Predictive Inference Is Free with the Jackknife+-after-Bootstrap

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Abstract

Ensemble learning is widely used in applications to make predictions in complex decision problems—for example, averaging models fitted to a sequence of samples bootstrapped from the available training data. While such methods offer more accurate, stable, and robust predictions and model estimates, much less is known about how to perform valid, assumption-lean inference on the output of these types of procedures. In this paper, we propose the jackknife+-after-bootstrap (J+aB), a procedure for constructing a predictive interval, which uses only the available bootstrapped samples and their corresponding fitted models, and is therefore “free” in terms of the cost of model fitting. The J+aB offers a predictive coverage guarantee that holds with no assumptions on the distribution of the data, the nature of the fitted model, or the way in which the ensemble of models are aggregated—at worst, the failure rate of the predictive interval is inflated by a factor of 2. Our numerical experiments verify the coverage and accuracy of the resulting predictive intervals on real data.

Keywords: Assumption-free inference; Bagging; Bootstrapping; Conformal inference; Ensemble learning; Exchangeability; Jackknife; Predictive inference; Stability

1 Introduction

Ensemble learning is a popular technique for enhancing the performance of machine learning algorithms. It is used to capture a complex model space with simple hypotheses which are often significantly easier to learn, or to increase the accuracy of an otherwise unstable procedure (see Hastie et al., 2009; Polikar, 2006; Rokach, 2010, and references therein). While ensembling can provide substantially more stable and accurate estimates, relatively little is known about how to perform provably valid inference on the resulting output. Particular challenges arise when the distribution of the data is unknown, and/or when working with a highly complex base algorithm whose behavior is difficult to characterize theoretically. To consider a motivating example, suppose that our data consist of feature vectors \( X \in \mathbb{R}^p \) and a real-valued response \( Y \in \mathbb{R} \). Even in an idealized scenario where we might be certain that these data follow a linear model, it is still not clear how we might perform inference on the bagged regression function obtained by, say, running the Lasso on multiple bootstrapped samples of the data and averaging the result.

To address the problem of inference for ensemble predictions, we propose a method for constructing a predictive confidence interval for a new observation, without any additional calls to the base regression algorithm, and is therefore “free” in terms of the cost of model fitting. When run at a target predictive coverage level of \( 1 - \alpha \), our method provably provides at least \( 1 - 2\alpha \) coverage in the worst case, with no assumptions aside from requiring independent and identically distributed data or stability of the underlying base regression algorithm. The procedure we propose is constructed by combining model ensembling with the recently proposed jackknife+ method for predictive inference (Barber et al., 2019).

Our main contributions are as follows.

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We propose the jackknife+-after-bootstrap (J+aB), a novel method for constructing a predictive confidence interval for ensemble predictions.

We prove that the coverage is at worst $1 - 2\alpha$ for the assumption-free theory. This lower bound is non-asymptotic, and holds for any sample size and any distribution of the data.

We verify that coverage is approximately $1 - \alpha$ empirically.

2 Background and Related Work

2.1 Problem Statement

Suppose we are given $n$ independent and identically distributed (i.i.d.) observations

$$(X_1, Y_1), \ldots, (X_n, Y_n) \overset{iid}{\sim} P$$

for some probability distribution $P$ on $\mathbb{R}^p \times \mathbb{R}$. Given the available training data, we would now like to be able to predict the value of the response $Y_{n+1}$ for a new data point with features $X_{n+1}$, where we assume that $(X_{n+1}, Y_{n+1})$ is drawn from the same probability distribution $P$. A common framework is to fit a regression model $\hat{\mu} : \mathbb{R}^p \to \mathbb{R}$ by applying some regression algorithm to the training data $\{(X_i, Y_i)\}_{i=1}^n$, and then predicting $\hat{\mu}(X_{n+1})$ as our best estimate of the unseen test response $Y_{n+1}$. However, the question arises: How can we quantify the likely accuracy or error level of these predictions? For example, can we use the available information to build an interval around our estimate $\hat{\mu}(X_{n+1}) \pm$ (some margin of error) that we believe is likely to contain $Y_{n+1}$?

More generally, we aim to build a predictive interval $\hat{C}(X_{n+1}) \subseteq \mathbb{R}$ that maps the test features $X_{n+1}$ to an interval (or more generally, a set) believed to contain $Y_{n+1}$. Implicitly, $\hat{C}$ is a function of the training data $\{(X_i, Y_i)\}_{i=1}^n$.

2.2 Distribution-Free Prediction

A predictive interval $\hat{C}$ satisfies distribution-free predictive coverage at level $1 - \alpha$ if

$$P\left[Y_{n+1} \in \hat{C}(X_{n+1})\right] \geq 1 - \alpha$$

for any distribution $P$ of the data. This probability is with respect to the distribution of the $n+1$ training and test data points (as well as any additional source of randomness used in obtaining $\hat{C}$); the bound must hold uniformly over all distributions $P$.

Distribution-free prediction methods have garnered attention in recent years as wrapper methods for complex machine learning algorithms such as neural networks. The use of holdout or validation sets is a common, and computationally inexpensive, way to avoid overfitting and ensure distribution-free predictive coverage [Papadopoulos 2008, Vovk 2013, Lei et al. 2018], while methods such as cross-validation or leave-one-out cross-validation (also called the “jackknife”) stabilize the results in practice but require some assumptions to analyze theoretically [Steinberger and Leeb 2016, 2018, Barber et al. 2019]. Distribution-free guarantees are also obtained by the conformal prediction methodology of Vovk et al. (2005) (see also Lei et al. 2018).

2.2.1 The Jackknife and Jackknife+ Methods

Our method is inspired by the recent jackknife+ of [Barber et al. 2019]. As suggested by the name, the jackknife+ is a simple modification of the jackknife approach to constructing predictive confidence intervals.

To define these methods, we begin by introducing some notation. Let $\mathcal{R}$ denote any regression algorithm, which maps a training data set of any size to a fitted regression function, which is a function mapping a new $X$ to a predicted $Y$. We will write $\hat{\mu} = \mathcal{R}(\{(X_i, Y_i)\}_{i=1}^n)$ for the fitted function obtained via the full training data set, and will also write $\hat{\mu}_{-i} = \mathcal{R}(\{(X_j, Y_j)\}_{j=1,j\neq i}^n)$ for the fitted function obtained if data point $i$ is removed from the training set.
Let \( q^+_{\alpha,n}(v_i) \) and \( q^-_{\alpha,n}(v_i) \) denote the upper and the lower \( \alpha \)-quantiles of the empirical distribution of a collection of \( n \) values indexed by \( i \), that is to say,
\[
q^+_{\alpha,n}(v_i) = \left\lfloor (1 - \alpha)(n + 1) \right\rfloor \text{th smallest value of } v_1, \ldots, v_n,
\]
and \( q^-_{\alpha,n}(v_i) = -q^+_{\alpha,n}(-v_i) \). The usual jackknife prediction interval is given by
\[
\hat{C}^\alpha_{\alpha,n}(x) = \hat{\mu}(x) \pm q^+_{\alpha,n}\{R_i\} = \left[q^-_{\alpha,n}\{\hat{\mu}(x) - R_i\}, q^+_{\alpha,n}\{\hat{\mu}(x) + R_i\}\right],
\]
where \( R_i = |Y_i - \hat{\mu}_i(X_i)| \) is the \( i \)-th leave-one-out residual. The construction is based on the idea that the \( R_i \)'s are good estimates of the test residual \( |Y_{n+1} - \hat{\mu}_i(X_{n+1})| \), because the data used to train \( \hat{\mu}_i \) is independent of \( (X_i, Y_i) \). Perhaps surprisingly, fully assumption-free theoretical guarantees are impossible to achieve for the jackknife construction (see [Barber et al., 2019 Theorem 2]).

The jackknife+ applies a simple modification to jackknife that leads to an assumption-free, nonasymptotic coverage guarantee. This is done by replacing \( \hat{\mu} \) in the above interval with \( \hat{\mu}_i \)'s:
\[
\hat{C}^{1+\alpha}_{\alpha,n}(x) = \left[q^-_{\alpha,n}\{\hat{\mu}_i(x) - R_i\}, q^+_{\alpha,n}\{\hat{\mu}_i(x) + R_i\}\right].
\]

It can be shown that \( \hat{C}^{1+\alpha}_{\alpha,n}(X_{n+1}) \) satisfies
\[
\Pr\left[Y_{n+1} \in \hat{C}^{1+\alpha}_{\alpha,n}(X_{n+1})\right] \geq 1 - 2\alpha
\]
for any sample size \( n \), irrespective of the data distribution and the choice of regression method. Intuitively, the reason that the original jackknife fails to achieve such a guarantee without additional assumptions is that the test residual \( |Y_{n+1} - \hat{\mu}_i(X_{n+1})| \) is not quite comparable with the leave-one-out residuals \( |Y_i - \hat{\mu}_i(X_i)| \); the former always uses one more observation to train the regression algorithm compared to the latter. The jackknife+ correction restores the symmetry, making assumption-free theory possible.

### 2.3 Ensemble Methods

In this paper, we are concerned with ensemble predictions that apply a base regression method to different training sets generated from the training data by a resampling procedure. Specifically, we begin by creating multiple training data sets of size \( m \),
\[
S_1 = (i_{1,1}, \ldots, i_{1,m}), \ldots, S_B = (i_{B,1}, \ldots, i_{B,m}),
\]
where each index \( i_{b,k} \) is chosen from the set \( \{1, \ldots, n\} \) indexing the training data points. (Since \( S_b \) might contain the same index \( i \) multiple times, formally we consider \( S_b \) to index a multiset of the original training data.) For each \( b \), we then compute a fitted function \( \hat{\mu}_b \) on the \( b \)-th training data set \( S_b \). These \( B \) fitted regression functions are finally aggregated using some aggregation function \( \varphi \), which maps a collection of predictions \( \hat{\mu}_1(x), \ldots, \hat{\mu}_B(x) \) to a single final prediction \( \hat{\varphi}(x) \) for any feature vector \( x \in \mathbb{R}^p \).

This ensemble construction is formalized in Algorithm 1. To make this construction more concrete, we consider a few common examples:

- The training data sets \( S_b \) may be chosen by bootstrapping, i.e., drawing \( m \) indices from \( \{1, \ldots, n\} \) uniformly at random with replacement, or by subsampling, i.e., drawing \( m \) indices from \( \{1, \ldots, n\} \) uniformly at random without replacement. We typically would choose the ratio \( m/n \) to be a constant, e.g., \( m = n \) for bootstrapping, or \( m = n/2 \) for subsampling.
- Common choices for the base algorithm \( \mathcal{R} \) might be a linear or generalized linear regression, a penalized or constrained version of linear regression such as the Lasso, a neural net, or a regression tree.
- The aggregation function \( \varphi \) is often chosen to be the median, mean, or trimmed mean.

For any base algorithm \( \mathcal{R} \), when \( \varphi \) is chosen to be mean aggregation, the ensemble method run with bootstrapped \( S_b \)'s is referred to as bagging ([Breiman, 1996]), while if we instead use subsampled \( S_b \)'s, then this ensemble procedure is referred to as subagging ([Bühlmann and Yu, 2002]).

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1 Formally, we define \( \varphi \) as a map from \( \bigcup_{k \geq 0} \mathbb{R}^k \rightarrow \mathbb{R} \), mapping any collection of predictions in \( \mathbb{R} \) to a single aggregated prediction. (If the collection is empty, we would simply output zero or some other default choice). \( \varphi \) lifts naturally to a map on vectors of functions, by writing \( \hat{\varphi}(\hat{\mu}_1, \ldots, \hat{\mu}_B) \), where \( \hat{\varphi}(x) \) is defined for each \( x \in \mathbb{R} \) by applying \( \varphi \) to the collection \( (\hat{\mu}_1(x), \ldots, \hat{\mu}_B(x)) \).
Algorithm 1 Ensembled learning

\textbf{Input:} Data \(\{(X_i, Y_i)\}_{i=1}^n\)

\textbf{Output:} Ensembled regression function \(\hat{\mu}_\phi\)

\begin{algorithmic}
\For {\(b = 1, \ldots, B\)}
\State Draw \(S_b = (i_{b,1}, \ldots, i_{b,m})\) by sampling uniformly at random, with or without replacement, from \(\{1, \ldots, n\}\).
\State Compute \(\hat{\mu}_b = R((X_{i_{b,1}}, Y_{i_{b,1}}), \ldots, (X_{i_{b,m}}, Y_{i_{b,m}}))\).
\EndFor
\State Define \(\hat{\mu}_\phi = \varphi(\hat{\mu}_1, \ldots, \hat{\mu}_B)\).
\end{algorithmic}

2.3.1 Can We Apply Jackknife$\+$ to an Ensemble?

An ensembled model \(\hat{\mu}_\phi\) provides a point prediction at any new \(X_{n+1}\), but how can we estimate its accuracy—that is, what information do we have about the likely error, \(|Y_{n+1} - \hat{\mu}_\phi(X_{n+1})|\)? While ensembling is generally understood to provide a more robust and stable prediction as compared to the underlying base algorithm, there are substantial difficulties in developing inference procedures for ensemble methods with theoretical guarantees. For one thing, ensemble methods are frequently used with highly discontinuous and nonlinear base learners, and aggregating many of them leads to models that defy an easy analysis. The problem is compounded by the fact that ensemble methods are typically employed in settings where good generative models of the data distribution are either unavailable or difficult to obtain. Thus, we would naturally want to use distribution-free predictive inference methods whose validity does not depend on knowing the distribution of the data or characterizing the behavior of the regression algorithm.

We might therefore consider applying a method such as jackknife$\+$ or conformal prediction to the ensembled model. However, the computational cost of such a procedure is prohibitive. In the case of jackknife$\+$, each ensembled model requires \(B\) many calls to the underlying base algorithm \(R\), which is then repeated \(n\) many times—that is, Algorithm 1 is run once for each leave-one-out regression—for a total of \(Bn\) many calls to \(R\). Therefore, we should not naively apply the jackknife$\+$ “wrapper” to an ensembled regression.

2.4 Related Work

Many ensemble methods can be cast as particular instances of bootstrap aggregating or bagging [Breiman, 1996]. Some of the earlier theoretical works were concerned with studying the impact of bagging on improving accuracy compared to the base method [Bühlmann and Yu, 2002; Buja and Stuetzle, 2006; Friedman and Hall, 2007]. These works are primarily focused on quantifying the improvement over the base (non-ensembled) algorithm.

The literature that deals with precise uncertainty quantification of ensemble estimators is substantially leaner. Meinshausen (2006); Athey et al. (2019); Lu and Hardin (2019) proposed methods for estimating conditional quantiles derived from the popular random forests [Ho, 1995; Breiman, 2001]. These methods can be used to construct valid prediction intervals, but their guarantees are necessarily approximate or asymptotic, and rely on additional conditions. By contrast, Sexton and Laake (2009); Wager et al. (2014); Mentch and Hooker (2016) studied methods for estimating the variance of the random forest estimator of the conditional mean by applying, in order, the jackknife-after-bootstrap (not jackknife$\+$) [Efron, 1992] or the infinitesimal jackknife [Efron, 2014] or U-statistics theory. Roy and Larocque (2019) propose a heuristic for constructing prediction intervals with such variance estimates. For a comprehensive survey of statistical work related to random forests, we refer the reader to the literature review by Athey et al. (2019).

While our proposed methods are designed to be deployed in conjunction with bootstrap or ensemble methods, in flavor they are more closely linked to the growing literature on assumption-free predictive inference (see Vovk et al. 2005; Lei et al., 2018, and references there in). Our paper is most closely related to the jackknife$\+$ of Barber et al. (2019). More recently, Kuchibhotla and Ramdas (2019) looked at aggregating conformal inference after subsampling or bootstrapping. Their work proposes ensembling multiple runs of an inference procedure, while in contrast our present work seeks to provide inference for ensemble methods.

As mentioned in Section 2.3.1 applying jackknife$\+$ (or, equivalently, jackknife) as a “wrapper” around an ensembled algorithm is computationally burdensome, with \(Bn\) many calls to the base learner (where
$B$ is the number of samples used for constructing an ensemble, and $n$ is the sample size). To reduce this computational burden while ensuring distribution-free theoretical guarantees, we can instead consider using a holdout set to assess the predictive accuracy of an ensembled model, as studied by, e.g., [Papadopoulos et al. (2002); Papadopoulos and Haralambous (2011)]. However, when the sample size $n$ is limited, we will achieve more accurate predictions with a cross-validation or jackknife type method, which avoids reducing the sample size in order to obtain a holdout set.

Finally, our work is most closely related to the idea of “out-of-bag” prediction intervals proposed for the jackknife, as a computationally efficient alternative to the naive idea of applying jackknife directly to an ensembled algorithm and thus requiring $Bn$ calls to the base learner. Specifically, defining the function

$$\hat{\mu}_\varphi \setminus i = \varphi(\{\hat{\mu}_b : b = 1, \ldots, B, S_b \not\ni i\}),$$

which ensembles all models $\hat{\mu}_b$ whose subsample $S_b$ does not train on the $i$th data point, [Johansson et al. (2014)] propose a prediction interval of the form

$$\hat{\mu}_\varphi(X_{n+1}) \pm q^+_{\alpha,n}(R_i) \quad \text{where} \quad R_i = |Y_i - \hat{\mu}_{\varphi \setminus i}(X_i)|. \tag{2}$$

[Zhang et al. (2019)] provide a theoretical analysis of this type of prediction interval, ensuring that predictive coverage holds asymptotically under additional assumptions. [Devtyarov and Nouretdinov (2010); Lofstrom et al. (2013); Boström et al. (2017); Bostrom et al. (2017); Linusson et al. (2019)] study variants of this type of method, but distribution-free coverage is not guaranteed in any of these proposed methods.

### 3 The Jackknife+-after-Bootstrap Method

The key observation behind our method is that, by exploiting the structure of the ensemble, it is possible to obtain $n$ many leave-one-out regressors—that is, for each $i = 1, \ldots, n$, we need a fitted regression that does not depend on the data point $i$—with the same number of calls to the base regression method. To obtain the $i$-th leave-one-out fitted predictor $\hat{\mu}_{\varphi \setminus i}$, we will simply aggregate the original models $\hat{\mu}_1, \ldots, \hat{\mu}_B$ with the caveat that we exclude any $\hat{\mu}_b$ whose training data set $S_b$ includes data point $i$.

**Algorithm 2** Jackknife+-after-Bootstrap (J+aB)

**Input:** Data $\{(X_i, Y_i)\}_{i=1}^n$

**Output:** Predictive interval $\hat{C}_{\alpha,n,B}^{J+aB}$

for $b = 1, \ldots, B$

for $m = 1, \ldots, B$

Draw $S_b = (i_{b,1}, \ldots, i_{b,m})$ by sampling uniformly at random (with or without replacement, as desired) from $\{1, \ldots, n\}$.

Compute $\hat{\mu}_b = R((X_{i_{b,1}}, Y_{i_{b,1}}), \ldots, (X_{i_{b,m}}, Y_{i_{b,m}}))$.

end for

end for

Aggregate $\hat{\mu}_{\varphi \setminus i} = \varphi(\{\hat{\mu}_b : b = 1, \ldots, B, S_b \not\ni i\})$.

Compute the residual, $R_i = |Y_i - \hat{\mu}_{\varphi \setminus i}(X_i)|$.

end for

Compute the jackknife+-after-bootstrap prediction interval: at each $x \in \mathbb{R}$,

$$\hat{C}_{\alpha,n,B}^{J+aB}(x) = \left[q^+_{\alpha,n}(\hat{\mu}_{\varphi \setminus i}(x) - R_i), q^+_{\alpha,n}(\hat{\mu}_{\varphi \setminus i}(x) + R_i)\right].$$

To run the jackknife+-after-bootstrap (J+aB) method given in Algorithm 2, we can see that all $n$ leave-one-out models $\hat{\mu}_{\varphi \setminus i}$ are computed by aggregating subsets of the same underlying list of fitted models $\hat{\mu}_1, \ldots, \hat{\mu}_B$. Therefore, the cost of J+aB is essentially the same as that of ensembled learning (Algorithm 1) in any setting where the dominant computational cost comes from model training rather than model aggregation or function evaluation. For example, this will hold if $\varphi$ is the mean or median while $R$ is an expensive method such as a neural net.

Thus, for a prediction task, instead of a point estimate obtained by ensemble learning (Algorithm 1), we can provide a more informative prediction interval via jackknife+-after-bootstrap (Algorithm 2), essentially “for free.”
4 Theory

We make two assumptions, one on the data distribution and the other on the ensemble algorithm.

**Assumption 1** (i.i.d. data). The training and test data are i.i.d.: \((X_1, Y_1), \ldots, (X_n, Y_n), (X_{n+1}, Y_{n+1}) \sim \mathcal{P}\), where \(\mathcal{P}\) is any distribution on \(\mathbb{R}^p \times \mathbb{R}\).

**Assumption 2** (symmetric algorithms). For \(k \geq 1\), any fixed \(k\)-tuple \(((x_1, y_1), \ldots, (x_k, y_k)) \in \mathbb{R}^p \times \mathbb{R}\), and any permutation \(\sigma\) on \(\{1, \ldots, k\}\), it holds that \(\mathcal{R}((x_1, y_1), \ldots, (x_k, y_k)) = \mathcal{R}((x_{\sigma(1)}, y_{\sigma(1)}), \ldots, (x_{\sigma(k)}, y_{\sigma(k)}))\) and \(\varphi(y_1, \ldots, y_k) = \varphi(y_{\sigma(1)}, \ldots, y_{\sigma(k)})\).

In other words, the base regression algorithm \(\mathcal{R}\) and the aggregation \(\varphi\) are both invariant to the ordering of the input arguments.\(^2\)

Assumption 1 is fairly standard in the distribution-free prediction literature (Vovk et al., 2005; Lei et al., 2018; Barber et al., 2019) (in fact, as in the conformal prediction literature, our results only require exchangeability of the \(n + 1\) data points—the i.i.d. assumption is a familiar special case). Assumption 2 is a natural condition in the setting where the data points are i.i.d. and therefore should logically be treated symmetrically.

4.1 Assumption-Free Guarantees

In this section, we establish a coverage guarantee for the jackknife+-after-bootstrap prediction interval, with no assumptions on the data, the base algorithm, or the aggregation procedure. One interesting requirement is that the number of subsamples, \(B\), is required to be random for this result to hold—we discuss this point later on.

**Theorem 1.** Fix any integers \(\tilde{B} \geq 1\) and \(m \geq 1\), any base algorithm \(\mathcal{R}\), and any aggregation function \(\varphi\). Suppose jackknife+-after-bootstrap (Algorithm 2) is run with \(B \sim \text{Binomial}(\tilde{B}, (1 - \frac{1}{n+1})^m)\) (in the case of sampling with replacement) or \(B \sim \text{Binomial}(\tilde{B}, 1 - \frac{m}{n+1})\) (in the case of sampling without replacement). Then, under Assumptions 1 and 2, the jackknife+-after-bootstrap prediction interval satisfies

\[
P \left[ Y_{n+1} \in \hat{C}_{a,n,B}(X_{n+1}) \right] \geq 1 - 2\alpha,
\]

where the probability holds with respect to the random draw of the training data \((X_1, Y_1), \ldots, (X_n, Y_n)\), the test data point \((X_{n+1}, Y_{n+1})\), and \(B\).

This theorem shows that the distribution-free coverage guarantee of the jackknife+ extends immediately to the jackknife+-after-bootstrap with one intriguing twist: the number of bootstrapped or subsampled training sets, \(B\), must be drawn at random rather than chosen in advance. In practice, we do not expect this to make any meaningful difference to the output of the algorithm (concentration of the Binomial distribution ensures that the random \(B\) constructed in the theorem is essentially constant, as long as \(\tilde{B}\) is large). In Section 4.2 we will formalize the idea that, for aggregating maps \(\varphi\) that are not overly sensitive to slight changes in the number of input models, running the jackknife+-after-bootstrap with a fixed choice of \(B\) is also valid. However, for assumption-free guarantees that do not rely on stability of the aggregating map \(\varphi\), the theoretical arguments allowing us to obtain distribution-free coverage require this random \(B\) in an interesting way.

4.1.1 Why Do We Need a Random \(B\)?

To see why \(B\) needs to be random in order to establish Theorem 1, it is instructive to go over the jackknife+ theory and understand how exchangeability is used in the proof to obtain a lower-bound on the coverage. The proof of the jackknife+ coverage guarantee (Barber et al., 2019 Theorem 1) is based on the observation that

\(^2\)If \(\mathcal{R}\) and/or \(\varphi\) involve any randomization—for example if \(\varphi\) operates by sampling from the collection of predictions—then we can require that the outputs are equal in distribution under any permutation of the input arguments, rather than requiring that equality holds deterministically. In this case, the coverage guarantees in our theorems hold on average over the randomization in \(\mathcal{R}\) and/or \(\varphi\), in addition to the distribution of the data.
We now prove the distribution-free guarantee of Theorem 1. Our proof follows the main idea of the jackknife+ Algorithm 3 and therefore the resulting array of residuals \( (\hat{\mu}_{\cdot i})_{i=1}^{n} \) and \( (\mu_{\cdot i})_{i=1}^{n} \) of subsamples \( \mu \) and \( \hat{\mu} \) and therefore the resulting array of residuals \( (\hat{\mu}_{\cdot i})_{i=1}^{n} \) and \( (\mu_{\cdot i})_{i=1}^{n} \) of subsamples \( \mu \) and \( \hat{\mu} \)

Data
Input: 

of leave-one-out fitted predictors \( \hat{\mu}_{\cdot i}, \) the residual for the new observation exceeds the residual for the \( i \)-th observation in magnitude. In other words, if \( Y_{n+1} \notin \mathcal{E}_{\alpha,n}(X_{n+1}) \) then

\[
\sum_{i=1}^{n} \mathbb{I}\left[ \left| Y_{n+1} - \hat{\mu}_{\cdot i}(X_{n+1}) \right| > \left| Y_{i} - \hat{\mu}_{\cdot i}(X_{i}) \right| \right] \geq (1 - \alpha)(n + 1).
\]

Initially, it may seem that we cannot use exchangeability of the training and test data to study this event, since each training data point \( i \) appears in every \( \hat{\mu}_{\cdot i} \) where \( j \neq i \), while the test point \( n + 1 \) is not used in any fitted model.

However, we can embed these \( n \) leave-one-out models \( (\hat{\mu}_{\cdot i})_{i=1}^{n} \) into a larger collection in order to restore exchangeability. Consider the \( (n + 1) \times (n + 1) \) array of leave-two-out fitted predictors \( (\hat{\mu}_{\cdot i,j})_{1 \leq i,j \leq n+1} \). Since the \( n + 1 \) data points are assumed to be i.i.d., and this array constructs leave-two-out fitted models for each possible pair, the resulting \( (n + 1) \times (n + 1) \) array is exchangeable, i.e., its distribution does not change if we permute the rows/columns. As \( \hat{\mu}_{n+1,i} = \hat{\mu}_{\cdot i} \) for \( i = 1, \ldots, n \), any statement we make with \( \hat{\mu}_{n+1,i} \)'s, which are embedded in the \( (n + 1) \times (n + 1) \) exchangeable array, is related back to \( \hat{\mu}_{\cdot i} \)'s, and thus, to the jackknife+ interval. This construction underlies the theory for the jackknife+.

If we attempt to apply the jackknife+ proof for the J+aB algorithm, however, issues arise immediately. In particular, consider defining \( \hat{\mu}_{\cdot i,j} = \varphi((\hat{\mu}_{i} : S_{b} \neq i, j)) \), the aggregation of all fitted models \( \hat{\mu}_{i} \) whose underlying subsampled or bootstrapped data set \( S_{b} \) does not include either \( i \) or \( j \). For each \( i = 1, \ldots, n \), we have \( \hat{\mu}_{\cdot i,n+1} = \hat{\mu}_{\cdot i} \), exactly as for the jackknife+ proof, and so it would seem that we can prove coverage of the jackknife+-after-bootstrap method by way of this larger \( (n + 1) \times (n + 1) \) array of \( \hat{\mu}_{\cdot i,j} \)’s.

Unfortunately, though, this larger array is not exchangeable—the jackknife+-after-bootstrap algorithm subtly violates symmetry even though \( \mathcal{R} \) and \( \varphi \) are themselves symmetric. This is mostly easily seen by noting that there are always exactly \( B \) many subsampled or bootstrapped training data sets \( S_{b} \) that do not include the test observation \( n + 1 \), whereas for any training observation \( i = 1, \ldots, n \) the number of \( S_{b} \)'s that do not contain \( i \) is usually smaller. It turns out that this issue can easily be addressed by simply drawing \( B \) from a Binomial distribution, as we will see next.

4.1.2 Proof of Theorem 1

We now prove the distribution-free guarantee of Theorem 1. Our proof follows the main idea of the jackknife+ guarantee (Barber et al., 2019, Theorem 1)—we lift the jackknife+-after-bootstrap method, which requires the construction of \( n \) many leave-one-out ensemble models \( \hat{\mu}_{\cdot i} \), to an \( (n + 1) \times (n + 1) \) array of leave-two-out models. Unlike the jackknife+ theory, here we must take care to ensure exchangeability within the collection of subsamples \( S_{b} \). Here we sketch the argument; for completeness, full details are given in Appendix A.

Algorithm 3 Lifted jackknife+-after-bootstrap residuals

Input: Data \( \{(X_{i}, Y_{i})\}_{i=1}^{n+1} \)

Output: Residuals \( (R_{ij} : i \neq j \in \{1, \ldots, n + 1\}) \)

for \( b = 1, \ldots, B \) do

\[\begin{align*}
& \text{Draw } S_{b} = (i_{b,1}, \ldots, i_{b,m}) \text{ uniformly at random, with or without replacement, from } \{1, \ldots, n + 1\}. \\
& \text{Compute } \hat{\mu}_{b} = \mathcal{R}((X_{i_{b,1}, Y_{i_{b,1}}}), \ldots, (X_{i_{b,m}, Y_{i_{b,m}}})).
\end{align*}\]

end for

for pairs \( i \neq j \in \{1, \ldots, n + 1\} \) do

\[\begin{align*}
& \text{Aggregate } \mu_{\cdot i,j} = \varphi((\hat{\mu}_{b} : S_{b} \neq i, j)). \\
& \text{Compute the residual, } R_{ij} = |Y_{i} - \hat{\mu}_{\cdot i,j}(X_{i})|.
\end{align*}\]

end for

Consider the “lifted” Algorithm 3. We can see that Algorithm 3 treats the \( n + 1 \) data points symmetrically, and therefore the resulting array of residuals \( (R_{ij} : i \neq j \in \{1, \ldots, n + 1\}) \) is exchangeable. Now, for each \( i = 1, \ldots, n + 1 \), define \( \mathcal{E}_{i} \) as the event that

\[
\sum_{j \in \{1, \ldots, n + 1\} \setminus \{i\}} \mathbb{I}[R_{ij} > R_{ji}] \geq (1 - \alpha)(n + 1).
\]
By a simple counting argument and exchangeability, it can be shown that \( P[\tilde{E}_{n+1}] \leq 2\alpha \), but we need to relate the event \( \tilde{E}_{n+1} \), defined based on the lifted jackknife+-after-bootstrap construction, to the original jackknife+-after-bootstrap interval \( \tilde{C}_{\alpha,n,B}^1(X_{n+1}) \). Let \( B = \sum_{b=1}^B \mathbb{1}[\tilde{S}_b \neq n + 1] \), the number of \( \tilde{S}_b \)'s containing only training data, in the lifted construction, and let \( 1 \leq b_1 < \cdots < b_B \leq B \) be the corresponding indices. Note that the distribution of \( B \) is Binomial, as specified in the theorem. Now, for each \( k = 1, \ldots, B \), define \( S_k = \tilde{S}_{b_k} \). We can observe that each \( S_k \) is an independent uniform draw from \( \{1, \ldots, n\} \) (with or without replacement). Therefore, we can equivalently consider running \( J + aB \) (Algorithm 2) with these particular subsamples or bootstrapped samples \( S_1, \ldots, S_B \). Furthermore, for each \( i = 1, \ldots, n \), this ensures that \( \tilde{\mu}_{\varphi \setminus i}(\cdot) = \tilde{\mu}_{\varphi \setminus i} \), that is, the leave-one-out models of the jackknife+-after-bootstrap methods coincide with the leave-two-out models of the lifted jackknife+-after-bootstrap. Thus, we have constructed a coupling of the jackknife+-after-bootstrap with its lifted version.

Now, define \( E_{n+1} \) as the event that

\[
\sum_{i=1}^n \mathbb{1}[|Y_{n+1} - \tilde{\mu}_{\varphi \setminus i}(X_{n+1})| > R_i] \geq (1 - \alpha)(n + 1),
\]

where \( R_i = |Y_i - \tilde{\mu}_{\varphi \setminus i}(X_i)| \) as before. By the coupling we have just constructed, we can see that the event \( E_{n+1} \) is exactly equivalent to the lifted event \( \tilde{E}_{n+1} \), and thus, \( P[E_{n+1}] = P[\tilde{E}_{n+1}] \leq 2\alpha \). It can be verified that if jackknife+-after-bootstrap fails to cover, i.e., if \( Y_{n+1} \notin \tilde{C}_{\alpha,n,B}^1(X_{n+1}) \), then the event \( E_{n+1} \) must occur, completing the proof.

### 4.2 Guarantees with Stability

Most ensembles that are encountered in practice exhibit concentrating behavior as \( B \to \infty \) with respect to the resampling distribution. For such ensembles, we expect the performance at large \( B \)'s to be all similar, as the jackknife+-after-bootstrap prediction intervals are converging to a fixed (conditional on the data) interval as we resample more and more sets. Intuitively, this happens for aggregations that are stable to adding or removing a small number of models in the collection.

To formalize this, let \( E^* \) denote the expectation with respect to the resampling measure—that is, conditioning on all the data points, we take the expectation with respect to the random subsamples \( S_1, \ldots, S_B \). For example, if \( \varphi(\cdot) = \text{mean}(\cdot) \) is the mean aggregation, then in that case we have

\[
E^*[\tilde{\mu}_{\text{mean}}(X_{n+1})] = E[\tilde{\mu}_1(X_{n+1})|(X_1, Y_1), \ldots, (X_n, Y_n), X_{n+1}],
\]

the expected prediction from the model \( \tilde{\mu}_1 \) fitted on training sample \( S_1 \), where the expectation is taken with respect to the draw of \( S_1 \).

**Assumption 3 (Ensemble stability).** For \( \varepsilon \geq 0 \) and \( \delta \in (0, 1) \), it holds for each \( i = 1, \ldots, n \) that

\[
P[|\tilde{\mu}_{\varphi \setminus i}(X_i) - E^*[\tilde{\mu}_{\varphi \setminus i}(X_i)]| > \varepsilon] \leq \delta.
\]

Here \( \tilde{\mu}_{\varphi \setminus i} \) is the ensembled leave-one-out model defined in Algorithm 2. To gain intuition for this assumption, we consider the mean aggregation as a canonical example, and verify that in that case this assumption holds for any bounded regression method.

**Proposition 1.** Suppose that \( \varphi(\cdot) = \text{mean}(\cdot) \) is the mean aggregation, and suppose the base regression method \( \mathcal{R} \) always outputs a bounded regression function, i.e., \( \mathcal{R} \) maps any training data set to a function \( \hat{\mu} \) taking values in a bounded range \( [l, u] \), for fixed constants \( l < u \). Then, for any \( \varepsilon > 0 \), Assumption 3 is satisfied with

\[
\delta = 2 \exp\left(-\frac{2\sqrt{B}\theta\varepsilon^2}{(u - l)^2}\right) + \exp\left(-\frac{(\sqrt{B} - 1)^2\theta^2}{2}\right),
\]

where \( \theta = (1 - \frac{1}{n})^m \) in the case of bagging (i.e., the \( S_b \)'s are bootstrapped samples, drawn with replacement), or \( \theta = 1 - \frac{m}{n} \) in the case of subagging (i.e., the \( S_b \)'s are subsamples drawn without replacement).
In other words, for large $B$, mean aggregation satisfies ensemble stability for any bounded base regression algorithm. (The proofs for this result, and all theoretical results in this section, are given in Appendix A.)

To study coverage properties under this notion of stability, we first define the $\varepsilon$-inflated jackknife+-after-bootstrap prediction interval as

$$
\hat{C}_{\alpha,n,B}^{\varepsilon,J+aB}(x) = \left[ q_{\alpha,n}(\hat{\mu}_{\varphi,i}(x) - R_i) - \varepsilon, q_{\alpha,n}(\hat{\mu}_{\varphi,i}(x) + R_i) + \varepsilon \right],
$$

for any $\varepsilon \geq 0$. We then have the following guarantee:

**Theorem 2.** Under $(\varepsilon, \delta)$-ensemble stability (Assumption 3), the $2\varepsilon$-inflated jackknife+-after-bootstrap prediction interval satisfies

$$
\Pr \left[ Y_{n+1} \in \hat{C}_{\alpha,n,B}^{2\varepsilon,J+aB}(X_{n+1}) \right] \geq 1 - 2\alpha - 4\sqrt{\delta}.
$$

It is worth going over the difference between Theorem 1 and Theorem 2. Theorem 1 gives an assumption-free lower-bound of $1 - 2\alpha$ on the coverage, but the coverage is over all randomness, including that of the Binomial draw. By contrast, the $\approx 1 - 2\alpha$ coverage guarantee of Theorem 2 holds for a fixed value of $B$ used to run Algorithm 2, but at the cost of requiring the ensembled algorithm $\hat{R}_{\alpha,B}$ to satisfy ensemble stability.

In contrast to the above notion of ensemble stability, Steinberger and Leeb (2018); Barber et al. (2019) study coverage of jackknife and jackknife+ under (non-ensembled) algorithmic stability, requiring that—a for a regression method $\hat{R}$—we have

$$
\Pr \left[ |\hat{\mu}_{\varphi,i}(X_{n+1}) - \hat{\mu}(X_{n+1})| > \varepsilon^* \right] \leq \delta^*,
$$

meaning that predictions of the fitted model $\hat{\mu}$ on a new test point are typically only slightly perturbed if we remove one training point. In this setting, jackknife and jackknife+ were shown to each guarantee approximately $1 - \alpha$ coverage.

We can take a lifted version of this assumption, requiring that it holds on the aggregated models (in expectation over the subsampling process):

$$
\Pr \left[ |E^* [\hat{\mu}_{\varphi,i}(X_{n+1})] - E^* [\hat{\mu}_{\varphi}(X_{n+1})]| > \varepsilon^* \right] \leq \delta^*.\tag{4}
$$

It is possible to have ensemble stability without algorithmic stability—for example, a bounded regression method might still be highly unstable relative to adding/removing a single data point (thus violating algorithmic stability), while Proposition 4 ensures that under mean aggregation, ensemble stability will hold. However, in the case of mean aggregation, in some settings a bagged or subagged estimator is understood to have superior stability properties, as measured by the variance or the mean squared error, compared to the base estimator (Bühlmann and Yu 2002; Buja and Stuetzle 2006; Friedman and Hall 2007). That is, the ensemble models might satisfy condition (4) at a small value of $\varepsilon^*$, even though (non-ensembled) models produced by the base algorithm $\hat{R}$ only satisfy algorithmic stability (3) at relatively large $\varepsilon^*$.

If both types of stability are satisfied, then the following result yields a coverage bound that is approximately $1 - \alpha$, rather than $1 - 2\alpha$ as above:

**Theorem 3.** Assume that $(\varepsilon, \delta)$-ensemble stability (Assumption 3) holds, and in addition, the ensembled model satisfies algorithmic stability (when averaged over the subsampling process), i.e., (4). Then the $2\varepsilon + 2\varepsilon^*$-inflated jackknife+-after-bootstrap prediction interval satisfies

$$
\Pr \left[ Y_{n+1} \in \hat{C}_{\alpha,n,B}^{(2\varepsilon + 2\varepsilon^*)J+aB}(X_{n+1}) \right] \geq 1 - \alpha - 3\sqrt{\delta} - 4\sqrt{\delta^*}.
$$

5 Experiments

Our experimental results aim to verify the coverage properties of jackknife+-after-bootstrap using different base algorithms, and to compare the performances of jackknife+-after-bootstrap with the original jackknife+ method (computed without ensembling). Code for reproducing all results and figures are available online.

[https://www.stat.uchicago.edu/~rina/jackknife+-after-bootstrap_realddata.html]
5.1 Data

We use the same three real data sets as in Barber et al. (2019), performing the same preprocessing steps on the data.

The Communities and Crime (Communities) data set (Redmond and Baveja, 2002) contains information on 1994 communities with \( d = 99 \) covariates. The response \( Y \) is the per capita violent crime rate.

The BlogFeedback (Blog) data set (Buza, 2014) contains 52397 blog posts with \( d = 280 \) covariates. The response is the number of comments left on the blog post in the following 24 hours, which we transform as \( Y = \log(1 + \#\text{comments}) \).

The Medical Expenditure Panel Survey 2016 (MEPS) data set (from the Agency for Healthcare Research and Quality) is described in Ezzati-Rice et al. (2008). The response is a composite score measuring use of medical services. There are 33005 data points with \( d = 107 \) covariates after the preprocessing steps following Barber et al. (2019). Since the distribution of the response is highly skewed, we use the transformation \( Y = \log(1 + \text{utilization score}) \).

5.2 Setup and Procedures

In all experiments, we fixed \( \alpha = 0.1 \) for a target coverage level of 90%. In each of 10 trials, a fixed \( n = 200 \) number of points were randomly sampled without replacement from the whole data set, and were used to train
Table 1: The performances of jackknife+-after-bootstrap \((m = n\) and sampling with replacement) and jackknife+ on all data sets for different base regression methods. (Results are averages over 10 independent training / test splits).

| Data set        | Base algorithm | Method | Coverage (SE) | Width (SE) |
|-----------------|----------------|--------|---------------|------------|
| Communities     | Ridge          | Jackknife+ | 0.907 (0.006) | 0.486 (0.011) |
|                 |                | J+AB    | 0.904 (0.005) | 0.478 (0.010) |
|                 | RF             | Jackknife+ | 0.935 (0.008) | 0.727 (0.020) |
|                 |                | J+AB    | 0.904 (0.007) | 0.500 (0.015) |
|                 | NN             | Jackknife+ | 0.910 (0.008) | 0.593 (0.018) |
|                 |                | J+AB    | 0.910 (0.012) | 0.575 (0.025) |
| MEPS            | Ridge          | Jackknife+ | 0.882 (0.008) | 4.193 (0.062) |
|                 |                | J+AB    | 0.890 (0.010) | 4.195 (0.062) |
|                 | RF             | Jackknife+ | 0.939 (0.005) | 5.720 (0.096) |
|                 |                | J+AB    | 0.912 (0.005) | 4.108 (0.058) |
|                 | NN             | Jackknife+ | 0.939 (0.005) | 4.762 (0.069) |
|                 |                | J+AB    | 0.910 (0.005) | 4.473 (0.070) |
| Blog            | Ridge          | Jackknife+ | 0.895 (0.008) | 3.011 (0.148) |
|                 |                | J+AB    | 0.895 (0.008) | 2.991 (0.148) |
|                 | RF             | Jackknife+ | 0.909 (0.008) | 3.165 (0.126) |
|                 |                | J+AB    | 0.902 (0.004) | 2.620 (0.063) |
|                 | NN             | Jackknife+ | 0.904 (0.006) | 3.111 (0.091) |
|                 |                | J+AB    | 0.896 (0.007) | 3.046 (0.102) |

both the jackknife+ and the jackknife+-after-bootstrap. We ran the jackknife+-after-bootstrap (Algorithm 2) using sampling with replacement with mean aggregation. We varied \(m\), the size of each bootstrap replicate, from \(m = 0.1n\) to \(m = n\) with an increment of \(0.1n\). Fixing \(\tilde{B} = 200\), a total of \(B \sim \text{Binomial}(\tilde{B}, (1 - \frac{1}{n+1}))^m\) bootstrap replicates were drawn at each run.

For comparison purposes, we chose the same three base regression algorithms as used in (Barber et al., 2019) — namely, ridge regression (RIDGE), random forests (RF) and neural networks (NN), with the same settings as used in Barber et al. (2019). We do not optimize these algorithms, as we are only interested in how the jackknife+-after-bootstrap performs with these models, and how it compares to the jackknife+.

### 5.3 Results

Table 1 displays the resulting average coverage and average interval width for each data set and each base algorithm, where for the jackknife+-after-bootstrap, the size of each bootstrap replicate is \(m = n\). Figure 1 displays the results over the range of \(m\) values for the MEPS data with RF as the base algorithm; due to limited space the remaining combinations are shown visually in the Appendix C. Note that the coverage of the jackknife+ is necessarily constant with respect to \(m\) because the method has no resampling; it is mainly displayed for ease of comparison with the jackknife+-after-bootstrap.

Although the assumption-free lower-bound on the coverage is only \(1 - 2\alpha\) for both the jackknife+-after-bootstrap and the jackknife+, Table 1 and Figure 1 make clear that both methods yield intervals with above or close to \(1 - \alpha\) coverage on average. The behavior is consistent for all data set and base regression method combinations we consider, as well as across all \(m\) in the case of the jackknife+-after-bootstrap.

Also noteworthy is that, when RF is used as the base algorithm, the jackknife+-after-bootstrap consistently yields shorter — and therefore more informative — intervals than the jackknife+. By contrast, there is little

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4The RF base algorithm we use subsamples the features but not the observations.
difference in interval widths for Ridge or NN, presumably because the base regression methods are not of the type to be greatly improved by bagging. This point is worth considering when choosing a method. In the case of RF, the jackknife+-after-bootstrap is likely to yield more efficient intervals at a comparable computational cost.

6 Conclusion

We propose the jackknife+-after-bootstrap, a computationally efficient method for constructing predictive intervals with assumption-free coverage guarantee, in the setting of ensemble learning. The jackknife+-after-bootstrap provides a mechanism for quantifying uncertainty in ensemble predictions that is both straightforward to implement and easy to interpret, and can therefore be easily integrated into existing ensembled models.

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A Additional Proofs

A.1 Proof of Theorem 1

For completeness, we give the full details of the proof of Theorem 1; a sketch of the proof is presented in Section 4.1.2 of the main paper.

Denote Algorithm 3 by \( \hat{A} \). We view \( \hat{A} \) as mapping a given input \( \{(X_i,Y_i)\}_{i=1}^{n+1} \) and a collection of subsamples or bootstrapped samples \( \hat{S}_1,\ldots,\hat{S}_B \) to a matrix of residuals \( R \in \mathbb{R}^{(n+1) \times (n+1)} \), where

\[
R_{ij} = \begin{cases} 
|Y_i - \hat{\mu}_{i,j}(X_i)| & \text{if } i \neq j, \\
0 & \text{if } i = j.
\end{cases}
\]

For any permutation \( \sigma \in \{1,\ldots,n+1\} \), let \( \Pi_\sigma \) stand for its matrix representation—that is, \( \Pi_\sigma \in \{0,1\}^{(n+1) \times (n+1)} \) has entries \( (\Pi_\sigma)_{\sigma(i),i} = 1 \) for each \( i \), and zeros elsewhere. Furthermore, for each subsample or bootstrapped sample \( \hat{S}_b = \{i_{b,1},\ldots,i_{b,m}\} \), write \( \sigma(\hat{S}_b) = \{\sigma(i_{b,1}),\ldots,\sigma(i_{b,m})\} \).

We now claim that

\[
R \overset{d}{=} \Pi_\sigma R \Pi_\sigma^T, \quad (5)
\]

for any fixed permutation \( \sigma \in \{1,\ldots,n+1\} \). Here \( R \) is the residual matrix obtained by a run of Algorithm 3; namely,

\[
R = \hat{A} \left( (X_1,Y_1),\ldots,(X_{n+1},Y_{n+1}); \hat{S}_1,\ldots,\hat{S}_B \right).
\]

To see why (5) holds, observe that deterministically, we have

\[
\Pi_\sigma R \Pi_\sigma^T = \hat{A} \left( (X_{\sigma(1)},Y_{\sigma(1)}),\ldots,(X_{\sigma(n+1)},Y_{\sigma(n+1)}); \sigma(\hat{S}_1),\ldots,\sigma(\hat{S}_B) \right).
\]

Furthermore, we have

\[
\left( (X_1,Y_1),\ldots,(X_{n+1},Y_{n+1}) \right) \overset{d}{=} \left( (X_{\sigma(1)},Y_{\sigma(1)}),\ldots,(X_{\sigma(n+1)},Y_{\sigma(n+1)}) \right)
\]

by Assumption 1 and

\[
\left( \hat{S}_1,\ldots,\hat{S}_B \right) \overset{d}{=} \left( \sigma(\hat{S}_1),\ldots,\sigma(\hat{S}_B) \right)
\]

since subsampling or resampling treats all the indices the same. Finally, the subsamples or bootstrapped samples (i.e., the \( \hat{S}_b \)'s) are drawn independently of the data points (i.e., the \( (X_i,Y_i) \)'s). Combining these calculations yields (5).

Next, given \( R \), define a “tournament matrix” \( A = A(R) \) as

\[
A_{ij} = \begin{cases} 
1 & \text{if } R_{ij} > R_{ji}, \\
0 & \text{if } i = j.
\end{cases}
\]

It is easily checked that \( A(\Pi_\sigma R \Pi_\sigma^T) = \Pi_\sigma A(R) \Pi_\sigma^T \), and hence (5) implies that

\[
A \overset{d}{=} \Pi_\sigma A(P) \Pi_\sigma^T. \quad (6)
\]

Let \( S_\alpha(A) \) be the set of row indices with row sums greater than or equal to \((1-\alpha)(n+1)\), i.e.,

\[
S_\alpha(A) = \left\{ i = 1,\ldots,n+1 : \sum_{j=1}^{n+1} A_{ij} \geq (1-\alpha)(n+1) \right\}.
\]

The argument of Step 3 in the proof of Barber et al. (2019) Theorem 1) applies to the lifted J+aB “tournament matrix” \( A \), and it holds deterministically that

\[
|S_\alpha(A)| \leq 2\alpha(n+1). \quad (7)
\]
On the other hand, if \( j \) is any index, and \( \sigma \) is any permutation that swaps indices \( n + 1 \) and \( j \), then

\[
\mathbb{P}[n + 1 \in S_\alpha(A)] = \mathbb{P}[j \in S_\alpha(\Pi_\sigma AP_i^T)] = \mathbb{P}[j \in S_\alpha(A)].
\]

The first two events are the same, and the second equality uses (6). Thus,

\[
\mathbb{P}[n + 1 \in S_\alpha(A)] = \frac{1}{n + 1} \sum_{j=1}^{n+1} \mathbb{P}[j \in S_\alpha(A)] = \frac{1}{n + 1} \mathbb{E} \left[ \sum_{j=1}^{n+1} \mathbb{I}[j \in S_\alpha(A)] \right] = \frac{\mathbb{E}[S_\alpha(A)]}{n + 1} \leq 2\alpha. \tag{8}
\]

Note that the event \( [n + 1 \in S_\alpha(A)] \) is exactly the event \( \hat{E}_{n+1} \), defined in Section 4.1.2. As described in the proof sketch in Section 4.1.2 of the main paper, we can couple this lifted event to the event \( \mathcal{E}_{n+1} \), also defined in Section 4.1.2 in terms of the actual jackknife-+ after-bootstrap, as follows. Let \( B = \sum_{b=1}^B \mathbb{I}[S_b \notin n + 1] \), the number of \( S_b \)'s containing only training data, and let \( 1 \leq b_1 < \cdots < b_B \leq B \) be the corresponding indices. Note that the distribution of \( B \) is Binomial, as specified in the theorem. Now, for each \( k = 1, \ldots, B \), define \( S_k = S_{b_k} \). We can observe that each \( S_k \) is an independent uniform draw from \( \{1, \ldots, n\} \) (with or without replacement). Therefore, we can equivalently consider running \( J + aB \) (Algorithm 2) with these particular subsamples or bootstrapped samples \( S_1, \ldots, S_B \), in which case it holds deterministically that

\[
\mu_{\tilde{\varphi}_{n+1,i} = \mu_{\tilde{\varphi}_i} \text{ for each } i = 1, \ldots, n} \quad \text{this ensures that} \quad |Y_{n+1} - \mu_{\varphi_{n+1,i}}(X_{n+1})| = |Y_{n+1} - \mu_{\varphi_{i}}(X_{n+1})| \quad \text{and} \quad |Y_i - \mu_{\varphi_{i,n+1}}(X_i)| = |Y_i - \mu_{\varphi_{i}}(X_i)|, \quad \text{and thus,}
\]

\[
\mathbb{P}[\mathcal{E}_{n+1}] = \mathbb{P}[\hat{E}_{n+1}] \leq 2\alpha.
\]

Finally, as in Step 1 in the proof of Barber et al. (2019, Theorem 1), it easily follows from the definition of \( \hat{C}_{\alpha,n,B} \) that if \( Y_{n+1} \notin \hat{C}_{\alpha,n,B}(X_{n+1}) \) then the event \( \hat{E}_{n+1} \) must occur. Indeed, if \( Y_{n+1} \notin \hat{C}_{\alpha,n,B}(X_{n+1}) \), then either \( Y_{n+1} \) falls below the lower bound, i.e.,

\[
\sum_{i=1}^{n} \mathbb{I}[Y_{n+1} - \mu_{\varphi_{i}}(X_{n+1}) < |Y_i - \mu_{\varphi_{i}}(X_i)|] \geq (1 - \alpha)(n + 1),
\]

or \( Y_{n+1} \) exceeds the upper bound, i.e.,

\[
\sum_{i=1}^{n} \mathbb{I}[Y_{n+1} - \mu_{\varphi_{i}}(X_{n+1}) > |Y_i - \mu_{\varphi_{i}}(X_i)|] \geq (1 - \alpha)(n + 1),
\]

and the above two expressions imply

\[
\sum_{i=1}^{n} \mathbb{I}[|Y_{n+1} - \mu_{\varphi_{i}}(X_{n+1})| > |Y_i - \mu_{\varphi_{i}}(X_i)|] \geq (1 - \alpha)(n + 1).
\]

Therefore, we conclude that

\[
\mathbb{P}[Y_{n+1} \notin \hat{C}_{\alpha,n,B}(X_{n+1})] \leq 2\alpha,
\]

thus proving the theorem.

### A.2 Proof of Proposition 1

By exchangeability, it suffices to prove the statement for a single \( i \in \{1, \ldots, n\} \). Fix \( i \), and let \( B_i \) denote the number of \( S_b \)'s not containing the index \( i \), i.e., \( B_i = \sum_{b=1}^B \mathbb{I}[S_b \notin i] \). For any fixed \( \gamma \in (0,1) \),

\[
\mathbb{P}^* \left[ |\mu_{\text{mean}}(X_i) - \mathbb{E}^*[\mu_{\text{mean}}(X_i)]| > \varepsilon \right] 
\leq \mathbb{P}^* \left[ |\mu_{\text{mean}}(X_i) - \mathbb{E}^*[\mu_{\text{mean}}(X_i)]| > \varepsilon \right. \quad \text{and} \quad B_i \geq \gamma \theta B \] \] \] \[ + \mathbb{P}^* \left[ B_i < \gamma \theta B \right].
\]

(As for our earlier notation \( \mathbb{E}^* \), here \( \mathbb{P}^* \) denotes expectation with respect to the random collection of subsamples or bootstrapped samples \( S_1, \ldots, S_B \), conditional on the data \( (X_1, Y_1), \ldots, (X_n, Y_n) \).)
The arithmetic mean aggregation function, $\varphi_{\text{mean}}$, satisfies
\[
\sup_{y_1, \ldots, y_B} |\varphi_{\text{mean}}(y_1, \ldots, y_B) - \varphi_{\text{mean}}(y_1, \ldots, y_{b-1}, y_{b'}, y_{b+1}, \ldots, y_B)| \leq \frac{u - \ell}{B_i}, \quad b = 1, \ldots, B_i.
\]
Thus, by McDiarmid’s inequality \cite[Theorem 6.2]{Boucheron2013},
\[
P^* \left[ |\hat{\mu}_{\text{mean}}(X_i) - E^*[\hat{\mu}_{\text{mean}}(X_i)]| > \varepsilon \mid B_i \geq \gamma \theta B \right] \leq 2 \exp \left( -\frac{2B\gamma \theta \varepsilon^2}{(u - \ell)^2} \right), \quad (9)
\]
On the other hand, $B_i \sim \text{Binomial}(B, \theta)$, where $\theta = (1 - \frac{1}{n})^m$ in the case of sampling with replacement, or $\theta = 1 - \frac{m}{n}$ for sampling without replacement. The Chernoff inequality for the binomial \cite[Chapter 2]{Boucheron2013} implies
\[
P[B_i < \gamma \theta B] \leq \exp \left(-\frac{B (1-\gamma)^2 \theta^2}{2}\right). \quad (10)
\]
Combining \eqref{eq:9} and \eqref{eq:10},
\[
P^* \left[ |\hat{\mu}_{\text{mean}}(X_i) - E^*[\hat{\mu}_{\text{mean}}(X_i)]| > \varepsilon \right] \leq 2 \exp \left(-\frac{2B\gamma \theta \varepsilon^2}{(u - \ell)^2}\right) + \exp \left(-\frac{B (1-\gamma)^2 \theta^2}{2}\right).
\]
Taking $\gamma = 1/\sqrt{B}$ yields
\[
P^* \left[ |\hat{\mu}_{\text{mean}}(X_i) - E^*[\hat{\mu}_{\text{mean}}(X_i)]| > \varepsilon \right] \leq 2 \exp \left(-\frac{2\sqrt{B}\theta \varepsilon^2}{(u - \ell)^2}\right) + \exp \left(-\frac{(\sqrt{B} - 1)^2 \theta^2}{2}\right).
\]

### A.3 Proof of Theorems \[\text{2} \text{ and } 3\]

Put $\hat{\mu}_{\varphi,i} = E^*[\hat{\mu}_{\varphi \setminus i}]$, where we recall that $E^*$ is the expectation conditional on the data. Let $R^*_{\varphi}$ denote the regression algorithm mapping data to $\hat{\mu}_{\varphi,i}$, i.e.,
\[
R^*_{\varphi} : \{(X_i, Y_i)\}_{i=1}^m \mapsto E^*[\varphi \left( \{ (X_{b,i}, Y_{b,i}) \}_{b=1}^m : b = 1, \ldots, B', B' \sim \text{Binomial}(B, \theta) \} \},
\]
where $\theta = \theta(n) = (1 - \frac{1}{n+1})^m$ (in the case of sampling with replacement) or $\theta = \theta(n) = 1 - \frac{m}{n+1}$ (in the case of sampling without replacement). We emphasize that $n$ here refers to the size of the sample being fed through $R^*_\varphi$ (e.g., each leave-one-out regressor $\hat{\mu}_{\varphi,i}$ is trained on $n - 1$ data points, so in this case, $\theta = \theta(n-1)$). $R^*_\varphi$ is a deterministic function of the data, since it averages over the random draw of the subsamples or bootstrapped samples. Furthermore, it is a symmetric regression algorithm (i.e., satisfies Assumption \[2\]). Fix some $\alpha' \in (0, 1)$ to be determined later, and construct the jackknife+ interval
\[
\hat{C}^{\ast+}_{\alpha',n}(x) = \left[q_{\alpha',n}(\hat{\mu}_{\varphi,i}(x) - R^*_i), q_{\alpha',n}(\hat{\mu}_{\varphi,i}(x) + R^*_i)\right],
\]
where $R^*_i = |Y_i - \hat{\mu}_{\varphi \setminus i}(X_i)|$ is the leave-one-out residual for this new regression algorithm. By \cite[Theorem 1]{Barber2019}, $C^{\ast+}_{\alpha',n}$ satisfies
\[
P \left[ Y_{n+1} \in \hat{C}^{\ast+}_{\alpha',n}(X_{n+1}) \right] \geq 1 - 2\alpha'. \quad (11)
\]
If, additionally, $R^*_\varphi$ satisfies the algorithmic stability condition \eqref{eq:3} given in Section 4.2 of the main paper, then by \cite[Theorem 5]{Barber2019}, the $2\varepsilon^*$-inflated jackknife+ interval
\[
\hat{C}^{\ast+\ast+}_{\alpha',n}(x) = \left[q_{\alpha',n}(\hat{\mu}_{\varphi,i}(x) - R^*_i) - 2\varepsilon^*, q_{\alpha',n}(\hat{\mu}_{\varphi,i}(x) + R^*_i) + 2\varepsilon^*\right]
\]
satisfies
\[
P \left[ Y_{n+1} \in \hat{C}^{\ast+\ast+}_{\alpha',n}(X_{n+1}) \right] \geq 1 - \alpha' - 4\sqrt{\delta^*}. \quad (12)
\]
Next, by Assumption 3 for each $i = 1, \ldots, n$,

$$
P \left[ \left| \hat{\mu}_{\varphi, i}(X_i) - \hat{\mu}_{\varphi, i}(X_i) \right| > \varepsilon \right] \leq \delta. \tag{13}$$

Let $\alpha' = \alpha - \sqrt{\delta}$. By the above argument, to prove the theorems, it suffices to show

$$\hat{C}_{\alpha,n,B}(X_{n+1}) \geq \hat{C}_{\alpha',n}(X_{n+1})$$

with probability at least $1 - 2\sqrt{\delta}$ in order to complete the proof of Theorem 2 or

$$\hat{C}_{\alpha,n,B}(X_{n+1}) \geq \hat{C}_{\alpha',n}(X_{n+1})$$

in order to complete the proof of Theorem 3. In fact, these two claims are proved identically—we simply need to show that

$$\hat{C}_{\alpha,n,B}(X_{n+1}) \geq \hat{C}_{\alpha',n}(X_{n+1})$$

with the choice $\varepsilon' = 0$ for Theorem 2 or $\varepsilon' = \varepsilon^*$ for Theorem 3.

To complete the proof, then, we establish the bound (14). Suppose $\hat{C}_{\alpha,n,B}(X_{n+1}) \geq \hat{C}_{\alpha',n}(X_{n+1})$. We have that either

$$q_{\alpha,n} \left\{ \hat{\mu}_{\varphi, i}(X_{n+1}) + R_i \right\} + 2\varepsilon < q_{\alpha',n} \left\{ \hat{\mu}_{\varphi, i}(X_{n+1}) + R_i \right\}$$

or

$$q_{\alpha,n} \left\{ \hat{\mu}_{\varphi, i}(X_{n+1}) - R_i \right\} - 2\varepsilon > q_{\alpha',n} \left\{ \hat{\mu}_{\varphi, i}(X_{n+1}) - R_i \right\},$$

where $R_i = |Y_i - \hat{\mu}_{\varphi, i}(X_i)|$. As in the proof of Barber et al. [2019] Theorem 5, this implies that

$$\left| \hat{\mu}_{\varphi, i}(X_{n+1}) - \hat{\mu}_{\varphi, i}(X_{n+1}) \right| + \left| \hat{\mu}_{\varphi, i}(X_i) - \hat{\mu}_{\varphi, i}(X_i) \right| \geq 2\varepsilon$$

for at least $[(1 - \alpha)(n+1)] - [(1 - \alpha')(n+1)] - 1 \geq \sqrt{\delta}(n+1)$ many indices $i = 1, \ldots, n$. Thus,

$$P \left[ \hat{C}_{\alpha,n,B}(X_{n+1}) \geq \hat{C}_{\alpha',n}(X_{n+1}) \right]$$

$$\leq \sum_{i=1}^{n} P \left[ \hat{\mu}_{\varphi, i}(X_{n+1}) - \hat{\mu}_{\varphi, i}(X_{n+1}) \right] + \hat{\mu}_{\varphi, i}(X_i) - \hat{\mu}_{\varphi, i}(X_i) \right| > 2\varepsilon \right] \geq \sqrt{\delta}(n+1)$$

$$\leq \frac{1}{\sqrt{\delta}(n+1)} \sum_{i=1}^{n} \left[ \hat{\mu}_{\varphi, i}(X_{n+1}) - \hat{\mu}_{\varphi, i}(X_{n+1}) \right] + \hat{\mu}_{\varphi, i}(X_i) - \hat{\mu}_{\varphi, i}(X_i) \right| > 2\varepsilon \right]$$

$$\leq \frac{2n}{\sqrt{\delta}(n+1)} \left[ \hat{\mu}_{\varphi, i}(X_{n+1}) - \hat{\mu}_{\varphi, i}(X_{n+1}) \right] \geq \varepsilon \right].$$

The second inequality is the Markov’s inequality, and the last step uses the exchangeability of the data points. Plugging in (13),

$$P \left[ \hat{C}_{\alpha,n,B}(X_{n+1}) \geq \hat{C}_{\alpha',n}(X_{n+1}) \right] \leq 2\sqrt{\delta},$$

implying (14). This completes the proofs for Theorems 2 and 3.

### B Jackknife-minmax-after-bootstrap

As in Barber et al. [2019], we may also consider the jackknife-minmax-after-bootstrap, which constructs the interval

$$\hat{C}_{\alpha,n,B}(x) = \left[ \min_i \hat{\mu}_{\varphi, i}(x) - q_{\alpha,n} \left\{ R_i \right\}, \max_i \hat{\mu}_{\varphi, i}(x) + q_{\alpha,n} \left\{ R_i \right\} \right].$$

The original jackknife-minmax satisfies $1 - \alpha$ lower bound on the coverage, and the same modification of the jackknife+ proof is applicable here, ensuring a $1 - \alpha$ lower bound on the coverage of the jackknife-minmax-after-bootstrap with the same caveat of a random $B$. However, as for the non-ensembled version, the method is too conservative, and is not recommend for practice.
C Supplementary Experiments

Figures 2 and 3 below show average coverage and average width, respectively, for all pairs of base regression method (RIDGE or RF or NN) and data set (COMMUNITIES or MEPS or BLOG). The precise experimental setup was described in Section 5. We remark that under RF and NN, the jackknife+-after-bootstrap returns markedly narrower intervals than the jackknife+, although both methods cover at \( \approx 1 - \alpha \) level. Under RIDGE, there is almost no difference between the jackknife+-after-bootstrap and the jackknife+ when it comes to the width of the intervals for all three data sets.
Figure 2: Average coverage results on all three data sets with three different base regression methods as \( m/n \) changes. The lines show the average, and the shaded areas show +/- one standard error, over 10 trials. The black dash-dotted line is the \( 1 - \alpha \) target coverage.
Figure 3: Average width results on all three data sets with three different base regression methods as $m/n$ changes. The lines show the average, and the shaded areas show $\pm$ one standard error, over 10 trials.