

DENSITY ESTIMATION FOR GROUPED DATA WITH APPLICATION TO LINE TRANSECT SAMPLING

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Line transect sampling is a method used to estimate wildlife populations, with the resulting data often grouped in intervals. Estimating the density from grouped data can be challenging. In this paper, we propose a kernel density estimator of wildlife population density for such grouped data. Our method uses a combined cross-validation and smoothed bootstrap approach to select the optimal bandwidth for grouped data. Our simulation study shows that with the smoothing parameter selected with this method, the estimated density from grouped data matches the true density more closely than with other approaches. Using smoothed bootstrap, we also construct bias-adjusted confidence intervals for the value of the density at the boundary. We apply the proposed method to two grouped data sets, one from a wooden stake study where the true density is known, and the other from a survey of kangaroos in Australia.

1. Introduction. In ecology, it is often of great interest to study the abundance of wildlife populations. A common approach for estimating the abundance of a biological population is distance sampling (Barabesi, 2000; Barabesi et al, 2002; Chen, 1996), of which line transect sampling is an example. A comprehensive review of distance sampling can be found in Burnham et al (1980) and Buckland et al (2001).

In such studies, the detectability of individual data points often varies with the distance and selection biases are common. In the basic line transect scheme, for example, a number of lines of total length L are randomly placed in the region of interest. Observers then move along these lines and record the perpendicular distance of each detected animal from the line. Animals further away from the lines are more likely to be missed and this can be modeled via a detection probability function $p(x)$ that represents the conditional probability of detecting an animal, given that the animal is at perpendicular distance x from the line. Buckland et al (2001) showed that the density function of observed distances, denoted $f(x)$, can be obtained from $p(x)$ by re-scaling $p(x)$ to integrate to 1.

In line transect sampling, it is assumed that the line transects are placed independently of the animal population so that the animals are distributed

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uniformly in distance from the lines. The decrease in observations with distance is then attributed to the detection function $p(x)$.

Several assumptions about $p(x)$ are also often made. Since animals are more likely to be missed with increasing distance from the observer, $p(x)$ is assumed to be monotonically decreasing with x . Furthermore, it is assumed that $p(0) = 1$ and $p'(0) = 0$, where p' is the derivative of p with respect to x , the former representing the assumption that an animal on the line will not be missed. By adding the assumption that $\int_0^\infty p(x) dx < \infty$, [Burnham and Anderson \(1976\)](#) showed that the average number of animals per unit area, D , can be estimated with

$$(1.1) \quad \hat{D} = \frac{n\hat{f}(0)}{2L},$$

where n is the number of observations, L the total length of the line transects and $\hat{f}(0)$ is an estimate of $f(0)$.

The rather unintuitive formula (1.1) can be better understood as follows; suppose that a strip of width $2w$ and total length L is surveyed and n animals are detected. The animal density is then given by

$$D = \frac{n}{2wLP_a},$$

where P_a is the unconditional detection probability of an animal in the strip of area $2wL$, which can be expressed as

$$P_a = \frac{1}{w} \int_0^w p(x) dx.$$

With $f(x) = p(x)/\int_0^w p(x) dx$, and $p(0) = 1$, one can show

$$P_a = \frac{1}{wf(0)},$$

giving (1.1).

Due to the difficulty in measuring distances, the observations are often grouped into convenient distance markers, such as multiples of five or ten. Thus estimation of animal populations using line transect sampling involves estimating a density function f from grouped data. In particular, the value of the density at the boundary, specifically, at $x = 0$, is of interest.

Various estimation techniques have been proposed for use with line transect data. [Buckland et al \(2001\)](#) introduced parametric modeling of f , of which Fourier series estimators ([Burnham et al, 1980](#)) form a subclass. Other methods include kernel density estimation ([Chen, 1996](#); [Mack and Quang,](#)

1998) and semiparametric methods (Barabesi, 2000; Barabesi et al, 2002). The reader is asked to refer to the cited works for details on these methods.

Parametric methods work well if the model is correct. Also, in smaller data sets, the data may be grouped into as few as 3 or 4 groups. In these cases, parametric models using covariate information will be useful (Marques and Buckland, 1992). Here, we focus on nonparametric methods, in particular, on kernel density estimation using grouped data. In the context of line transect sampling, the aim will be the estimation of $f(0)$. However, our proposed method for bandwidth selection in density estimation from grouped data has applications beyond line transect sampling (see Section 7).

Nonparametric estimation of $f(0)$ has a number of challenges in the grouped data setting:

1. DENSITY ESTIMATION FROM GROUPED DATA: When data are grouped, using risk function estimators such as the cross-validation score function to choose the optimal smoothing parameter can be problematic since the risk function estimators tend to be monotone decreasing functions of the smoothing parameter. As a result, using cross-validation for optimal smoothing parameter selection may lead to undersmoothing.
2. DENSITY ESTIMATION AT THE BOUNDARY: Since distances are non-negative, the support of the density should not include any negative values. To satisfy this condition, one must modify the original kernel density estimator to remove any boundary bias.
3. OBTAINING CONFIDENCE INTERVALS: The standardized form of the nonparametric estimator \hat{f} can be expressed as the sum of two terms:

$$\frac{\hat{f}(x) - f(x)}{\sqrt{\text{Var}(\hat{f}(x))}} = \frac{\hat{f}(x) - \text{E}(\hat{f}(x))}{\sqrt{\text{Var}(\hat{f}(x))}} + \frac{\text{E}(\hat{f}(x)) - f(x)}{\sqrt{\text{Var}(\hat{f}(x))}}.$$

While the first term converges to the standard normal distribution by the central limit theorem, in nonparametric inference the second term is not negligible because of the bias-variance trade-off. Common smoothing techniques require the bias and the standard error to be of the same order. Therefore, confidence intervals based on the traditional form of $\hat{f}(x) \pm z_{\alpha/2} \sqrt{\text{Var}(\hat{f}(x))}$ do not necessarily achieve the nominal level.

Note that the second and third points above are also common issues in nonparametric inference for ungrouped data as well. Chen (1996) and Mack and Quang (1998) used kernel methods to address these two issues for ungrouped data. Barabesi et al (2002) developed a semiparametric method

for grouped data, but used the traditional form of the confidence interval for $f(0)$. Optimal bandwidth selection plays an important role in addressing the second and third issues whether data are grouped or not. In this work, we develop an inference procedure that addresses all three issues together.

Specifically, we propose a combined cross-validation and smoothed bootstrap procedure to select the optimal bandwidth in kernel density estimation with grouped data and to construct bias-adjusted confidence intervals for the density at the boundary. To adjust for the boundary bias, we employ a symmetrization technique introduced by [Buckland \(1992\)](#). Our methods can be easily extended to multivariate cases. We are not aware of any other work that addresses all aforementioned issues together.

The paper is organized as follows. [Section 2](#) provides a brief overview of kernel density estimators and includes a description of the symmetrization technique for kernel density estimates at the boundary. In [Section 3](#), we introduce a smoothed bootstrap approach for bandwidth selection for grouped data. [Section 4](#) explains our approach for constructing bias-adjusted confidence intervals for $f(0)$ and the animal population density D . We present two case studies in [Section 5](#), one using data from a wood stake study and the other from a survey of kangaroos in Australia. [Section 6](#) shows the performance of the proposed method in simulation studies with data generated from artificially constructed densities commonly used to test kernel density estimators as well as with a simulated line transect data set. Concluding remarks follow in [Section 7](#).

2. Inference for $f(0)$. Suppose that we have a sample X_1, \dots, X_n from the density function $f(x)$. The nonparametric kernel density estimator of $f(x)$ is given by

$$\hat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{x - X_j}{h}\right),$$

where h is the bandwidth and K is a bounded, symmetric kernel function integrating to one. In kernel methods, the choice of the bandwidth is more crucial than the choice of kernel. The bandwidth specifies the amount of smoothing applied to the data and controls the performance of $\hat{f}_h(x)$. For grouped data, the choice of h will be addressed in [Section 3](#). We use the Gaussian kernel throughout this paper.

In line transect sampling, the interest is in the value of the density at the boundary $x = 0$, $f(0)$, since this quantity is related to the animal population density. It is well known that kernel estimators suffer from high bias near boundaries ([Wasserman, 2005](#)). [Barabesi \(2000\)](#) used local likelihood density

estimation to reduce this boundary bias, and Barabesi et al (2002) extended this approach to grouped data. We will instead employ the symmetrization technique used in Chen (1996), originally suggested by Buckland (1992). The key idea of the symmetrization technique is to duplicate the data by reflecting the data about the boundary: we replace each data value x_i with x_i and its reflection $-x_i$ about 0. Then we assume that the data consist of values y_1, \dots, y_{2n} where $y_{2i-1} = x_i$ and $y_{2i} = -x_i$. Thus, $X = |Y|$ and we have

$$f(x) = g(x) + g(-x),$$

where g is the density of y . The kernel estimator of g is

$$\hat{g}_h(x) = \frac{1}{2nh} \sum_{k=1}^{2n} K\left(\frac{x - y_k}{h}\right) = \frac{1}{2nh} \sum_{i=1}^n \left[K\left(\frac{x - x_i}{h}\right) + K\left(\frac{x + x_i}{h}\right) \right],$$

so that we have, as the kernel estimator of $f(0)$,

$$\hat{f}_h(0) = 2\hat{g}_h(0) = \frac{1}{nh} \sum_{k=1}^{2n} K\left(\frac{0 - y_k}{h}\right) = \frac{2}{nh} \sum_{i=1}^n K\left(\frac{x_i}{h}\right),$$

where the last equality is due to the symmetry of the Gaussian kernel about zero.

3. Bandwidth Selector for Grouped Data. Here, we first describe the cross-validation method and the smoothed bootstrap method for bandwidth selection with ungrouped data. After highlighting difficulties with using these methods with grouped data, we introduce a combined cross-validation and smoothed bootstrap strategy that can deal with such grouped data.

In density estimation, the performance of the density estimate \hat{f}_h is highly sensitive to the choice of the smoothing parameter h and one often selects the optimal smoothing parameter from observed data using some criterion of performance. A common criterion is the risk function, $R(f, \hat{f}_h)$, defined to be the expectation of a loss function, $L(f, \hat{f}_h)$, often chosen to be the integrated squared error (ISE):

$$L(f, \hat{f}_h) = \text{ISE} = \int [\hat{f}_h(x) - f(x)]^2 dx.$$

The risk function can be written as a sum of the squared bias term and the variance term,

$$R(f, \hat{f}_h) = \text{E} \left(L(f, \hat{f}_h) \right) = \int \text{bias}^2(\hat{f}_h(x)) dx + \int \text{Var}(\hat{f}_h(x)) dx,$$

hence the optimal smoothing parameter is chosen to balance the tradeoff between the bias and the variance.

The integrated squared estimator (ISE) can be written as

$$\begin{aligned} \text{ISE} &= \int [\hat{f}_h(x) - f(x)]^2 dx \\ (3.1) \quad &= \int \hat{f}_h^2(x) dx - 2 \int \hat{f}_h(x) f(x) dx + \int f^2(x) dx. \end{aligned}$$

Since the last term on the right-hand side of (3.1) is independent of h , minimizing ISE is equivalent to minimizing the first two terms. As f is not known, the middle term has to be estimated, usually by cross-validation or bootstrap.

With cross-validation, this middle term is estimated by

$$-\frac{2}{n} \sum_{i=1}^n \hat{f}_h^{-i}(X_i),$$

where

$$\hat{f}_h^{-i}(x) = \frac{1}{h(n-1)} \sum_{j \neq i}^n K\left(\frac{x - X_j}{h}\right)$$

is the kernel estimate of f with the i -th data point removed. Thus the cross-validation function is

$$\text{CV}(h) = \int \hat{f}_h^2(x) dx - \frac{2}{n} \sum_{i=1}^n \hat{f}_h^{-i}(X_i),$$

and the value of h that minimizes this function is chosen as the bandwidth. An asymptotic justification of the cross-validation procedure can be found in [Stone \(1984\)](#).

The bootstrap is an alternative to cross-validation for bandwidth selection ([Taylor, 1989](#)). However, the nonparametric bootstrap method of sampling the data points with replacement and obtaining bootstrap density estimates from the bootstrap samples cannot capture the bias since the bootstrap estimates are unbiased. Thus, the smoothed bootstrap is used instead. This involves obtaining an initial density estimate, $\hat{f}(x; h_{in})$, using a *pilot* bandwidth value h_{in} and obtaining smoothed bootstrap samples by drawing samples from this initial density estimate. The optimal bandwidth is then the value of h that minimizes

$$(3.2) \quad \text{BMISE}(h) = \mathbb{E}_S \int [\hat{f}^S(x; h) - \hat{f}(x; h_{in})]^2 dx,$$

where \hat{f}^S is the kernel density estimate for the smoothed bootstrap sample generated from $\hat{f}(x; h_{in})$ and E_S represents the mean over the smoothed bootstrap sampling distribution. This smoothed bootstrap approach can often perform better than cross-validation. See the work done by [Faraway and Jhun \(1990\)](#) and [Jones et al. \(1996\)](#) for the details. [Faraway and Jhun \(1990\)](#) recommended choosing the pilot estimate with cross-validation.

The cross-validation and smoothed bootstrap methods described above work well with ungrouped data. In practice, however, data are often binned or rounded to some extent. Suppose we have a mesh $\{t_k\}_{k=0}^K$ specifying K intervals. The actual data (X_1, \dots, X_n) is not recorded as such, but instead is of the form $(v_1, n_1), \dots, (v_K, n_K)$ where n_k is the count in the bin $B_k = [t_{k-1}, t_k)$ and v_k is typically taken to be the midpoint of the bin B_k . Often the bin size $\delta_k = t_k - t_{k-1}$ is constant for all k , but this is not required in our proposed method.

It is well known that using the cross-validation function to select the smoothing parameter leads to undersmoothing if the proportion of tied data is larger than some threshold ([Silverman, 1986](#)). Indeed, any reasonable risk function estimate may not work as a criterion for choosing the optimal smoothing parameter if there is significant overlapping in the data.

This can be explained heuristically. Since the risk function can be written as a sum of a squared bias term and a variance term, selecting the bandwidth that minimizes the risk function selects the amount of smoothing that balances the bias and the variance. When data are grouped, however, there are additional biases so that the squared bias term dominates the variance term in the risk function. As a smaller bandwidth reduces the bias, using the risk function produces undersmoothing. In density estimation, this means that the selected optimal bandwidth will be close to 0.

To address this problem, we propose a new bandwidth selection procedure for kernel density estimation using a combined cross-validation and smoothed bootstrap strategy. To estimate $f(0)$ in line transect sampling, we use this new method for bandwidth selection (Steps 2-6 below) together with the symmetrization technique of [Section 2](#) (Step 1).

Suppose we have grouped data with a number of counts within each bin. The estimation procedure involves the following steps:

1. Apply the symmetrization technique to $X_i, i = 1, \dots, n$ to obtain $Y = (Y_1, \dots, Y_{2n})$. Note that X is binned, so many of the X_i 's, and thus the Y_i 's, overlap. This symmetrization step is performed to reduce the boundary bias in the estimation of $f(0)$. The remaining steps form the smoothed bootstrap procedure for bandwidth selection for grouped data.

2. For each bin $k = 1, \dots, K$, generate noise from the uniform $[-\delta_k/2, \delta_k/2]$ distribution and add them to the data points, so that the data points no longer overlap. Let $Y^U = (Y_1^U, \dots, Y_{2n}^U)$ denote the new data.
3. Use cross-validation to calculate the optimal bandwidth for Y^U .
4. Repeat Steps 2 and 3 1000 times and let the average of the optimal bandwidths be h_{in} . An initial density estimate $\hat{g}(y; h_{in})$ is then obtained using h_{in} as the pilot bandwidth.
5. Generate B smoothed bootstrap samples $Y^S = (Y_1^S, \dots, Y_{2n}^S)$ from $\hat{g}(y; h_{in})$.
6. With the smoothed bootstrap samples, evaluate BMISE as a function of h and find the value of h that minimizes $\text{BMISE}(h)$, denoted h_S .
7. Compute $\hat{f}(0) = 2 \cdot \hat{g}(0; h_S)$

In short, we are using a smoothed bootstrap approach with the pilot bandwidth h_{in} found using cross-validation on grouped data with random noise added to them. Note that the smoothed bootstrap in Step 5 above produces bootstrap samples Y^S from $\hat{g}(y; h_{in})$, and the optimal bandwidth h_S is chosen based on Y^S not Y^U . Thus the choice of h_S is not directly affected by the dependence created in the symmetrization step.

Remark 1: Smoothed bootstrap samples can be generated from $\hat{g}(y; h_{in})$ by rejection sampling, but can be generated more simply as follows:

1. Use the naive bootstrap to resample Y_1^*, \dots, Y_{2n}^* from Y_1^U, \dots, Y_{2n}^U .
2. Generate z_i from $K(\cdot)$. In our case, since we are using the Gaussian kernel, we generate z_i from the standard normal.
3. Set $Y_i^S = Y_i^* + h_{in} \cdot z_i$ for $i = 1, \dots, 2n$.

Remark 2: A referee suggested using a different noise distribution than the uniform in Step 2 above, specifically, that the noise distribution be proportional to the detection function. As our method is intended for applications besides distance sampling, we decide not to pursue this here.

4. Confidence Intervals for $f(0)$ and D . In this section, we construct bootstrap confidence intervals for $f(0)$ based on the kernel density estimates. Constructing confidence intervals for densities requires accounting for the bias that is not captured in the naive bootstrap procedure. [Hall \(1992\)](#) proposed two methods to account for the bias: explicit bias estimation and undersmoothing. The former method involves estimating the leading term of the bias explicitly to obtain a bias-adjusted bootstrap t -confidence interval. The leading term of the bias is a functional of the second derivative of f and [Hall \(1992\)](#) suggested using a plug-in kernel estimator of the derivative. In the undersmoothing method, a sub-optimal

bandwidth of a smaller order than the optimal bandwidth is chosen to make $[E(\widehat{f}(x)) - f(x)]/\sqrt{\text{Var}(\widehat{f}(x))}$ negligible.

Assuming that the maximum number d for which the d -th derivative, $f^{(d)}$ exists and is known, Hall (1992) compared the two approaches and recommended the undersmoothing method. However, in practice the value of d is usually unknown. Furthermore, there are no useful guidelines for the choice of the plug-in kernel estimator of the derivative and the amount of undersmoothing.

Thus, we propose using smoothed bootstrap to estimate the bias of the kernel density estimate and construct several confidence intervals based on our smoothed bootstrap procedure. These confidence intervals are based on studentized and non-studentized pivot statistics. We use these confidence intervals in our simulation and case studies.

To construct confidence intervals, we first follow Steps 1 to 7 in Section 3 to generate smoothed resamples. For smoothed resample $X_b^S, b = 1, \dots, B$, define

$$\widehat{f}_b^S(x; h_S) = \frac{1}{nh_S} \sum_{i=1}^n K\left(\frac{x - X_{i,b}^S}{h_S}\right).$$

Define the pivot statistic $R_{n,b}^S(x) = \widehat{f}_b^S(x; h_S) - \widehat{f}(x; h_{in})$. If we let r_α^S denote the α sample quantile of $(R_{n,1}^S, \dots, R_{n,B}^S)$, then a $100(1 - \alpha)\%$ bootstrap pivot confidence interval for $f(x)$ is

$$(4.1) \quad (\widehat{f}(x; h_S) - r_{1-\alpha/2}^S, \widehat{f}(x; h_S) - r_{\alpha/2}^S).$$

Faraway and Jhun (1990) used a similar pivot statistic to construct simultaneous confidence bands for f .

An alternative is to construct confidence intervals based on a studentized version of the above pivot statistic. It is known that studentized confidence intervals are more accurate since these intervals are second-order accurate (Wasserman, 2005).

With a suitable estimator $\widehat{\sigma}_b^S$ of the standard deviation $\sigma(x)$ of $\widehat{f}(x)$, we can use the studentized pivot

$$U_{n,b}^S = \frac{\widehat{f}_b^S(x; h_S) - \widehat{f}(x; h_{in})}{\widehat{\sigma}_b^S(x)},$$

yielding a $100(1 - \alpha)\%$ bootstrap studentized pivotal interval

$$(4.2) \quad (\widehat{f}(x; h_S) - u_{1-\alpha/2}^S \widehat{\sigma}(x), \widehat{f}(x; h_S) - u_{\alpha/2}^S \widehat{\sigma}(x)),$$

where u_α^S is the α sample quantile of $(U_{n,1}^S, \dots, U_{n,B}^S)$. Please refer to the Appendix for details on how to obtain $\widehat{\sigma}_b^S$.

To construct a confidence interval of D , we use equation (1.1). Here there is additional variability in \hat{D} due to n being random. Buckland et al (2001) showed that the standard error of \hat{D} is given by

$$\hat{\sigma}_D = \hat{D} \sqrt{\left(\frac{\text{Var}(n)}{n^2} + \left[\frac{\hat{\sigma}(0)}{\hat{f}(0)} \right]^2 \right)}.$$

If we follow the common practice of using the Poisson for the distribution of n , $\text{Var}(n)$ can be estimated by the value of n , and the above expression simplifies to

$$\hat{\sigma}_D = \hat{D} \sqrt{\left(\frac{1}{n} + \left[\frac{\hat{\sigma}(0)}{\hat{f}(0)} \right]^2 \right)}.$$

We use this latter formula in our analyses and simulation study.

Using the same approach of defining a studentized pivot statistic, we get the following $100(1 - \alpha)\%$ confidence interval for D :

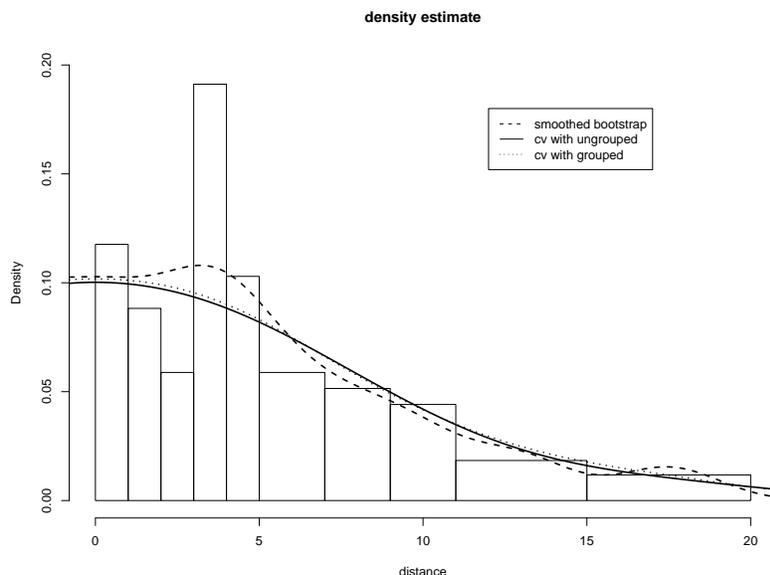
$$(\hat{D} - w_{1-\alpha/2}^S \hat{\sigma}_D, \hat{D} + w_{\alpha/2}^S \hat{\sigma}_D),$$

where w_α^S is the α sample quantile of the pivot statistics $W_{n,1}^S, \dots, W_{n,B}^S$ computed from the bootstrap sample, and $\hat{\sigma}_D$ is as given above. See the Appendix for details.

5. Case Studies. We next look at two case studies, involving a wooden stake data set and a survey of kangaroos in Australia. All computation, including implementation of our smoothed bootstrap method, was done with the R statistical language (R Development Core Team, 2008). The code will be available as supplemental material at the *Annals of Applied Statistics* website.

5.1. *Stake data in Utah.* We consider here a wooden stakes data set from Logan, Utah, which was also analyzed by Burnham et al (1980); Barabesi (2000); Barabesi et al (2002). This data set was collected as part of a larger study on line transect sampling. In particular, 150 wooden stakes were put within 20m of a transect line in a meadow near Logan, Utah. The length of the transect line was 1000m and the actual density of stakes was known to be $D = 37.5$ stakes/hectare. An observer walked along the transect line and searched visually for the stakes.

Out of 150 stakes, 68 were observed. The actual perpendicular distances of the identified stakes from the transect line are given in Table 6 of Burnham et al

FIG 1. *Wooden stakes with kernel density estimates*

(1980). We notice that more than one stake are found at some distances. In an actual application these distances are not known, but are estimated by the observer. With ten distance categories with end points 1, 2, 3, 4, 5, 7, 9, 11, 15, 20, the data then consist of counts of 8, 6, 4, 13, 7, 8, 7, 6, 5, 4 in the ten distance categories. Note that the intervals do not have the same length.

Fig 1 shows a histogram of the relative frequencies and kernel density estimates with bandwidths obtained using different selection methods.

The density estimate with the smoothed bootstrap bandwidth seems a better fit and also yields the estimate $\hat{f}(0) = 0.1033$, or $\hat{D} = 35.11$, which is closer to the true density $D = 37.5$. For both grouped and ungrouped data, we received the warning message: *minimum occurred at one end of the range* from R and the lower bounds of the bandwidth range were chosen as optimal bandwidths with cross-validation. With cross-validation bandwidth selectors based on ungrouped data and grouped data, we found $\hat{D} = 34.07$ and $\hat{D} = 34.58$ respectively.

Burnham et al (1980) fit Fourier series models to the ungrouped and grouped data to obtain confidence intervals for D . As pointed out in Mack and Quang (1998), the Fourier series method requires specifying a horizon, the maximum sighting distance, which is not well defined for grouped data.

Barabesi (2000) suggested a local likelihood method to make inference for

TABLE 1
Confidence intervals for D

Method	95% Interval
Fourier series method with ungrouped data (Burnham et al, 1980)	(32.28,45.72)
Fourier series method with grouped data (Burnham et al, 1980)	(23.95,40.90)
Local likelihood (Barabesi, 2000)	(27.20,52.09)
Local least squares (Barabesi et al, 2002)	(22.13,49.25)
Smoothed bootstrap	(26.65,45.57)

$f(0)$, but the method is mainly developed for ungrouped data. Barabesi et al (2002) used density estimation with local least squares to obtain estimates for D , with bandwidth chosen using a plug-in method. While their method can be used for grouped data, the resulting confidence interval for $f(0)$ does not account for the estimation bias.

Table 1 shows the confidence interval we constructed from the wood stake data using the bootstrap method described in Section 4. For comparison, we have also included in the table confidence intervals obtained from the above-mentioned references. While all confidence intervals cover the true value $D = 37.5$, there are interesting differences.

First note that the first confidence interval is based on the ungrouped data and thus it is the shortest. Information is lost when data are grouped, and it is expected that the other confidence intervals will not be as precise. The second confidence interval is based on the Fourier series method, applied to the grouped data. This is a parametric method based on the maximum likelihood estimator and the length of this confidence interval is shorter than other confidence intervals using the grouped data. The confidence interval on the third line is based on a method developed for ungrouped data but applied to the grouped data. Notice the much wider confidence interval obtained as a result. While the fourth confidence interval is valid it fails to consider the estimation bias. Note that our confidence interval is shorter than other nonparametric confidence intervals.

5.2. *Kangaroo survey data from Australia.* Southwell and Weaver (1993) compared various density estimation techniques for line transect data using a data set of kangaroo sightings collected at two locations in Australia, Wallaby Creek and Tidbinbilla Nature Reserve.

The line-transect work was conducted in a 1.5km^2 region in Wallaby Creek and in a 0.2km^2 region in Tidbinbilla Nature Reserve. At each site, a grid of equally-spaced parallel lines were marked, 100m and 50m apart respectively at Wallaby Creek and Tidbinbilla Nature Reserve. An observation session would consist of first randomly selecting a transect and a direction.

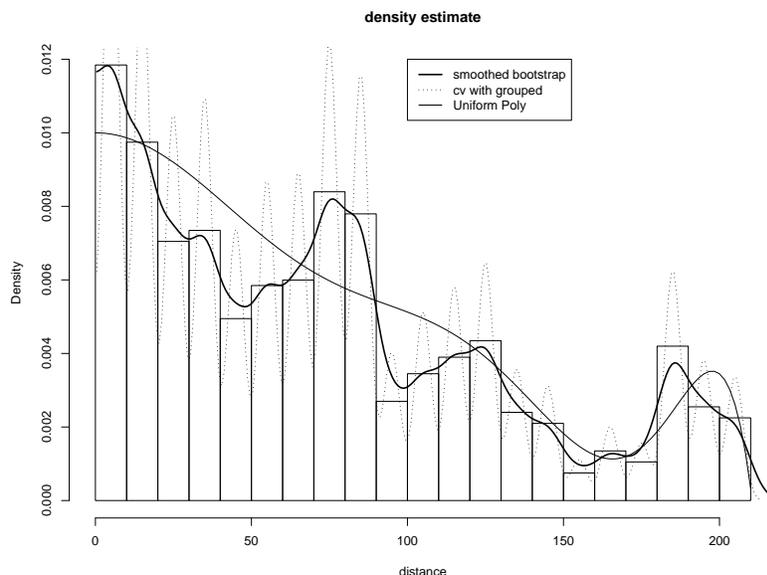


FIG 2. *Eastern grey kangaroo in Wallaby Creek with kernel density estimates*

An observer would traverse that transect, then another line transect 400m (Wallaby Creek) or 200m (Tidbinbilla) away, and so on, alternating the direction with each subsequent line transect. Each observation session would focus on a particular species, the eastern grey kangaroo (*Macropus giganteus*) or red-necked wallaby (*M. rufogriseus*) in Wallaby Creek and the red kangaroo (*M. rufus*) in Tidbinbilla.

The kangaroos at both locations were used to the presence of humans. This allowed the line transects to be more closely spaced than would normally be done. Furthermore, it is also then relatively straightforward to perform a census of the kangaroo populations. Thus the true kangaroo population sizes are known, and serve as a point of comparison for the line-transect estimation techniques. Here, we will only use their data on sightings of the eastern grey kangaroo in Wallaby Creek.

Figure 2 shows a histogram of the eastern grey kangaroo data, together with kernel density estimates obtained using optimal bandwidths selected using cross-validation on the grouped data and using our smoothed bootstrap method. Also shown is a density estimate obtained using the Distance software program (Thomas et al., 2009). This density estimate was obtained from the model with a Uniform key function and polynomial adjustment to the tails. This model was selected from among the other alternatives using

AIC as the criterion.

The cross-validation approach yields a density that essentially has a peak at every bin, while the density obtained with the Distance software program suggests that too much smoothing may have been applied. The density estimates obtained from the models with the next two smallest AIC values, using hazard-rate and half-normal key functions with cosine adjustments, also suggests over-smoothing (not shown). The density estimate based on our smoothed bootstrap approach attains a better fit to the data, with a good balance between smoothing and retaining the peaks.

The true density D is known to be 44 animals per km^2 . Using the smoothed bootstrap approach, we obtained $\hat{D} = 43.71$ and a 95% confidence interval of (37.63, 50.51). For comparison, with the line transect estimate based on the Uniform model with polynomial adjustment, we have $\hat{D} = 39.16$ with 95% confidence interval (34.91, 43.94).

6. Simulation. This section contains two parts. Section 6.1 studies the performance of the bandwidth selection procedure together with the symmetrization technique for estimating $f(0)$ using simulated line transect data.

As our method is applicable to areas beyond line transect sampling, it is of interest to explore its performance under a variety of settings. In Section 6.2 we apply our bandwidth selection method to data generated from artificially constructed densities. These densities are mixtures of normals and while such densities are not considered likely in real applications, they are nevertheless commonly used in the density estimation community to assess different methods. Here, the aim is to estimate the whole density function using the selected bandwidth.

6.1. *Simulation study 1.* Here, we consider a simulated line transect data set that was generated by [Buckland et al \(2001\)](#) for comparing various line transect data analyses. We briefly describe it below, referring the reader to [Buckland et al \(2001\)](#) for more details.

The data set was simulated so that the assumptions for line transect sampling hold. It was based on the context of line transect sampling using 12 parallel line transects of varying lengths within a region of irregular shape. The detection function used was the half-normal and the true values of $f(0)$ and D are 0.0798 m^{-1} (to three significant figures) and 79.79 objects per km^2 . The model was set up so that the expected number of observations was 96, The simulated data set has 105 observations. The original data set was ungrouped, but was grouped in various ways by [Buckland et al \(2001\)](#) for use with some of the methods considered there. We use the data which had

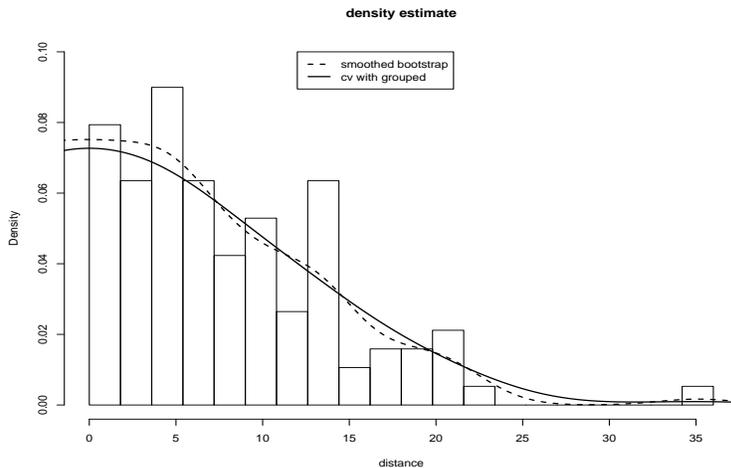


FIG 3. Histogram of the simulated transect line sampling data together with kernel density estimates with bandwidths selected using smoothed bootstrap and cross-validation with grouped data.

been grouped into 20 groups of equal width. Figure 3 shows a histogram of the raw data.

We applied smoothed bootstrap and cross-validation for grouped data to this data set. The resulting density estimates are shown in Figure 3. Estimates of $f(0)$ and D are shown in Table 2. This table also contains estimates taken from Table 4.2 of Buckland et al (2001), obtained using parametric models fit to the data. These involve fitting a key function (uniform, half-normal or hazard-rate) to the data and then applying an adjustment (cosine, polynomial or Hermite) to the tails.

Since the true detection function is half-normal, it is not surprising that the half-normal (with Hermite adjustment) gave an estimate of $f(0)$ closest to the true value. The estimate obtained with smoothed bootstrap was closer to the true value than the cross-validation estimate and the estimates obtained using the uniform model. Note that to get D , the expected value $E(n) = 96$ was used in the formula (1.1), while for the estimates, $n = 105$ was used.

We note also that the simulated data had an outlier and Buckland et al (2001) recommended truncating about 5% of the data, corresponding to dropping six of the largest observations in this case. After truncation, $f(0)$

TABLE 2

Estimates of $f(0)$ using smoothed bootstrap, cross-validation and from several parametric models fit by [Buckland et al \(2001\)](#).

Method	$\hat{f}(0)$	\hat{D}
Smoothed bootstrap	0.0751	82.14
Cross-validation	0.0726	79.44
Uniform + cosine	0.0732	80.06
Uniform + polynomial	0.0681	74.43
Half-normal + Hermite	0.0794	86.87
Hazard-rate + cosine	0.0769	84.06
True value	0.0798	79.79

and \hat{D} were 0.0844 and 87.98 using the half-normal model with Hermite adjustment. Our method is nonparametric, and hence we do not make assumptions about the form of the density. In particular, our estimate $\hat{f}(0)$ is robust to outliers in the tails because the kernel estimate is based on *local* smoothing. Hence the presence of outliers does not adversely affect the estimation of $f(0)$ and our method does not require truncation.

Using the formulas in Section 4, we obtained standard errors of 0.017 and 20.36 for $\hat{f}(0)$ and \hat{D} respectively assuming the Poisson distribution as the sampling distribution for n . Nominal 95% confidence intervals for $f(0)$ and D , obtained by bootstrap, were (0.061, 0.092) and (67.18, 101.33) respectively.

With a normal approximation approach in [Buckland et al \(2001\)](#), 95% confidence intervals for D are (60.14, 113.60) and (59.36, 116.30) (with truncation).

6.2. *Simulation study 2.* In this section, we present results from a simulation study testing the effectiveness of our bandwidth selection method for estimating the whole density function from binned data, a special case of grouped data.

We used four mixture normal densities taken from [Marron and Wand](#)

TABLE 3

Parameters for mixture normal densities

Model	density	$\sum_{k=1}^K p_k N(\mu_k, \sigma_k^2)$
1	Gaussian	$N(0, 1)$
2	Separated bimodal	$\frac{1}{2}N\left(-\frac{3}{2}, \left(\frac{1}{2}\right)^2\right) + \frac{1}{2}N\left(\frac{3}{2}, \left(\frac{1}{2}\right)^2\right)$
3	Claw	$\frac{1}{2}N(0, 1) + \sum_{k=0}^4 \frac{1}{10}N\left(\frac{k}{2} - 1, \left(\frac{1}{10}\right)^2\right)$
4	Asymmetric Claw	$\frac{1}{2}N(0, 1) + \sum_{k=-2}^1 \frac{2^{k-1}}{30}N\left(k + \frac{1}{2}, \left(\frac{2^{-k}}{10}\right)^2\right)$

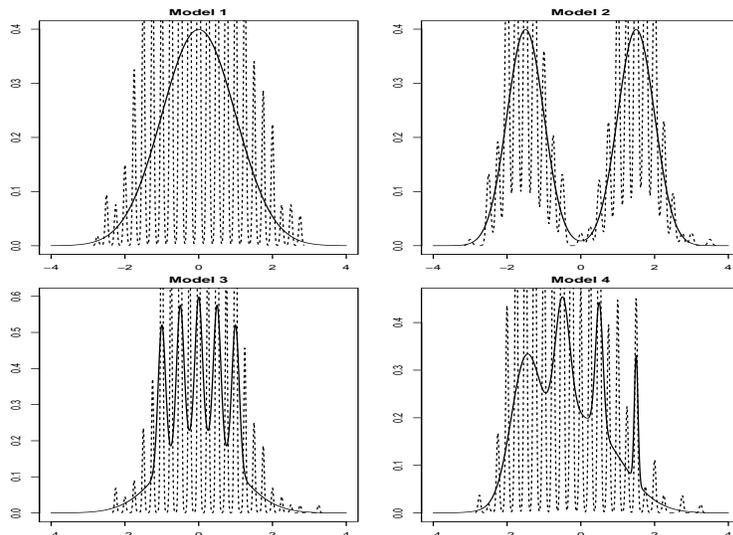


FIG 4. Plots showing the true densities of the 4 models we considered (solid lines) and the kernel density estimates (dashed lines) using the cross-validation optimal bandwidths obtained from the binned data, h_{cv}^{bin} .

(1992). The parameters for the mixture densities are shown in Table 3 and plots of these densities are shown in Figure 4 (solid lines). All simulation studies were implemented using the R. We generated a sample of size 500 from each of these densities and binned the data using a bin size of 0.25.

Thus we have two data sets for each model, one raw and one binned. Optimal bandwidth selection using cross-validation was applied to each data set, yielding bandwidth values $h_{cv,i}^{raw}$ and $h_{cv,i}^{bin}$ for $i = 1, \dots, 4$, which are cross-validation optimal bandwidths obtained from the i -th raw data set and i -th binned data set respectively. In R, this is done using the function `bw.ucv`. Since this is an optimization problem, a built-in range of bandwidths is used in the function. For all models we considered, applying the function to the binned data sets yielded the warning message “*minimum occurred at one end of the range*”, suggesting that the optimal bandwidths found using cross-validation are near 0.

Each pair of selected bandwidths are then used with the *binned* data to obtain kernel density estimates. The results are shown in Figures 4 and 5, which are respectively plots of the kernel density estimators using $h_{cv,i}^{bin}$ and $h_{cv,i}^{raw}$.

Figure 4 shows the problem of using cross-validation on the binned data to obtain optimal bandwidths. As can be seen, the selected bandwidths $h_{cv,i}^{bin}$

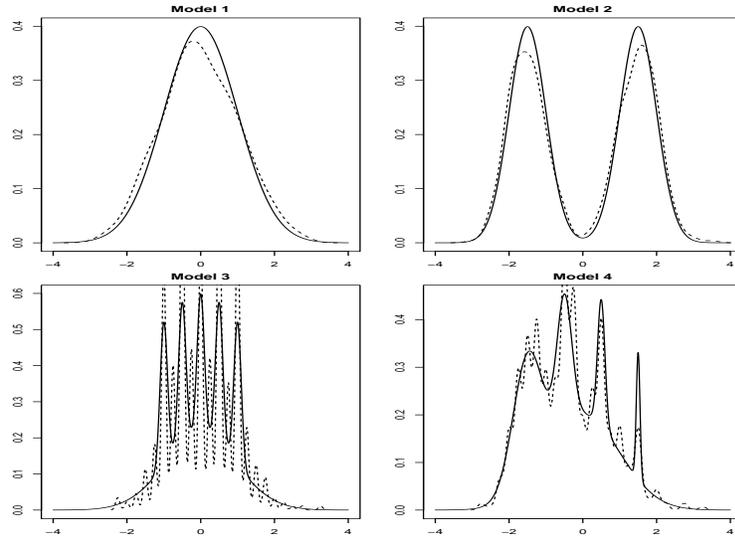


FIG 5. Plots showing the true densities of the 4 models we considered (solid lines) and the kernel density estimates (dashed lines) using the cross-validation optimal bandwidths obtained from the original, raw data, h_{cv}^{raw} .

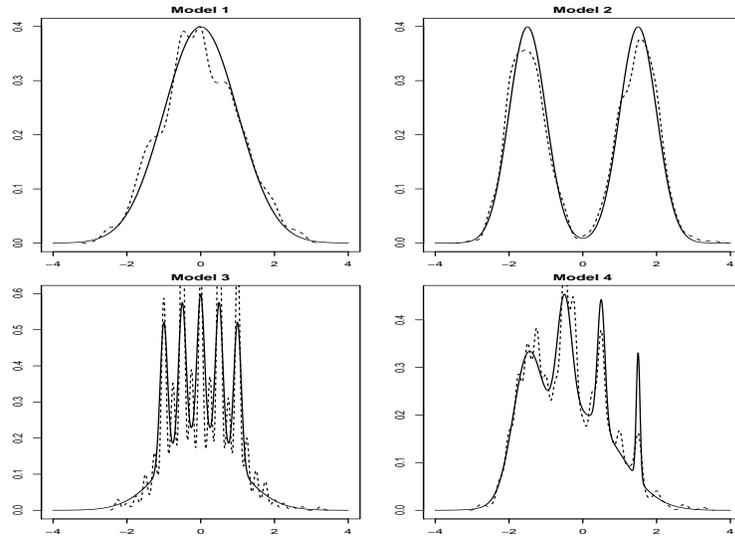


FIG 6. Plots showing the true densities of the 4 models we considered (solid lines) and the kernel density estimates (dashed lines) using the initial bandwidths h_{in} obtained from Step 4 of the smoothed bootstrap procedure.

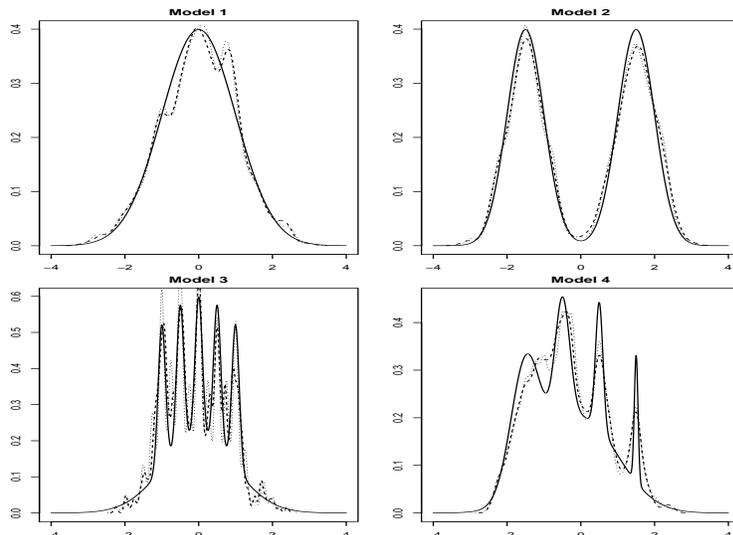


FIG 7. Plots showing the true densities of the 4 models we considered (solid lines) and the kernel density estimates (dashed lines) using optimal bandwidths selected using smoothed bootstrap, h_S . The dashed lines are density estimates using cross validation optimal bandwidth from the original, raw data

are too small, resulting in severe under-smoothing (dashed lines). In Figure 5 we find that if the underlying true density is relatively smooth (models 1 and 2), using the optimal bandwidths for the raw data, $h_{cv,i}^{raw}$, on the binned data works well. However, if the true density is less smooth, using $h_{cv,i}^{raw}$ is not appropriate for the binned data. Thus methods such as that proposed by Chiu (1991) that aim to obtain approximations to h_{cv}^{raw} may not work if the true density is not sufficiently smooth.

Figure 6 shows plots of kernel density estimates using the pilot bandwidths h_{in} obtained from Step 4 of our procedure described in Section 3. These plots are similar to those in Figure 5, with density estimates close to the true densities if the true densities are sufficiently smooth, but with severe under-smoothing otherwise.

Plots of kernel densities estimates using the smoothed bootstrap optimal bandwidths h_S are shown in Figure 7 (dotted lines). For comparison, the kernel density estimates using h_{cv}^{raw} with the raw data (the best case scenario) are also shown in dashed lines. Note that the dotted lines are very close to the dashed lines in spite of some information loss due to the binning. It is clear that in all the models we considered, the resulting density estimates are much smoother and closer to the true densities than using h_{cv}^{bin} , h_{cv}^{raw} or

h_{in} on the binned data. Table 4 summarizes the optimal bandwidth values chosen by different bandwidth selectors.

TABLE 4
Bandwidth comparisons for mixture normal densities

Model	CV with raw data	CV with binned data	Initial bandwidth	Smoothed bootstrap
1	0.316	0.034	0.154	0.154
2	0.191	0.054	0.148	0.144
3	0.058	0.028	0.066	0.074
4	0.093	0.034	0.101	0.112

7. Concluding Remarks. In this paper, we introduced a combined cross-validation and smoothed bootstrap approach for obtaining kernel density estimates from grouped data. Our simulation results show that the smoothing parameter found using our method produced density estimates that matched the true density most closely compared with competing methods.

In line transect sampling, it is the value of the density at the boundary, specifically $f(0)$, that is of interest, since the estimate of $f(0)$ is used to estimate the animal population density. We showed that the symmetrization technique of [Chen \(1996\)](#) together with our bandwidth selection procedure was able to produce good estimates of both the stake density and the eastern grey kangaroo density.

There are some limitations to our method. For application to line transect sampling, we are restricted to data that is sufficiently large and grouped into about 10 intervals. With smaller data sizes, the data may be grouped into as few as 3 or 4 intervals. In such cases, we do not expect a nonparametric kernel method to work well. Often, a parametric model involving covariates is used instead.

The methodology developed in this paper has wider potential application in other scientific areas. For example, economists often want to make inference for income distributions in developing countries where only grouped data are available to outsiders ([Wu and Perloff, 2007](#)). In astronomy, [Efron and Tibshirani \(1996\)](#) applied a semiparametric density estimator to the estimation for density of galaxy for which counts on a fine grid are variables. Complex survey data are another possible application ([Bellhouse and Staffor, 1999](#)). We will explore some of these applications in future work.

APPENDIX A: ESTIMATION OF $\sigma^2(X)$

We describe how to estimate the variance $\sigma^2(x)$ of $\hat{f}(x)$. It can be shown that

$$\sigma^2(x) = \frac{1}{nh^2} \int K\left(\frac{x-y}{h}\right)^2 f(y)dy - \frac{1}{n} \left[\frac{1}{h} \int K\left(\frac{x-y}{h}\right) f(y) \right],$$

and [Hall \(1992\)](#) proposed the following estimator of $\sigma(x)$:

$$[\hat{\sigma}(x)]^2 = \frac{1}{nh} \left[\frac{1}{nh} \sum_{i=1}^n K\left(\frac{x-X_i}{h}\right)^2 - h\hat{f}(x)^2 \right].$$

With our smoothed bootstrap samples, we can estimate the variance by

$$[\hat{\sigma}_b^S(x)]^2 = \frac{1}{nh_S} \left[\frac{1}{nh_S} \sum_{i=1}^n K\left(\frac{x-X_{i,b}^S}{h_S}\right)^2 - h_S \hat{f}_b^S(x; h_S)^2 \right],$$

and use $\hat{\sigma}_b^S(x)$ in the studentized pivot statistic $U_{n,b}^S$.

APPENDIX B: CONFIDENCE INTERVAL FOR D

[Chen \(1996\)](#) showed that

$$\frac{\hat{D} - D - \widehat{\text{bias}}(\hat{D})}{\hat{\sigma}_D} \rightarrow N(0, 1),$$

where $\widehat{\text{bias}}(\hat{D}) = nf^{(2)}(0)h^2/(2L)$ and $f^{(2)}$ is the second derivative of f .

Based on the same approach that we used to obtain a confidence interval for $f(0)$, we define a studentized pivot statistic:

$$W_{n,b}^S = \frac{\hat{D}_b^S - \hat{D}_{h_{in}}}{\hat{\sigma}_{b,D}^S},$$

where

$$\begin{aligned} \hat{D}_{h_{in}} &= \frac{n\hat{f}(0; h_{in})}{2L}, & \hat{D}_b^S &= \frac{n\hat{f}_b^S(0; h_S)}{2L}, \\ \hat{\sigma}_{b,D}^S &= \hat{D}_b^S \sqrt{\left(\frac{\text{Var}(n)}{n^2} + \left[\frac{\hat{\sigma}_b^2(0)}{\hat{f}_b^S(0; h_S)} \right]^2 \right)}. \end{aligned}$$

With B bootstrap samples, we get values $W_{n,1}^S, \dots, W_{n,B}^S$. A $100(1 - \alpha)\%$ confidence interval for D is then given by

$$(\hat{D} - w_{1-\alpha/2}^S \hat{\sigma}_D, \hat{D} - w_{\alpha/2}^S \hat{\sigma}_D),$$

where w_α^S is the α sample quantile of $(W_{n,1}^S, \dots, W_{n,B}^S)$.

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