent and, thus, we choose the Šidák over the Bonferroni adjustment (cf. for example [Dic14]) since they are less conservative.

| Selection rule          | Prediction accuracy   | AUC            |
|-------------------------|-----------------------|----------------|
| default (single best)   | Bootstrap tilting (BT)| BT             |
|                         | Wald                  | DeLong         |
|                         | Wilson                | Hanley-McNeil  |
|                         | Clopper-Pearson (CP)  |                |
| top 10%                 | MABT                  | MABT           |
|                         | BT + Šidák            | BT + Šidák     |
|                         | Wald + Šidák          | DeLong + Šidák |
|                         | Wilson + Šidák        | Hanley-McNeil + Šidák |
|                         | CP + Šidák            |                |
| within 1 SE             | Multiplicity-adj. BT (MABT) | MABT          |
|                         | BT + Šidák            | BT + Šidák     |
|                         | Wald + Šidák          | DeLong + Šidák |
|                         | Wilson + Šidák        | Hanley-McNeil + Šidák |
|                         | CP + Šidák            |                |

Table 1: Listing of the considered interval procedures per performance measure and selection rule.

3.2 Results

Next we present the results from 5000 simulation runs for each combination of simulation parameters. Figure 5 presents the overall observed coverage probabilities of the seven interval methods over all simulation experiments, i. e.
over all performance measures (prediction accuracy, AUC), selection rules (single best, top 10%, within 1 standard error), sample sizes (200, 400 for prediction accuracy and 400, 600 for AUC, i.e. evaluation sample sizes 50, 100 and 100, 150, respectively), for both validation performance estimation variants (with and without cross-validation), and both feature generation methods (A, B). Overall, our proposed approach yields the most reliable observed coverage probabilities.

For brevity, we only present a selection of more detailed results here, which are the most competitive approaches in terms of coverage probability and size of the lower confidence bounds. The individual arguments why we dismiss certain results from presentation here can be found in the Supplement Document. For prediction accuracy, this leaves us with the following competition: Wilson unadjusted confidence bounds for the single best performing model; default bootstrap tilting confidence bounds for the single best performing model; our proposed maxT-type multiplicity-adjusted bootstrap tilting confidence bounds for the best model of the within one standard error selection of models. For AUC, the competition is the same as for prediction accuracy with DeLong replacing Wilson. In any case, for pres-election, the validation performance is computed using the cross-validation estimate from the learning data. Since we split the data into 50% training, 25% validation, and 25% evaluation data, for the selected results presented here, this is effectively a 75%/25% learning/evaluation split because for cross-validation we use both the training and validation data.

In the results we see that our proposed confidence bounds are somewhat conservative in the simpler setups, i.e. feature case A with prediction accuracy, and less conservative in the more complex setups, i.e. feature case B or in case of AUC, cf. Figures 6 and 7. At the same time, the adverse effect of conservatism is not pronounced and does not directly translate into smaller lower bounds, cf. Figures 8 and 9. Similar observations have already been made in [Hal88], where other conservative bootstrap intervals were not directly related to larger intervals. Also, the confidence bounds from our proposed method are less variable than the competing methods. Regarding tightness, we cannot draw a final conclusion, cf. Figures 10 and 11. Note however that in some AUC simulation configurations the default bootstrap tilting and the DeLong method yield too liberal intervals such that the comparison of our proposed confidence bounds to those in terms of size of the lower bound and tightness is unfair. (Too liberal intervals are identified as those whose coverage falls below $0.9469 = 1 - \alpha - \sqrt{(1 - \alpha) \cdot \alpha/5000}$ which is the desired coverage probability minus one standard error due to the finite number of simulation runs.) Nevertheless, especially in case of the smaller sample size, there is a visible gain in final model performance, cf. Figures 12 and 13.

4 Data Example

In this Section, we apply the proposed approach on the Breast Cancer Wisconsin Diagnostic Data Set from the UCI Machine Learning Repository, cf. [DG17], which consists of 698 observations on nine characteristics of cell nuclei present in digitized images of a fine needle aspirate of breast mass. The goal is to predict malignant tissue, which is the label in 241 cases. We split the data randomly into 523 observations for learning (75%) and 175 for evaluation (25%). In the learning phase, 100 lasso models with equidistant tuning parameters between 0 and $\lambda_{\text{max}} = 0.3829133$ are trained and ten-fold cross-validated performances on the learning data are obtained for each of the candidate models. We employ the single best, top 10%, and within 1 standard error selection rules on the validation performances, refit the preselected models on the entire learning set, and select the one model with the highest evaluation performance among them for confidence bound estimation. We compute all the different interval procedures from all three selection strategies for comparison here (cf. Table 1). For the bootstrap-based confidence bounds we use 10,000 bootstrap resamples in case of prediction accuracy and 2000 resamples in case of AUC. In case of the prediction accuracy, for the within 1 SE and top 10% selection rules, the default bootstrap tilting (BT), Clopper-Pearson (CP), Wald, and Wilson confidence bounds use Šidák-adjusted significance levels of about 0.0043 ($m = 12$ preselected models) and 0.0085 ($m = 6$); in case of the AUC, these levels are 0.0057 ($m = 11$) and 0.0023 ($m = 22$), respectively.

Table 2 presents the results for the accuracy. The proposed confidence bounds (MABT) turn out to be among the largest; the MABT confidence bound from the within 1 SE selection is only being outperformed in the default pipeline by the Wald confidence bound, which however are questionable in terms of coverage probability. In Table 3 the results for the AUC are shown. The MABT bounds are about as large as the BT bound from the default pipeline and only slightly smaller than the DeLong and Hanley-McNeil bounds. Note however that the latter two turn out to be too liberal in our simulations and, thus, the DeLong and Hanley-McNeil bounds are questionable.

In summary, while our proposed MABT confidence bounds turned out to be reliable regarding coverage probability in our simulation experiments (cf. Section 3), in this real-data example they turn out competitive regarding the size of the lower confidence bound.
Figure 5: Observed coverage probability for each of the interval methods over all the simulation experiments. BT denotes the default bootstrap tilting confidence bounds, CP denotes the Clopper-Pearson bounds, HMcN denotes the Hanley-McNeil bounds, and MABT denotes our proposed bounds.

Figure 6: Prediction accuracy: observed coverage for the various simulation configurations. BT denotes the default bootstrap tilting confidence bounds and MABT denotes our proposed bounds.
Figure 7: AUC: observed coverage for the various simulation configurations. BT denotes the default bootstrap tilting confidence bounds and MABT denotes our proposed bounds.

Figure 8: Prediction accuracy: lower confidence bound estimates. BT denotes the default bootstrap tilting confidence bounds and MABT denotes our proposed bounds. Bounds that come from too liberal approaches are grayed out; comparing them to methods that reach the desired confidence is unfair.
Figure 9: AUC: lower confidence bound estimates. BT denotes the default bootstrap tilting confidence bounds and MABT denotes our proposed bounds. Bounds that come from too liberal approaches are grayed out; comparing them to methods that reach the desired confidence is unfair.

| no. m of preselected models | single best | top 10% | within 1 SE |
|-----------------------------|-------------|---------|-------------|
| performance                 |             |         |             |
| validation                  | 96.0        | 95.4–96.0 | 95.8–96.0 |
| evaluation                  | 96.0        | 95.4–96.0 | 96.0–96.0 |
| lower confidence bound      |             |         |             |
| BT                          | 92.9        | 90.7    | 91.3        |
| CP                          | 92.6        | 90.4    | 91.0        |
| MABT                        | –           | 92.0    | 92.8        |
| Wald                        | 93.6        | 92.1    | 92.4        |
| Wilson                      | 92.8        | 90.1    | 90.8        |

Table 2: Lower confidence bounds for the prediction accuracy. Our proposed MABT bound from the within 1 SE selection rule is only inferior to the default pipeline Wald bound, which however is questionable in terms of coverage probability.
Figure 10: Prediction accuracy: tightness of the lower bounds, i.e. the distance between the true performance to the lower bound. BT denotes the default bootstrap tilting confidence bounds and MABT denotes our proposed bounds. Bounds that come from too liberal approaches are grayed out; comparing them to methods that reach the desired confidence is unfair.

|                | single best | top 10%    | within 1 SE |
|----------------|-------------|------------|-------------|
| no. $m$ of preselected models | 1           | 11         | 22          |
| performance    |             |            |             |
| validation      | 99.2        | 99.2–99.2  | 99.1–99.2   |
| evaluation      | 99.4        | 99.4–99.4  | 99.4–99.4   |
| lower confidence bound |            |            |             |
| BT             | 98.4        | 97.8       | 97.7        |
| DeLong         | 98.8        | 98.6       | 98.9        |
| HMcN           | 98.7        | 98.8       | 98.8        |
| MABT           | –           | 98.3       | 98.4        |

Table 3: Lower confidence bounds from each approach for the AUC. Our proposed MABT bound are slightly smaller than the DeLong and the Hanley-McNeil bounds, which however are both questionable in terms of coverage probability.
Figure 11: AUC: tightness of the lower bounds, i.e. the distance between the true performance to the lower bound. BT denotes the default bootstrap tilting confidence bounds and MABT denotes our proposed bounds. Bounds that come from too liberal approaches are grayed out; comparing them to methods that reach the desired confidence is unfair.

Figure 12: Prediction accuracy: True performance of the final selected model. Note that BT and Wilson or BT and DeLong bounds, respectively, use the same default pipeline and, thus, select exactly the same final model.
Figure 13: AUC: true performance of the final selected model. Note that BT and Wilson or BT and DeLong bounds, respectively, use the same default pipeline and, thus, select exactly the same final model.
5 Discussion

We proposed multiplicity-adjusted bootstrap tilting confidence bounds that allow for valid inference when more than a single candidate predictive model is evaluated. This is especially beneficial in situations where data is scarce as it eases the allocation of data towards learning and evaluation. Other methods in the literature either do not estimate conditional performance or do so only indirectly (for instance, cross-validation and nested cross-validation, cf. [BHT21], respectively). This is different with the proposed approach, which directly estimates the conditional performance by resampling from the model’s predictions from the evaluation set.

The perhaps most prominent advantage of our proposed approach is that it can be universally applied. In principle, it works with any selection rule, any competition of prediction models, even from different model classes, and any performance measure as long as there is a version of it which accepts weights. Also, no additional model training is necessary, such that the additional computational burden is little.

In our simulation experiments, our proposed confidence bounds turn out to be reliable regarding coverage probability while still offering comparably large lower confidence bounds as competing methods. Also, the evaluation of multiple candidate models instead of a single one can lead to better final model selections. But with increasing sample size, these advantages decrease. In a real data example, the proposed confidence bounds perform comparably well to the competition, and were only outperformed by methods that show themselves to be too liberal in some situations.

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