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#### Abstract

In this paper, three smoothed bootstrap methods are introduced for bivariate data. Two of them are based on Nonparametric Predictive Inference for bivariate data with both parametric and non-parametric copulas [10, 28, 29, 30]. The nonparametric predictive inference methods combined with copulas use generalizations of Hill's  $A_{(n)}$  assumption [23] for bivariate data. The third smoothed bootstrap method is based on uniform kernels. All smoothed bootstrap methods are compared to Efron's bootstrap method for bivariate data [14] through simulations. The comparison is conducted in terms of the coverage of percentile confidence intervals for the Pearson, Kendall and Spearman correlations, while also two simple functions of the bivariate observations are considered. From the study, it is found that the smoothed bootstrap methods mostly perform better than Efron's method in case of data simulated from a symmetric distribution and in case of the correlation between the variables is low or medium, in particular for small data sets. In the case of high dependence level between the variables, Efron's bootstrap method provides better results for the Pearson, Kendall and Spearman correlations due to its restriction in sampling from the data only, contrary to the smoothed bootstrap methods, which allow more variation in sampling.

**Keywords:** Efron's bootstrap method, Hill's  $A_{(n)}$  assumption, kernels, nonparametric predictive inference, parametric and non-parametric copulas.

# 1 Introduction

The bootstrap approach [13] is a simple non-parametric method introduced to infer accuracy of statistical estimates. It has been widely used for a variety of statistical problems as it relies on few mathematical assumptions and it leads to provide good results [17]. In situations where only little information is available to support the use of a specific probability distribution for statistical inference, the bootstrap method is of great practical use [11].

Efron [13] introduced the bootstrap method for univariate real-valued data. The method uses the original data set to create multiple bootstrap samples by sampling with replacement, and based on each bootstrap sample the statistic of interest is calculated. The empirical distribution of the resulting values can be used to approximate the distribution of the statistic of interest. Many references describe Efron's bootstrap method with applications, e.g. Berrar [4], Davison and Hinkley [11] and Efron and Tibshirani [17]. Based on kernels, linear interpolation and histospline smoothing, several smoothed bootstrap methods have been introduced to obtain better results; see e.g. Banks [3], De Angelis and Young [12], Hall [20], Silverman and Young [36], Young [41] for more details.

In 1981, Efron [14] introduced the bootstrap method for univariate rightcensored data. It is very similar to the one for real-valued data. The bootstrap samples are created by resampling from the original data set, and the statistic of interest is computed based on each bootstrap sample. The empirical distribution of those resulting values can be used for analysis. Based on the right-censoring  $A_{(n)}$  assumption, proposed by Coolen and Yan [9], a new smoothed bootstrap method has been introduced for better results; see Al Luhayb [1] and Al Luhayb et al [2] for more details.

Efron and Tibshirani [16] presented the bootstrap method for bivariate real-valued data. This method is quite similar to the method for univariate data. Multiple bootstrap samples are created by sampling with replacement from the original data set, and the statistic of interest is calculated based on each bootstrap sample. The empirical distribution of the resulting values can be a good proxy for the distribution of the statistic of interest. However, Efron's bootstrap method provides poor results for small data sets.

This paper introduces three smoothed bootstrap methods based on Nonparametric Predictive Inference with parametric and non-parametric copulas and uniform kernels. Advantages of the new smoothed bootstrap methods are discussed on four aspects. First, simulation studies mostly show that the proposed methods provide better results than Efron's method when the data distribution is symmetric. Secondly, the smoothed bootstrap methods provide better results than Efron's method for small data sets. Thirdly, they can provide better estimates in case of low and medium dependence levels between the variables. Fourthly, bootstrap samples created in the new methods do not include tied observations, which can be an advantage compared to the bootstrap samples created by Efron's method.

This paper is organized as follows: Section 2 presents Efron's bootstrap methods for univariate data and bivariate data. Section 3 presents an overview of the combination of NPI with parametric and non-parametric copulas for bivariate data [10, 28, 29]. Section 4 introduces two smoothed bootstrap methods based on NPI with copulas for such data and it presents the third smoothed bootstrap method based on box kernels assigned to the original observations. An example with data from the literature is presented in Section 5 to illustrate application of the proposed smoothed bootstrap methods and Efron's method. Comparisons between the proposed smoothed bootstrap methods and Efron's bootstrap method for bivariate data are presented in Section 6. Section 7 presents concluding remarks.

#### Efron's bootstrap methods 2

This section introduces Efron's bootstrap methods for univariate and bivariate data. For univariate data, let the real-valued random quantities  $X_1, X_2, \ldots, X_n$  be independent and identically distributed with distribution F, and  $x_1, x_2, \ldots, x_n$  be the observations corresponding to the random quantities  $X_1, X_2, \ldots, X_n$ . Furthermore, let  $\theta(F)$  be the statistic of interest.

In 1979, Efron [13] presented the bootstrap method for univariate realvalued data. Multiple bootstrap samples of size n are created by sampling with replacement from the original data set and the statistic of interest is computed based on each bootstrap sample. Let B denote the number of bootstrap samples, it is important that quite a large number of such samples is used, e.g. B = 1000. This leads to B values of the test statistic, and the empirical distribution of these B values is used as an estimate for the distribution of the statistic of interest,  $\theta(F)$ .

For bivariate real-valued data, Efron and Tibshirani [16] generalized the bootstrap method and it is used for different measures of statistical accuracy, e.g. standard errors and confidence intervals of some statistics of interest. Let the random quantities  $(X_i, Y_i) \in \mathbb{R}^2$ , for  $i = 1, 2, \ldots, n$ , be independent and identically distributed with distribution H, and let the observation corresponding to  $(X_i, Y_i)$  be denoted by  $(x_i, y_i)$ . Furthermore, let the statistic of interest be  $\theta(H)$ . Multiple bootstrap samples, e.g. B = 1000, of size n are created by sampling with replacement from the observed data, and based on each bootstrap sample, the statistic of interest is calculated. This leads to B values, and the empirical distribution of these B values is used as a proxy for the distribution of the statistic of interest; this is the same basic idea as for univariate data.

To derive a bootstrap estimate of the standard error of the sample statistic  $\hat{\theta}$ , denoted by  $\hat{\sigma}_{boot}$ , the standard deviation of the *B* resulting values,  $\hat{\theta}^{*1}, \hat{\theta}^{*2}, \ldots, \hat{\theta}^{*B}$ , can be computed by

$$\hat{\sigma}_{boot} = \sqrt{\frac{\sum_{j=1}^{B} (\hat{\theta}^{*j})^2 - (\sum_{j=1}^{B} \hat{\theta}^{*j})^2 / B}{B-1}}$$
(1)

For standard errors, Efron and Tibshirani [17] considered B to be in the range 25 to 200; however for hypotheses tests and confidence intervals, B should be at least 1000 for good results. In this paper, we use B = 1000.

# 3 Combination of nonparametric predictive inference and copulas

In 1959, Sklar [37] introduced the copula concept, which is a multivariate cumulative distribution function with uniform marginals on [0, 1], which we denote by C(.,.) in the case of bivariate data. It enables modelling dependence between random variables and constructing multivariate distributions. In the literature, copulas have been widely used for a variety of statistical applications due to their ability to model the dependence between random variables separately from the marginal distributions. Parametric and non-parametric copulas have been presented in the literature, and most of them are symmetric, see [6, 24, 31, 40] for more details. If the variables X and Y are exchangeable then the corresponding copula is symmetric. This symmetry can be written as  $C(F_X(x), F_Y(y)) = C(F_Y(y), F_X(x))$ , where  $F_X(x)$  and  $F_Y(y)$  are the cumulative distribution functions of the variables X and Y, respectively.

Coolen-Maturi et al [10] and Muhammad et al [29] used parametric and non-parametric copulas in combination with nonparametric predictive inference (NPI) on the marginals. The methods provide a partially specified predictive distribution for one future bivariate observation, and they both consist of two steps. For these methods, NPI is first assumed for the individual variables, then a copula is assumed in the second step to take the dependence between the variables into account. If a parametric copula is assumed in the second step, the method is referred to as the semi-parametric predictive method. If a non-parametric kernel-based copula is assumed in the second step, the method is referred to as the non-parametric predictive method.

To describe the two predictive methods, we use the notations and definitions presented in [10, 28, 29]. Let  $(x_i, y_i)$ , for i = 1, 2, ..., n, be the n bivariate real-valued observations corresponding to n exchangeable bivariate random quantities with no ties. For simplicity, the observations of each individual variable are ordered and denoted by  $x_i$  and  $y_j$ . This leads to  $x_1 < x_2 < \ldots < x_i < \ldots < x_n$  and  $y_1 < y_2 < \ldots < y_j < \ldots < y_n$ . Hill [23]

 $A_{(n)}$  assumption is used for the marginals, so we have

$$P(X_{n+1} \in (x_{i-1}, x_i)) = \frac{1}{n+1}$$
 and  $P(Y_{n+1} \in (y_{j-1}, y_j)) = \frac{1}{n+1}$  (2)

for i, j = 1, 2, ..., n + 1, where  $x_0 = a_x$ ,  $y_0 = a_y$ ,  $x_{n+1} = b_x$  and  $y_{n+1} = b_y$  in case of finite support  $[a_x, b_x]$  for  $X_{n+1}$  and  $[a_y, b_y]$  for  $Y_{n+1}$ , or with  $x_0 = -\infty$ ,  $y_0 = -\infty$ ,  $x_{n+1} = +\infty$  and  $y_{n+1} = +\infty$  in case the support is not restricted.

To link the first step to the second step of the predictive methods, where the copula concept takes the dependence structure in the data into account [10], a natural transformation of the random variables is used. Let  $\tilde{X}_{n+1}$  and  $\tilde{Y}_{n+1}$  denote transformed versions of the random quantities  $X_{n+1}$  and  $Y_{n+1}$ , respectively, such that

$$(X_{n+1} \in (x_{i-1}, x_i), Y_{n+1} \in (y_{j-1}, y_j)) \iff \left(\tilde{X}_{n+1} \in (\frac{i-1}{n+1}, \frac{i}{n+1}), \tilde{Y}_{n+1} \in (\frac{j-1}{n+1}, \frac{j}{n+1})\right)$$
(3)

for  $i, j = 1, 2, \dots, n+1$ .

After the transformation, the  ${\cal A}_{(n)}$  assumptions for the marginals are as follows

$$P\left(\tilde{X}_{n+1} \in \left(\frac{i-1}{n+1}, \frac{i}{n+1}\right)\right) = P\left(X_{n+1} \in (x_{i-1}, x_i)\right) = \frac{1}{n+1}$$
(4)

$$P\left(\tilde{Y}_{n+1} \in \left(\frac{j-1}{n+1}, \frac{j}{n+1}\right)\right) = P\left(Y_{n+1} \in \left(y_{j-1}, y_j\right)\right) = \frac{1}{n+1}$$
(5)

Two important points should be mentioned here. First, the transformation leads from the real space  $\mathbb{R}^2$  to  $[0,1]^2$ , where  $[0,1]^2$  is partitioned into  $(n+1)^2$  equal-sized blocks based on the *n* observed bivariate observations, as illustrated in Figure 1. Secondly, the uniform marginal distributions have been discretized on  $[0,1]^2$ , so that each column and each row has probability  $\frac{1}{n+1}$ .

## 3.1 The semi-parametric predictive method

The semi-parametric predictive method [10, 28] is as follows. The NPI method is used for the marginals in the first step as described above, and a parametric copula is assumed to take the dependence structure between the variables into account [28], which is the second step. To estimate the copula parameter, it is possible to use the transformed data, where the original observations are replaced by  $\left(\frac{r_i^x}{n+1}, \frac{r_i^y}{n+1}\right)$ , where  $r_i^x$  is the rank of the observation  $x_i$ among the x-observations, and  $r_i^y$  is the rank of the observation  $y_i$  among the y-observations.

The above descriptions for the first and second steps of the semi-parametric predictive method show that the NPI approach used for the variables is combined with the parametric copula to provide a partially specified predictive

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Fig. 1 Presentation of the transformed space.

distribution for one future bivariate observation. A probability is assigned to each of the  $(n + 1)^2$  blocks by the following formula

$$h_{ij}(\hat{\beta}) = P\left(\tilde{X}_{n+1} \in (\frac{i-1}{n+1}, \frac{i}{n+1}), \tilde{Y}_{n+1} \in (\frac{j-1}{n+1}, \frac{j}{n+1})|\hat{\beta}\right)$$
(6)

for i, j = 1, 2, ..., n + 1, where  $P(.|\hat{\beta})$  represents the assumed copula-based probability for the transformed data based on the original data and estimated copula parameter  $\hat{\beta}$ . The probabilities  $h_{ij}$  satisfy three conditions.  $h_{ij} \ge 0$ .  $\sum_{i=1}^{n} h_{ij} = \frac{1}{n+1}$  for all  $j \in \{1, 2, ..., n+1\}$  and  $\sum_{j=1}^{n} h_{ij} = \frac{1}{n+1}$  for all  $i \in \{1, 2, ..., n+1\}$ . This implies  $\sum_{i,j} h_{ij} = 1$ .

The copula parameter can be estimated by multiple procedures presented in the literature, see [18, 19, 25] for more details. In this paper, two estimation methods are considered for the semi-parametric predictive method, and those methods are widely used in the literature. The first estimation method is referred to as pseudo maximum likelihood estimation (PMLE), where the log pseudo likelihood function is [19]

$$\ell^*(\beta) = \sum_{i=1}^n \ln\left(c_\beta(\frac{r_i^x}{n+1}, \frac{r_i^y}{n+1})\right)$$
(7)

where  $c_{\beta}(u,v) = \frac{\partial^2}{\partial u \partial v} C_{\beta}(u,v)$ , and  $C_{\beta}(u,v)$  is the cumulative distribution function of a parametric copula. The pseudo maximum likelihood estimator is the value  $\hat{\beta}$  that maximizes  $\ell^*$ .

The second estimation method is the inversion of Kendall's tau (Itau), where the Kendall's tau formula and its population version in terms of the copula are [19]

$$\tau = \frac{4}{n(n-1)}P - 1 \text{ and } \tau(C_{\beta}) = 4\int_0^1 \int_0^1 C_{\beta}(u,v) \ dC_{\beta}(u,v) - 1 \qquad (8)$$

where P is the summation of concordant pairs in the sample. To compute the concordant pairs, we first order the pairs  $(x_i, y_i)$ , for i = 1, 2, ..., n, based on the x observations from smallest to greatest and rank the y observations, then at each ordered pair, we compute the number of y ranks that are greater than the y rank of that ordered pair. The summation of the resulting values will be P.  $\tau$  is the sample Kendall's correlation. The Itau estimator is the value  $\hat{\beta}$  resulting from solving the equation  $\tau = \tau(C_{\beta})$ . Both estimation methods are available in the R package VineCopula [33].

For more accuracy in estimating the copula parameter, Genest et al [18] and Kojadinovic and Yan [25] showed that the pseudo maximum likelihood estimation is better than the inversion of Kendall's tau method with consideration to mean square error when the sample size is greater than 100 or Kendall's correlation  $\tau \geq 0.4$ ; otherwise, the Itau method provides more accurate estimates.

### 3.2 The non-parametric predictive method

In the non-parametric predictive method for bivariate data [28, 29], the NPI approach is used for the variables, as described before, as first step. For the second step, a kernel smoothing copula is used, and an estimated probability density function  $\hat{c}$  can be defined as [28]:

$$\hat{c}(x,y) = \frac{1}{nb_X b_Y} \sum_{i=1}^n K\left(\frac{x - F_X(\tilde{X}_i)}{b_X}, \frac{y - F_Y(\tilde{Y}_i)}{b_Y}\right)$$
(9)

where  $K : \mathbb{R}^2 \to \mathbb{R}$  is a bivariate kernel function,  $b_X, b_Y > 0$  are the bandwidths, which are the smoothing parameters, and  $F_X(\tilde{X}_i) = \frac{r_x^i}{n+1}$  and  $F_Y(\tilde{Y}_i) = \frac{r_y^i}{n+1}$ .

Now, the NPI approach assumed for the marginals is combined with the non-parametric kernel-based copula to take the dependence structure into account. The kernel K(.,.) in Equation (9) can be any kernel function, popular choices for kernels in such copulas are e.g. Gaussian, Epanechnikov or Uniform, which are available in the R package np [21]. The values  $h_{ij}$  can be found by the following equation

$$h_{ij}(\hat{c}) = P\left(\tilde{X}_{n+1} \in (\frac{i-1}{n+1}, \frac{i}{n+1}), \tilde{Y}_{n+1} \in (\frac{j-1}{n+1}, \frac{j}{n+1})|\hat{c}\right)$$
(10)

where i, j = 1, 2, ..., n + 1 and  $P(.|\hat{c})$  is the non-parametric kernel-based copula probability with estimated kernel density function  $\hat{c}$ . Note that the values  $h_{ij}$ satisfy the three conditions mentioned after Equation (6) in Subsection 3.1.

To implement this predictive method, it is important to choose the bandwidths  $b_X$  and  $b_Y$  for the kernel. In the literature, there is a range of recommendations for different scenarios, see e.g. [22, 26, 28, 35] for more details. In this paper, we use Equation (11) as the normal reference rule-of-thumb bandwidth.

$$b_Z = 1.06 \ \hat{A}_Z \ n^{-1} \tag{11}$$

where  $\hat{A}_Z = \min\left(\hat{\sigma}_Z, \frac{IQR(Z)}{1.349}\right)$ ,  $\hat{\sigma}_Z$  is the estimate of the standard deviation of the variable Z, IQR(Z) is the interquartile range of Z, the 1.349 value is the interquartile range of the standard normal distribution and n is the sample size.

# 4 Smoothed bootstrap methods

This section introduces the smoothed bootstrap methods for bivariate data based on the predictive methods presented in Section 3 and on uniform kernels. They are presented based on the theory of NPI and kernel methods, and then their performances are investigated and compared with Efron's method in terms of the coverage probability. Furthermore, they avoid ties, which occur in the bootstrap samples created by Efron's bootstrap method. The smoothed bootstrap method based on the semi-parametric predictive method is referred to by SBSP, and the one based on the non-parametric predictive method by SBNP. We call the smoothed bootstrap method based on uniform kernels the smoothed Efron's bootstrap and refer to it by SEB.

Let the random variables  $(X_i, Y_i) \in \mathbb{R}^2$ , for i = 1, 2, ..., n, be independent and identically distributed with distribution F, and let  $(x_i, y_i)$ , for i = 1, 2, ..., n, be the observations corresponding to these random variables. Furthermore, suppose that  $\theta(F)$  is the statistic of interest.

# 4.1 The SBSP method

Based on the original data set, the semi-parametric predictive method creates  $(n+1)^2$  squares dividing the sample space and this method assigns probabilities  $h_{ij}(\hat{\beta})$  to those squares by Equation (6) [28]. For simplicity, the smoothed bootstrap algorithm for bivariate data based on the semi-parametric predictive method is described as follows [1]:

- 1. Apply the semi-parametric predictive method to the original data to create  $(n+1)^2$  squares and compute their estimated probabilities  $h_{ij}(\hat{\beta})$ .
- 2. Sample with replacement n squares with their estimated probabilities  $h_{ij}(\hat{\beta})$ , then draw one bivariate observation from each chosen square. This leads to create one smoothed bootstrap sample of size n, and it is denoted by  $D_{boot}^* = \{(x_1^*, y_1^*), (x_2^*, y_2^*), \dots, (x_n^*, y_n^*)\}.$
- 3. Calculate the statistic of interest,  $\hat{\theta}^* = \hat{\theta}(D^*_{boot})$ .

4. Perform Steps (2) and (3) *B* times to create *B* bootstrap samples with their statistics of interest  $\hat{\theta}^{*1}, \hat{\theta}^{*2}, \dots, \hat{\theta}^{*B}$ .

For the case of finite support, all squares dividing the sample space are finite. This enables uniform sampling from the selected squares during the bootstrap procedure. In contrast, when the sample space is infinite from any side, infinite shapes will occur, and this makes it impossible to sample uniformly from those infinite shapes. For this issue, we will use the idea proposed by BinHimd [5], Coolen and Himd [8] for the infinite intervals when the data is univariate, but the idea is generalized for two dimensional data. If an infinite shape is selected during the bootstrap procedure and the block's range is  $(-\infty, x_1)$  or  $(x_n, +\infty)$ , Normal distribution tails will be assumed with mean  $\mu$  and standard deviation  $\sigma$ , and these parameters are defined such that the probability in the interval is  $\frac{1}{n+1}$ . Therefore, the parameters are computed by

$$\hat{\mu} = \frac{x_{(1)} + x_{(n)}}{2}$$

$$\hat{\sigma} = \frac{x_{(n)} - \mu}{\Phi^{-1}(\frac{n}{n+1})}$$
(12)

where  $\Phi$  is the standard Normal cumulative distribution function.

After assuming the Normal distribution tails, a value is sampled from the left tail for  $(-\infty, x_1)$ , and a value is sampled from the right tail for  $(x_n, +\infty)$ . The x observation sampled from either tail of the Normal distribution will be considered as the x value of the bivariate future observation. For the case of infinite internals from either lower or upper bound, the block's range is  $(-\infty, y_1)$  or  $(y_n, +\infty)$ , the same method will be applied with regard to the variable Y. The y observation sampled from either tail will be considered as the y value of the bivariate future observation.

## 4.2 The SBNP method

In this smoothed bootstrap method, the non-parametric predictive method is used to divide the sample space into  $(n+1)^2$  squares based on the original data and to compute the probabilities  $h_{ij}(\hat{c})$  by Equation (10) [28]. For simplicity, the algorithm of this bootstrap can be described as follows [1]:

- 1. Apply the non-parametric predictive method to the original data to create  $(n+1)^2$  squares and compute their estimated probabilities  $h_{ij}(\hat{c})$ .
- 2. Sample with replacement n squares with their estimated probabilities  $h_{ij}(\hat{c})$ , then draw one bivariate observation from each chosen square. This leads to create one smoothed bootstrap sample of size n, and it is denoted by  $D_{boot}^* = \{(x_1^*, y_1^*), (x_2^*, y_2^*), \dots, (x_n^*, y_n^*)\}.$
- 3. Calculate the statistic of interest,  $\hat{\theta}^* = \hat{\theta}(D_{boot}^*)$ .
- 4. Perform Steps (2) and (3) *B* times to create *B* bootstrap samples with their statistics of interest  $\hat{\theta}^{*1}, \hat{\theta}^{*2}, \ldots, \hat{\theta}^{*B}$ .

For the case of infinite support, we follow the technique we described in Section 4.1 to sample observations from the Normal distribution tails for the infinite intervals.

# 4.3 Smoothed Efron's bootstrap

With Efron's bootstrap samples, ties occur due to the resampling procedure from the original data set to create the bootstrap samples. To avoid ties to occur in the bootstrap samples, we need to relax the resampling assumption of Efron's bootstrap method. In this section, a new smoothed bootstrap method is introduced based on uniform kernels assigned to the observed data points, and the method is referred to as smoothed Efron's bootstrap method, SEB. Each observation is surrounded by a block of size  $b_X \times b_Y$ , where the observation is located in the center of its corresponding block. Due to the distances among the observations and the size of blocks, the created blocks could be overlapping. To create one smoothed Efron's bootstrap sample, we sample n blocks with replacement, then sample one observation uniformly from each selected block. To illustrate the smoothed Efron's bootstrap method, n equal-sized blocks are created and assigned to the observed data points, as shown in Figure 2 for n = 4, where  $b_X$  and  $b_Y$  are computed by Equation (11), but we replace  $n^{-1}$  by  $n^{-\frac{1}{4}}$  to have more smoothness in sampling; we discuss the choice of bandwidths later for best performance in Section 6.2. The algorithm of this smoothed version of Efron's bootstrap is as follows [1]:

- 1. Create n blocks of size  $b_X \times b_Y$  with the observed data points at their center.
- 2. Sample *n* blocks with replacement, then sample one bivariate observation uniformly from each selected block. This step creates one smoothed bootstrap sample of size *n*, which is denoted by  $D_{boot}^* = \{(x_1^*, y_1^*), (x_2^*, y_2^*), \dots, (x_n^*, y_n^*)\}.$
- 3. Calculate the estimate of the statistic of interest,  $\hat{\theta}^* = \hat{\theta}(D_{hoot}^*)$ .
- 4. Perform Steps (2) and (3) *B* times in order to have *B* bootstrap estimates of the statistic  $\theta(F)$ ; this leads to  $\hat{\theta}^{*1}, \hat{\theta}^{*2}, \dots, \hat{\theta}^{*B}$ .

To illustrate the new smoothed bootstrap methods along with Efron's bootstrap method, we use one example from the literature in the following section.



Fig. 2 The kernels assigned to the observed data points.

# 5 Example

This section introduces an example using data from the literature on 30 elevenyear-old girls attending Heaton Middle School in Bradford [28]; the data are presented in Table 1 and Figure 3. For the 30 girls, the data set includes height in meters (m) and weight in kilogram (kg), and the body mass index (BMI), where BMI can be computed by

$$BMI = \frac{\text{Weight (kg)}}{[\text{Height (m)}]^2}$$
(13)

By using this data set, we want to estimate the Pearson correlation between height and weight for such girls, which we denote by  $\hat{r}$ , and the standard error of r along with the 90% bootstrap confidence interval for r based on the proposed bootstrap methods and Efron's bootstrap method. The sample Pearson, Kendall and Spearman correlations between height and weight are 0.742, 0.631, 0.807, respectively.

By each bootstrap method, 1000 bootstrap samples of size n = 30 are created. The Pearson correlation is computed based on each bootstrap sample, and this leads to 1000 values of estimates;  $\hat{r}^{*1}, \hat{r}^{*2}, \ldots, \hat{r}^{*1000}$ . By taking the mean of these 1000 values, the bootstrap estimate for r is derived, and its

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Height (m)	Weight (kg)	BMI	Height (m)	Weight (kg)	BMI
1.350	26.000	14.270	1.330	31.001	17.530
1.460	33.000	15.480	1.491	34.000	15.310
1.530	55.000	23.500	1.411	32.001	16.100
1.540	50.000	21.080	1.640	47.000	17.470
1.390	32.000	16.560	1.462	37.000	17.360
1.310	25.000	14.570	1.492	46.000	20.720
1.490	44.000	19.820	1.470	36.003	16.660
1.370	31.000	16.520	1.520	47.001	20.340
1.430	36.000	17.600	1.400	33.001	16.840
1.461	35.000	16.420	1.431	42.000	20.540
1.410	28.000	14.080	1.480	32.002	14.610
1.360	28.001	15.140	1.493	32.003	14.410
1.541	36.001	15.180	1.412	29.000	14.590
1.510	48.000	21.050	1.371	34.001	18.110
1.550	36.002	14.980	1.351	30.000	16.460

Table 1 The heights (m) and weights (kg) of 30 eleven-year-old girls.



Fig. 3 Heights (m) and corresponding weights (kg) values of 30 eleven-year-old girls.

standard error can be estimated by Equation (1). For the 90% bootstrap confidence interval, the lower and upper bounds are the 50th and 950th ordered values of the 1000 resulting values, respectively. All bootstrap estimates are presented in Table 2.

Table 2 presents the bootstrap estimates for r, SE(r) and the 90% confidence interval for r based on the smoothed bootstrap methods and Efron's bootstrap method. For the Pearson correlation r, all bootstrap methods show that there is a positive correlation between height and weight. The largest estimate is based on the SBSP method; the lowest estimate is based on the SBNP

Table 2 The estimated results for r, SE(r) and the 90% confidence interval for r based on each bootstrap method.

Method	$\hat{r}$	$SE(\hat{r})$	90% confidence interval
SBSP	0.791	0.069	(0.670, 0.884)
SBNP	0.652	0.120	(0.437,  0.830)
Efron	0.742	0.061	(0.639, 0.832)
SEB	0.720	0.063	(0.632, 0.834)

**Table 3** The estimated results for  $\theta$ , SE( $\theta$ ) and the 90% confidence interval for  $\theta$  based on each bootstrap method.

Method	$\hat{ heta}$	$SE(\hat{\theta})$	90% confidence interval
SBSP	17.100	0.479	(16.350, 17.870)
SBNP	17.230	0.591	(16.310, 18.250)
Efron	17.110	0.455	(16.410, 17.900)
SEB	17.080	0.446	(16.360, 17.830)

method. The smoothed bootstrap method based on the non-parametric predictive method, SBNP, provides the largest estimate for the standard error of r and wider 90% confidence interval. This could be because the method has more variation in sampling. In contrast, Efron's method and the SEB method have smaller estimates for SE(r) and narrower confidence intervals due to their processes of sampling. In general, all bootstrap methods provide clear evidence of positive correlation between the variables as the sample size and the number of bootstrap samples are large and there is roughly linear relationship between the variables, as shown in Figure 3.

Another interest of using the data set is to estimate the mean  $\theta$  of the body mass index for all girls in such a population, and this is denoted by  $\hat{\theta}$ . It is aimed to quantify the uncertainty in this estimate by considering the standard error of  $\hat{\theta}$  along with the 90% bootstrap confidence interval for  $\theta$  based on the proposed bootstrap methods and on Efron's bootstrap method. The sample mean of the body mass index is 17.110.

Based on each bootstrap method, 1000 bootstrap samples of size n = 30 are created, and the mean of the body mass index is computed based on each bootstrap sample. This leads to 1000 estimates;  $\hat{\theta}^{*1}, \hat{\theta}^{*2}, \ldots, \hat{\theta}^{*1000}$ . The mean of these 1000 estimates is the bootstrap estimate for  $\theta$ , its standard error is estimated by Equation (1). For the 90% bootstrap confidence interval, the lower and upper bounds are the 50th and 950th ordered values of the 1000 estimates, respectively. All bootstrap estimates are presented in Table 3.

Table 3 presents the bootstrap estimates  $\theta$ , their standard errors SE( $\theta$ ) and the 90% confidence intervals for  $\theta$  based on the smoothed bootstrap methods and Efron's bootstrap method. For the mean  $\theta$  of the body mass index, all bootstrap methods provide nearly identical estimates. The largest estimate is based on the SBNP method; the lowest estimate is based on the SEB method. The smoothed bootstrap method based on the non-parametric predictive method, SBNP, provides the largest estimate for the standard error of

**Table 4** The estimated results for  $\theta$ , SE( $\theta$ ) and the 90% confidence interval for  $\theta$  based on Efron's bootstrap method and Banks' bootstrap method for univariate data.

Method	$\hat{ heta}$	$SE(\hat{\theta})$	90% confidence interval
$\mathrm{Efron}_U$	17.107	0.467	(16.338, 17.894)
Banks	17.148	0.470	(16.393, 17.927)

 $\theta$  and wider 90% confidence interval. This could be because the method has more variation in sampling. In contrast, Efron's method and the SEB method have smaller estimates for SE( $\theta$ ) and narrower confidence intervals due to their processes of sampling.

It is worth to compare the proposed bootstrap methods for bivariate data with the alternative bootstrap methods for univariate data when the function of interest is univariate and the data is bivariate as the case of BMI Example. Table 4 presents the bootstrap estimates  $\hat{\theta}$ , their standard errors SE( $\theta$ ) and the 90% confidence intervals for  $\theta$  based on Efron's bootstrap method and Banks' bootstrap method for univariate data. The results are nearly identical to those of the SBSP, SBNP, Efron and SEB methods, which are presented in Table 3.

# 6 Comparison of the bootstrap methods

In the literature, many statistical studies consider as primary requirement for confidence regions that the difference between the nominal and estimated coverage probabilities is small [3], and many simulations are considered with high confidence levels, e.g. 0.90, 0.95 and 0.99. However, Banks [3] considered the whole coverage probability scale to investigate the performance of bootstrap methods. Banks first divides the whole real line by the quantiles of the statistic of interest into a certain number of regions, then he investigates the distribution of coverage probabilities over those regions. In this paper, we create 10 confidence regions with nominal coverage probability 0.10 by

$$CR_{(i)} = \left(q_{\left(\frac{\alpha_{i+1}}{2}\right)}, q_{\left(\frac{\alpha_{i}}{2}\right)}\right) \cup \left(q_{\left(1-\frac{\alpha_{i}}{2}\right)}, q_{\left(1-\frac{\alpha_{i+1}}{2}\right)}\right)$$
(14)

where i = 1, 2, ..., 10,  $\alpha_{i+1} = \alpha_i - 0.10$ ,  $\alpha_1 = 1$  and  $q_{(z)}$  is the  $z^{th}$  quantile of the statistic of interest.

The null hypothesis is that the coverage probabilities are equal for the 10 confidence regions; each confidence region has confidence level 0.10, and the test is as follows

 $H_0$ : The coverage probabilities are equally distributed over the 10 regions.

 $H_1$ : Not all coverage probabilities are equal.

(15)

To perform this hypothesis test, Banks [3] used the chi-square goodness of fit test. Banks used this method to compare his smoothed bootstrap method to other bootstrap methods, namely smoothed Rubin's bootstrap [3], Efron's method [13] and Rubin's Bayesian bootstrap [32], and the best bootstrap

Table 5The copula families with the marginal distributions used to generate bivariatedata sets.

Scenario	Copula	X	Y	au
1	Normal	U(0,1)	U(0,1)	-0.75, -0.50, -0.25, 0, 0.25, 0.50, 0.75
2	Gumbel	U(0,1)	U(0,1)	0,0.25,0.50,0.75
3	Clayton	N(1, 1)	N(5, 3)	0.75

method is the one with the smallest chi-squared value,  $\chi^2$ . In other words, the best method is the one with the lowest discrepancy between the nominal and estimated coverage probabilities for a specific statistic. In this paper, we use this technique to compare the proposed bootstrap methods, presented in Section 4, and Efron's bootstrap method for bivariate data.

For the chi-squared goodness of fit test, the significance level is set equal to 0.05, the 95th percentile of the chi-squared distribution with 9 degrees of freedom is equal to 16.92. For a chi-squared test statistic value less than 16.92, the null hypothesis is not rejected. For a chi-squared test statistic value greater than 16.92, the null hypothesis is rejected, and in this case it is important to consider whether this is mostly due to over-coverage or under-coverage in the first regions,  $CR_{(1)}, CR_{(2)}$  and  $CR_{(3)}$ , which are located in the centre. For simplicity, we use the over (under) lines to indicate the over-(under-)coverage proportions in the first confidence regions. This helps to understand why a large chi-squared test statistic value is obtained.

To generate bivariate data sets and compare the proposed bootstrap methods with Efron's method, three copula families are considered with different Kendal correlation  $\tau$ , which has a one-to-one relationship with the copula parameter  $\beta$ , and different sample sizes n. For the first scenario, the Normal copula model is used. The marginal distributions of X and Y are both Uniform(0, 1). This scenario is considered because the Normal copula is symmetric and more appropriate [27]. For the second scenario, the Gumbel copula model is used. This copula is asymmetric and has strong right-tail dependence and relatively weak left-tail dependence [38]. The marginal distributions of X and Y are both Uniform(0,1). For the third scenario, the Clavton copula is used. This copula is asymmetric and models greater dependence in the negative tail than in the positive tail [28]. The marginal distribution of X is Normal( $\mu = 1, \sigma = 1$ ) and the marginal distribution of Y is Normal( $\mu = 5, \sigma = 3$ ). All these scenarios are specified in Table 5. For the first two scenarios, the standard Uniform is used for the marginals to investigate how the bootstrap methods perform in case of finite support, but for the third scenario, we use Normal distributions with different means and different standard deviations to show how the bootstrap methods perform in case of infinite support.

In the simulations, we use sample sizes n = 10, 50, 100, and the statistics of interest are the Pearson (r), Kendall  $(\tau)$  and Spearman  $(r_S)$  correlations, which are widely used in the literature to measure the dependence between the variables and to show the direction of the relationship between the variables,

whether is positive or negative. These statistics are as follows [7]

$$r = \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \overline{x})^2 \sum_{i=1}^{n} (y_i - \overline{y})^2}} \\ \tau = \frac{4}{n(n-1)}P - 1$$

$$r_S = 1 - \frac{6\sum_{i=1}^{n} d_i^2}{n(n^2 - 1)}$$
(16)

where *n* is number of observations,  $x_i$  and  $y_i$  are the observations of the variables X and Y, respectively, and  $\overline{x} = \frac{\sum_{i=1}^{n} x_i}{n}$  and  $\overline{y} = \frac{\sum_{i=1}^{n} y_i}{n}$ . *P* is the summation of concordant pairs in the sample.  $d_i$  is the difference between the  $x_i$  and  $y_i$  ranks.

We also investigate the estimated coverage proportions for the averages of  $T_1 = X + Y$  and  $T_2 = XY^2$ , which are referred to by  $\overline{T_1}$ , and  $\overline{T_2}$ , respectively. These statistics are considered to investigate the performance of bootstrap methods for some simple functions of X and Y.

For the smoothed bootstrap method based on the semi-parametric predictive method, the pseudo MLE method is used to estimate the copula parameter  $\beta$  when  $\tau \geq 0.4$  [19]; otherwise the inversion of Kendall's tau is used. For the smoothed bootstrap method based on the non-parametric predictive method, the Normal kernel is applied with the bandwidths calculated by Equation (11). To apply this method, we used the package np in R software [21].

## 6.1 First scenario

For the case of finite support, the first scenario listed in Table 5 is used to generate N = 1000 bivariate data sets, and based on those created data sets, the smoothed bootstrap methods are compared with Efron's method. Each bootstrap method is applied B = 1000 times for each created data set, and the statistic of interest is computed based on each bootstrap sample. This leads to 1000 resulting values, and based on these values, the 10 confidence regions can be derived by Equation (14). We then calculate the proportions of confidence regions which include the true statistic of interest. This procedure is repeated for all N = 1000 created data sets in order to observe the estimated coverage proportions for the true statistic of interest in the 10 confidence regions. Based on the proportions, the corresponding chi-squared value can be computed for each bootstrap method. Tables 6 to 10 present the chi-squared values obtained from the estimated coverage proportions for r,  $\tau$ ,  $r_S$ ,  $\overline{T_1}$  and  $\overline{T_2}$ , respectively, based on each bootstrap method.

Table 6 presents the chi-squared values for the Pearson correlation r based on each bootstrap method. For larger chi-squared values, we use over- and under-lines to illustrate the over- and under-coverage proportions in the first three confidence regions. When n = 10 and  $\tau = -0.25, 0, 0.25$ , the SBSP, SBNP and SEB methods provide large chi-squared values due to under-coverage, but

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	<i>n</i> =		10				50				100			
$\tau$	β	r	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
-0.75	-0.9239	-0.92	29.98	54.34	91.22	$\overline{79.36}$	12.32	7.32	14.96	13.06	16.82	12.08	9.82	4.16
-0.50	-0.7071	-0.69	15.04	11.06	<u>70.16</u>	14.58	9.28	15.70	7.66	6.18	7.32	7.34	6.62	10.32
-0.25	-0.3827	-0.37	<u>27.92</u>	<u>24.16</u>	<u>48.90</u>	<u>30.98</u>	7.46	12.02	9.48	4.40	$\overline{20.20}$	4.82	10.24	3.46
0	0	0	24.52	35.54	56.84	<u>34.62</u>	8.18	6.50	14.48	6.86	11.72	11.44	11.92	7.82
0.25	0.3827	0.37	<u>43.18</u>	20.44	<u>37.86</u>	<u>24.90</u>	8.96	8.04	9.94	5.96	17.56	10.62	<u>26.24</u>	15.98
0.50	0.7071	0.69	8.00	4.82	80.84	<u>24.94</u>	7.28	9.64	13.54	5.26	$\overline{21.22}$	11.04	4.78	11.14
0.75	0.9239	0.92	126.20	65.24	<u>116.46</u>	$\overline{64.38}$	17.32	7.72	<u>25.62</u>	14.86	$\overline{24.88}$	11.92	5.76	11.64

Table 6 The chi-squared values for the Pearson correlation r.



Fig. 4 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for r based on each bootstrap.

these methods lead to over-coverage when  $\tau = -0.75$  and 0.75. At this sample size for all levels of dependence, Efron's method always provides larger chisquared values due to under-coverage. As the sample size increases to 50 and 100, all these bootstrap methods perform mostly well. Figure 4 indicates the simulation results as the number of simulations for which the null hypothesis  $H_0$  is not rejected and the number of simulations for which the null hypothesis  $H_0$  is rejected due to over- and due to under-coverage, regardless of the sample size. This figure suggests that the SBNP method is the best method, followed by the SEB method. These two smoothed bootstrap methods do not reject  $H_0$ in 16 and 15 cases, respectively, out of 21 simulations.

In Table 7, the chi-squared values for Kendall's correlation  $\tau$  are presented. This statistic is computed based on the concordance of data, and the smoothed bootstrap methods influence the rank of observed data points by the probabilities  $\hat{h}_{ij}$  for blocks and by sampling uniformly from the chosen blocks during the bootstrap procedures. This influence can be seen for high dependence levels  $\tau$ , in particular for the SEB method. As the sample size increases to 50 and 100, the SBSP and SBNP methods mostly perform well. The SBSP method provides small chi-squared values because the Normal copula is assumed in the semi-parametric predictive method and the same parametric copula is used to

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1	ı =		1	0			50	D		100				
$\tau$	β	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	
-0.75	-0.9239	$\overline{261.68}$	65.06	70.50	63.92	5.96	14.08	19.08	<u>69.00</u>	6.60	13.50	16.26	86.06	
-0.50	-0.7071	53.06	$\overline{52.00}$	$\overline{18.70}$	$\overline{104.02}$	8.14	7.56	3.60	9.20	3.10	10.26	10.08	6.66	
-0.25	-0.3827	8.78	$\overline{21.00}$	12.70	32.22	7.66	5.08	5.76	3.98	14.90	$\overline{17.18}$	18.30	11.60	
0	0	<u>17.98</u>	14.54	$\overline{33.54}$	$\overline{21.74}$	8.34	3.78	12.28	6.14	8.58	15.82	9.62	14.90	
0.25	0.3827	<u>18.60</u>	16.38	6.86	$\overline{28.68}$	11.12	8.86	9.58	9.92	<u>19.92</u>	13.98	16.72	13.18	
0.50	0.7071	5.44	71.66	$\overline{24.74}$	$\overline{103.40}$	16.94	6.94	8.40	8.98	11.28	8.32	10.44	10.12	
0.75	0.9239	$\overline{259.48}$	$\overline{92.50}$	$\overline{149.00}$	$\overline{73.92}$	$\overline{23.72}$	$\overline{24.94}$	11.38	20.02	19.76	10.20	12.18	46.66	

**Table 7** The chi-squared values for the Kendall correlation  $\tau$ .



Fig. 5 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $\tau$  based on each bootstrap.

create the data sets. Figure 5 shows that the SBNP method and Efron's bootstrap method are the methods which most often do not reject  $H_0$ ; they both do not reject  $H_0$  14 times and rejecting  $H_0$  7 times due to over-coverage in the first three confidence regions.

Table 8 presents the chi-squared values for Spearman's correlation  $r_S$ . This correlation is computed based on the difference between the ranks of the corresponding x and y observations, and the ranks may be influenced by the smoothed bootstrap methods due to their variation in sampling. For high dependence levels, e.g.  $\tau = -0.75, 0.75$ , the SEB method provides the largest chi-squared values compared to the other bootstrap methods, but with low dependence levels, it provides good results. The SBSP and SBNP methods along with Efron's method perform mostly well, but Efron's method is better, in particular for large data sets. To illustrate the performances of the bootstrap methods, Figure 6 presents the simulation results. This figure shows that the method, which most often does not reject  $H_0$ , is Efron's method due to the resampling process, which helps to not change the ranks of the corresponding x and y observations. This is contrary to the smoothed bootstrap methods, which have more variation in sampling. Efron's method is followed by the

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	<i>n</i> =			1	0			5	0		100			
$\tau$	β	$r_S$	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
-0.75	-0.9239	-0.92	$\overline{125.18}$	140.32	137.38	410.24	4.46	22.26	10.02	142.30	14.38	8.38	7.86	94.86
-0.50	-0.7071	-0.69	39.38	34.02	38.24	$\overline{69.18}$	7.12	7.72	6.70	9.40	11.66	8.38	9.18	9.80
-0.25	-0.3827	-0.37	10.82	10.52	5.80	$\overline{27.80}$	6.84	6.88	8.12	6.34	15.06	8.18	10.66	7.00
0	0	0	<u>17.58</u>	15.46	14.72	$\overline{18.64}$	11.74	3.12	7.34	11.62	7.48	6.98	6.98	15.96
0.25	0.3827	0.37	<u>20.04</u>	8.64	6.26	19.84	5.50	15.04	15.92	20.32	13.70	12.38	13.36	12.00
0.50	0.7071	0.69	35.92	$\overline{51.54}$	39.00	70.34	13.40	4.18	9.34	14.08	16.90	12.48	3.58	9.70
0.75	0.9239	0.92	89.14	116.40	147.30	445.88	30.48	11.70	3.60	82.30	33.88	12.52	4.58	63.20

**Table 8** The chi-squared values for the Spearman correlation  $r_S$ .



Fig. 6 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $r_S$  based on each bootstrap.

SBNP method. Out of 21 different cases, Efron's method does not reject  $H_0$  17 times and the SBNP method does not reject  $H_0$  16 times.

In Tables 9 and 10, the chi-squared values for the averages of  $T_1$  and  $T_2$  are presented, respectively. When n = 10 for all dependence level situations, the smoothed bootstrap methods are better than Efron's method in distributing the coverage proportions for both statistics  $\overline{T_1}$  and  $\overline{T_2}$  over the 10 confidence regions. At this sample size, all chi-squared values corresponding to Efron's method are large due to under-coverage in the first three confidence regions. Having under-coverage in the first three confidence regions could be due to the resampling process. As the sample size increases to 50 and 100 with no regard to the dependence level, Efron's method mostly provides good results for both statistics  $\overline{T_1}$  and  $\overline{T_2}$ . This leads to not rejecting  $H_0$  in most cases, but the smoothed bootstrap methods perform better at these sample sizes. In Figures 7 and 8, the simulation results are presented to show the number of times that  $H_0$  is not rejected and the number of times that  $H_0$  is rejected due to over- and due to under-coverage in the first three confidence regions. These figures show that the SBSP and SBNP methods are the best in terms of providing small chi-squared values for  $T_1$ ; they both lead to not reject  $H_0$ 17 times for the 21 cases. For  $\overline{T_2}$ , the SBSP and SBNP methods perform well

	<i>n</i> =		10					50	)		100			
$\tau$	β	$\overline{T_1}$	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
-0.75	-0.9239	1	85.86	$\overline{131.72}$	47.60	8.16	9.08	9.68	11.30	4.76	12.40	15.44	13.92	7.64
-0.50	-0.7071	1	24.44	$\overline{23.84}$	<u>47.12</u>	<u>17.10</u>	8.54	5.88	10.14	5.26	10.80	12.48	18.02	11.46
-0.25	-0.3827	1	13.90	$\overline{18.16}$	<u>39.96</u>	<u>28.14</u>	7.32	7.04	12.88	7.54	7.94	16.00	<u>28.02</u>	<u>20.72</u>
0	0	1	15.76	11.24	<u>40.04</u>	<u>28.26</u>	10.92	4.08	10.82	11.20	12.46	<u>17.32</u>	<u>19.04</u>	16.56
0.25	0.3827	1	8.90	8.56	41.94	33.04	20.10	7.10	17.98	15.20	14.22	4.60	10.44	17.68
0.50	0.7071	1	18.10	10.76	<u>37.50</u>	29.56	10.12	5.38	6.90	9.72	7.42	12.28	9.80	10.42
0.75	0.9239	1	9.72	9.74	36.48	31.62	13.28	6.60	7.08	6.58	13.38	9.12	13.48	13.00

**Table 9** The chi-squared values for  $\overline{T_1}$ .



Fig. 7 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $\overline{T_1}$  based on each bootstrap.

in most cases, but the SBSP method is better, as it does not reject  $H_0$  in 17 cases while the SBNP method does not reject  $H_0$  in 15 cases.

In each case of dependence level  $\tau$  and sample size n, we compare the bootstrap methods by counting how often a method provides the lowest chisquared value, with no consideration whether the value leads to rejecting the null hypothesis  $H_0$  or not. For each statistic of interest, we count the number of times that each method provides the lowest chi-squared values among all values. For example when n = 10 and  $\tau = -0.75$  in Table 6, the chi-squared values corresponding to the SBSP, SBNP and SEB methods are 29.98, 54.34 and 79.36, respectively; and all these values are large due to over-coverage in the first three confidence regions. The chi-squared value corresponding to Efron's method is 91.22, which is large due to under-coverage. In this situation, we count one for the SBSP method because its chi-squared value is the lowest value among all. The summaries based on Tables 6 to 10 are presented in Table 11. Each score in this table is indicated with three numbers, which are the numbers of chi-squared values that lead to not reject  $H_0$  and reject  $H_0$  due to over-coverage and due to under-coverage, respectively.

In Table 11, the SBNP and SEB methods have the highest score for the Pearson's correlation r, which is 8, but the SEB method performs better than the SBNP method because the former does not reject  $H_0$  7 times while the

	<i>n</i> =		10					50	)		100				
τ	β	$\overline{T_2}$	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	
-0.75	-0.9239	0.090	49.10	$\overline{49.72}$	46.28	5.42	26.02	8.08	17.86	14.64	7.70	8.66	9.60	3.52	
-0.50	-0.7071	0.109	13.28	8.52	<u>98.94</u>	<u>44.70</u>	7.12	11.88	10.44	9.04	6.12	8.56	7.70	3.66	
-0.25	-0.3827	0.136	18.46	<u>17.26</u>	<u>91.22</u>	<u>75.34</u>	12.46	8.64	10.64	<u>19.38</u>	4.26	15.18	16.08	6.14	
0	0	0.167	10.04	17.02	<u>110.96</u>	<u>87.78</u>	1.80	4.94	7.56	12.14	4.54	15.62	21.80	13.76	
0.25	0.3827	0.197	8.12	$\overline{19.06}$	<u>87.32</u>	<u>73.42</u>	12.22	10.30	5.14	14.94	11.62	<u>21.78</u>	<u>17.76</u>	15.14	
0.50	0.7071	0.224	19.04	11.40	<u>71.12</u>	<u>61.26</u>	14.68	5.94	8.80	11.34	2.90	<u>17.94</u>	4.40	16.56	
0.75	0.9239	0.243	15.30	15.74	42.60	<u>36.12</u>	16.54	9.76	8.98	<u>18.94</u>	6.04	9.50	5.92	12.28	

**Table 10** The chi-squared values for  $\overline{T_2}$ .



Fig. 8 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $\overline{T_2}$  based on each bootstrap.

**Table 11** The summary of scores for the bootstrap methods for the five statistics of interest along with the number of chi-squared values of each score that lead to not reject  $H_0$  and reject  $H_0$  due to over-coverage and under-coverage, (# not rejecting  $H_0$ , # rejecting  $H_0$  due to over-coverage, # rejecting  $H_0$  due to under-coverage).

Function	SBSP	SBNP	Efron	SEB
r	2(0,1,1)	8 (6,0,2)	3(3,0,0)	8(7,1,0)
au	6(6,0,0)	6(6,0,0)	4(3,1,0)	5(3,2,0)
$r_S$	5(2,3,0)	5(4,1,0)	9(9,0,0)	3(3,0,0)
$\overline{T_1}$	6 (6,0,0)	9 (9,0,0)	0(0,0,0)	6(5,0,1)
$\overline{T_2}$	9(9,0,0)	6(5,0,1)	3(3,0,0)	3(3,0,0)

SBNP method does not reject  $H_0$  6 times. For the Kendall's correlation  $\tau$ , the SBSP and SBNP methods are the best with score 6; this could be due to the Normal copula, which is used for generating and for analysis when applying the SBSP method. The SBNP method scores 6 as well. For the same statistic of interest, the SEB method is the second best with score 5. For the Spearman's correlation  $r_S$ , Efron's method is the best with score 9 and all chi-squared values do not support the rejection of  $H_0$ . This result is rational because Efron's bootstrap method, which is sampling with replacement, does not affect the ranks of the corresponding x and y observations, contrary to the smoothed bootstrap methods, which have more variation in sampling. The

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<i>n</i> =			10					50	)		100				
τ	β	r	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	
0	1	0	<u>28.50</u>	9.84	<u>31.42</u>	<u>17.36</u>	6.00	7.98	13.40	9.08	7.80	8.80	7.10	5.68	
0.25	1.3333	0.36	<u>23.72</u>	<u>19.10</u>	33.02	<u>18.96</u>	16.86	14.52	13.08	7.88	14.12	6.28	9.86	5.32	
0.50	2	0.68	12.26	8.12	<u>68.14</u>	<u>25.66</u>	25.24	10.28	<u>21.92</u>	7.58	<u>19.40</u>	6.96	7.64	7.86	
0.75	4	0.92	16.58	$\overline{41.54}$	116.02	60.10	33.00	16.82	12.90	<u>35.94</u>	22.66	15.32	9.60	59.52	

**Table 12** The chi-squared values for the Pearson correlation r.



Fig. 9 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for r based on each bootstrap.

second best is the SBNP method with score 5, and 4 chi-squared values out of 5 lead to not reject  $H_0$ . For the average of  $T_1$ , the SBNP method is the best, followed by the SBSP method. For the average of  $T_2$ , the SBSP method is the best with score 9, and the SBNP method is the second best with score 6, and 5 chi-squared values out of 6 are not rejecting  $H_0$ . The SBSP and SBNP methods are the best for the averages of  $T_1$  and  $T_2$  and this could be because the SBSP and SBNP methods allow more variations in sampling to create the bootstrap samples than Efron's method and the SEB method.

## 6.2 Second scenario

From the second scenario presented in Table 5, multiple bivariate data sets are created. For the smoothed bootstrap method based on the semi-parametric predictive method, the Normal copula is assumed in order to compute the probabilities  $\hat{h}_{ij}$  by Equation (6). In this section, we want to investigate how the SBSP method performs when the copula model used for analysis is different to the model used to generate data sets.

The smoothed bootstrap methods are compared to Efron's bootstrap method through simulations with consideration to the second scenario presented in Table 5. The chi-squared values are presented in Tables 12 to 16 for  $r, \tau, r_S$  and the statistics  $\overline{T_1}$  and  $\overline{T_2}$ , and Figures 9 to 13 visualize the results, respectively. For the Pearson correlation r, the best method not rejecting  $H_0$ 

1	n = 10					50	)		100				
τ	β	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
0	1	14.40	$\overline{30.58}$	41.98	$\overline{26.98}$	6.84	4.78	10.32	8.10	12.84	12.28	5.66	11.46
0.25	1.3333	$\overline{31.68}$	$\overline{43.54}$	30.44	$\overline{62.58}$	<u>18.74</u>	13.46	12.88	12.88	<u>17.52</u>	4.14	3.18	3.40
0.50	2	<u>26.34</u>	52.60	36.94	98.36	<u>29.18</u>	8.06	9.74	8.92	<u>17.02</u>	11.22	3.14	4.98
0.75	4	303.20	$\overline{58.60}$	85.00	49.04	28.76	15.72	13.16	<u>33.10</u>	18.90	10.16	9.86	49.56

**Table 13** The chi-squared values the Kendall correlation  $\tau$ .



Fig. 10 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $\tau$  based on each bootstrap.

is the smoothed bootstrap method based on the non-parametric predictive method. The SBNP method does not reject  $H_0$  10 times out of 12 cases as shown in Figure 9. For the Kendall correlation  $\tau$ , the SBNP method and Efron's method provide the best results to not reject  $H_0$ . From Figure 10, the methods lead to not reject  $H_0$  8 times and they reject  $H_0$  4 times due to over-coverage occurring in the first three confidence regions. For the Spearman correlation  $r_S$ , the best method is Efron's method. As shown in Figure 11, Efron's method does not reject  $H_0$  9 times and it rejects  $H_0$  3 times due to over-coverage. For the statistics  $\overline{T_1}$  and  $\overline{T_2}$ , the SBSP method is the best to not reject  $H_0$  as illustrated in Figures 12 and 13. This bootstrap method leads to not reject  $H_0$  10 times for both statistics  $\overline{T_1}$  and  $\overline{T_2}$ . Efron's method and the SEB method always lead to under-coverage for  $\overline{T_1}$  and  $\overline{T_2}$  when the sample size is 10. For large data sets, both these bootstrap methods provide mostly good results.

Table 17 presents the summary of scores for each bootstrap method providing the lowest chi-squared values on each statistic of interest. For the Pearson's correlation r, the best method is the SEB method with score 5. For the Kendall's correlation  $\tau$ , Efron's method is the best with score 7, and in 6 cases, the method leads to not reject  $H_0$ . For the Spearman's correlation  $r_S$ and  $\overline{T_1}$ , the best method is the SBNP method, which scores 5 for these statistics, and all values in these cases indicate that the SBNP method distribute

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	n =		10				50				100			
τ	β	$r_S$	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
0	1	0.00	27.70	13.38	15.38	21.02	10.30	13.10	11.70	7.78	9.20	15.48	16.20	6.86
0.25	1.3333	0.36	<u>23.76</u>	23.48	20.86	36.52	19.74	5.74	11.26	9.58	13.42	7.56	12.16	15.94
0.50	2	0.68	42.74	44.46	29.50	69.06	18.92	5.18	7.04	6.82	16.28	5.70	5.72	7.94
0.75	4	0.92	123.14	<u>112.48</u>	105.14	<u>398.76</u>	18.00	<u>25.68</u>	10.70	<u>266.32</u>	12.02	<u>22.94</u>	15.02	<u>248.46</u>

**Table 14** The chi-squared values for the Spearman correlation  $r_S$ .



Fig. 11 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $r_S$  based on each bootstrap.

the coverage proportions equally over the 10 confidence regions; this bootstrap method does not support rejection  $H_0$ . The SBSP method is the second best for  $\overline{T_1}$ , and it is the best method for  $\overline{T_2}$ .

Through simulations, we observed some important issues that should be pointed out. First, as the sample size increases with high dependence levels, the SEB method mostly provides large chi-squared values for  $r, \tau$  and  $r_S$  due to under-coverage in the first three confidence regions. From this observation, it may be beneficial to use small bandwidths for this bootstrap method when the dependence level  $\tau$  is greater than 0.50 or less than -0.50,  $\tau > 0.50$  or  $\tau < -0.50$ . To illustrate this, the simulations based on the second scenario are repeated with different bandwidth sizes. Equation (11) is considered for small bandwidths, but for large bandwidths  $n^{-1}$  is replaced by  $n^{-\frac{1}{4}}$ . Note that increasing the bandwidth size leads to more variation in sampling, which may lead to bad results in the situation of high dependence between the variables X and Y. Table 18 presents the simulation results, and it shows that the SEB method with small bandwidths mostly provides better results.

Secondly, the Itau estimation method is better than the PMLE estimation method for estimating the copula parameter  $\beta$  when applying the semiparametric predictive method, in particular when the dependence level  $\tau \leq 0.4$ . This estimation technique leads to better results for the SBSP method for some statistics of interest. Thirdly, we assume the Normal copula to apply the semiparametric predictive method due to its ability to model negative and positive

	n =		10				50				100			
τ	β	$\overline{T_1}$	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
0	1	1	13.46	8.68	<u>48.98</u>	<u>42.68</u>	12.86	10.42	5.44	2.58	5.16	12.96	9.34	10.50
0.25	1.3333	1	13.46	11.88	<u>33.98</u>	<u>33.18</u>	13.28	$\overline{17.16}$	14.62	14.88	19.56	7.90	<u>16.96</u>	13.88
0.50	2	1	7.94	13.38	<u>35.64</u>	28.92	6.26	3.72	6.54	6.56	12.64	8.50	14.64	17.16
0.75	4	1	20.86	22.52	24.82	<u>27.12</u>	7.60	8.52	8.70	12.14	13.56	$\underline{21.94}$	<u>17.02</u>	12.22

**Table 15** The chi-squared values for the statistic  $\overline{T_1}$ .



Fig. 12 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $\overline{T_1}$  based on each bootstrap.

correlations. Fourthly, the smoothed bootstrap methods based on the semiparametric and non-parametric predictive methods may provide poor results for the correlations  $r, \tau$  and  $r_S$  when the data distribution is asymmetric, contrary to the first and second scenarios, and this will be investigated through simulations in the next section.

## 6.3 Third scenario

From the third scenario listed in Table 5, N = 1000 data sets are created. In this scenario, the Clayton copula is used with dependence level  $\tau = 0.75$ , and the marginal distributions are  $X \sim \text{Normal}(\mu = 1, \sigma = 1)$  and  $Y \sim \text{Normal}(\mu = 5, \sigma = 3)$ . This data distribution is asymmetric. For each generated data set, each bootstrap method is applied B = 1000 times and the same comparison technique as in Sections 6.1 and 6.2 is used again. Table 19 presents the simulation results, it shows that the SBSP and SBNP methods provide poor results for the Pearson's, Kendall's and Spearman's correlations. For the same statistics of interest but with large data sets, the SBSP method continues to perform poorly, but the SBNP method improves. This could be because we use the Normal copula, which is symmetric, with the SBSP method while the data distribution is asymmetric so that the simulation results continue to be bad even with large data sets. The simulation results based on the

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	n =		10				50				100			
τ	β	$\overline{T_2}$	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
0	1	0.167	8.46	18.20	<u>110.82</u>	<u>104.00</u>	9.36	9.54	7.40	4.96	8.54	6.80	9.30	10.00
0.25	1.3333	0.199	5.24	26.44	<u>109.44</u>	<u>99.06</u>	12.04	12.00	12.14	13.18	<u>34.80</u>	14.78	16.64	<u>17.72</u>
0.50	2	0.225	11.70	24.08	<u>83.70</u>	<u>68.78</u>	5.76	6.12	8.30	11.80	<u>23.40</u>	<u>17.14</u>	20.18	<u>21.70</u>
0.75	4	0.243	15.02	18.26	<u>78.00</u>	<u>54.00</u>	5.66	10.48	10.90	6.86	10.18	12.76	12.34	9.56

**Table 16** The chi-squared values for the statistic  $\overline{T_2}$ .



Fig. 13 The number of times that  $H_0$  is not rejected, and the number of times that  $H_0$  is rejected due to over-coverage and due to under-coverage for  $\overline{T_2}$  based on each bootstrap.

**Table 17** The summary of scores for the bootstrap methods for the five statistics of interest along with the number of chi-squared values of each score that lead to not reject  $H_0$  and reject  $H_0$  due to over-coverage and under-coverage, (# not rejecting  $H_0$ , # rejecting  $H_0$  due to over-coverage, # rejecting  $H_0$  due to under-coverage).

Function	SBSP	SBNP	Efron	SEB
r	2(2,0,0)	3(3,0,0)	2(2,0,0)	5(4,0,1)
au	2(1,0,1)	2(2,0,0)	7(6,1,0)	2(1,1,0)
$r_S$	1(1,0,0)	5(5,0,0)	4(1,3,0)	2(2,0,0)
$\overline{T_1}$	5(4,1,0)	5(5,0,0)	0(0,0,0)	2(2,0,0)
$\overline{T_2}$	6(6,0,0)	4(3,0,1)	0(0,0,0)	2(2,0,0)

**Table 18** The chi-squared values obtained from the coverage proportions for  $r, \tau$  and  $r_S$  using the SEB method with two bandwidth sizes, where the copula parameter  $\beta = 4$ .

n =	1	0	5	0	100			
Bandwidth	small $(n^{-1})$	large $(n^{-\frac{1}{4}})$	small $(n^{-1})$	large $(n^{-\frac{1}{4}})$	small $(n^{-1})$	large $(n^{-\frac{1}{4}})$		
r = 0.92	<u>85.10</u>	$\overline{60.10}$	<u>19.84</u>	35.94	11.30	<u>59.52</u>		
$\tau=0.75$	$\overline{91.18}$	$\overline{49.04}$	12.52	<u>33.10</u>	9.20	49.56		
$r_S=0.92$	15.22	398.76	25.76	266.32	<u>18.20</u>	248.46		

SBNP method are improved as the sample size increases because the probabilities  $h_{ij}$  over the  $(n+1)^2$  blocks become close to the model probabilities for

n =		10		50	)		100					
Function	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB	SBSP	SBNP	Efron	SEB
r = 0.89	37.54	<u>4341.90</u>	249.22	15.70	425.88	154.50	<u>33.40</u>	13.48	1488.24	34.22	<u>19.36</u>	12.44
$\tau=0.75$	$\overline{210.52}$	<u>5701.30</u>	$\overline{34.54}$	64.18	<u>70.46</u>	<u>297.40</u>	8.54	6.34	<u>42.84</u>	11.58	9.80	<u>18.66</u>
$r_S=0.91$	$\overline{185.64}$	$\underline{7369.40}$	87.42	19.40	37.02	142.04	7.04	11.44	<u>31.12</u>	7.42	8.94	10.34
$\overline{T_1} = 6.00$	27.14	<u>47.86</u>	50.04	44.28	12.56	5.54	6.80	5.60	7.68	10.62	12.62	13.94
$\overline{T_2} = 58.63$	89.92	236.22	183.74	<u>174.48</u>	18.52	17.40	12.68	10.28	10.20	3.40	7.60	20.28

Table 19 The chi-squared values obtained from the coverage proportions for the true statistics of interest with copula parameter  $\beta = 6$ .

the blocks. For  $\overline{T_1}$  and  $\overline{T_2}$ , the SBSP and SBNP bootstrap methods provide large chi-squared values when n = 10 due to under-coverage in the first three confidence regions. As the sample size increases, their results improve. In this scenario, all these bootstrap methods provide good results for large data sets.

# 7 Concluding remarks

This paper introduced three smoothed bootstrap methods for bivariate data based on the semi-parametric and non-parametric predictive methods and on uniform kernels. These bootstrap methods are compared to Efron's bootstrap method through simulations in terms of the coverage proportions for the Pearson, Kendall and Spearman correlations along with the averages of  $T_1$  and  $T_2$ , where  $T_1 = X + Y$  and  $T_2 = XY^2$ . In the simulations, we consider different dependence levels  $\tau$  and sample sizes n = 10, 50 and 100.

From the simulations, we observed some important features in the results that should be mentioned. First, for the case of a symmetric data distribution, the SBNP method mostly provides better results for the Pearson correlation rthan the other bootstrap methods. When we consider the Kendall correlation  $\tau$  and the Spearman correlation  $r_S$ , it is better to use Efron's method due to its resampling process. This process does not influence the rank of observations, which is used to compute these statistics of interest. For the statistics  $\overline{T_1}$ and  $\overline{T_2}$ , the SBSP and SBNP methods mostly provide the lowest discrepancies between the nominal and actual coverage proportions, in particular for small data sets. Secondly, for the case of an asymmetric data distribution, it may be beneficial to use either the SEB method or Efron's method. They mostly provide better results because they have less variation in sampling than the SBSP and SBNP methods. Thirdly, Efron's method and the SEB method with small bandwidth size perform well for  $r, \tau$  and  $r_S$  in case of high dependence between the variables, contrary to the SBSP and SBNP method, which decrease the correlation between the variables by their processes of sampling. Fourthly, the proposed smoothed bootstrap methods mostly provide better outcomes for all statistics when the dependence level is low or medium because the smoothed methods allow more variation in sampling, which lead to better estimates, in particular for small data sets. Lastly, it seems that with a large enough sample, Efron's method leads to bootstrap samples that reflect linear relations

between X and Y well and remain close to the real linear relation, while the smoothed methods, due to more variation in sampling, perform less well.

Due to the processes of sampling related to the smoothed bootstrap methods, ties occur with probability zero in the bootstrap samples, contrary to the bootstrap samples created by Efron's method. This helps to compute the statistic of interest easily; with Efron's bootstrap samples, there is a need to break the ties in some real applications, so more assumptions may be needed. For more details, we refer to [39], which describes the issue of ties in a storm characteristics example.

In running R codes, the SBSP method takes approximately four times as long as Efron's method. This is mainly due to fitting the Normal copula on each created data set to calculate the probabilities  $h_{ij}$ , sampling uniformly from the limited squares and getting observations from the fitted normal tails for the unlimited squares. However, the SBNP and SEB methods require approximately equal computation time as Efron's method.

This paper has introduced new smoothed bootstrap methods for bivariate data, and presented an initial investigation of their performance. Future research is needed to consider the performance in more detail and to compare the methods with more alternative bootstrap methods, e.g. those presented by Efron and Gong [15]. Extending the proposed bootstrap methods to non-iid data is also and important topic for future research [34]. The proposed methods can be generalized to multivariate data beyond 2 dimensions by using the NPI method with multi-dimensional copulas, this is left as a topic for future research.

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