

Bandwidth Selection for Weighted Kernel Density Estimation

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Abstract: Weighted kernel-density estimates (wKDE) are broadly used in many statistical areas, for instant, density estimation under right-censoring. However, bandwidth selection could be a problem by reweighting the kernels. In this paper, we investigate the methods of bandwidth selection for wKDE. Three mean integrated squared error based bandwidth selection methods are introduced. The least-squares cross-validation method, the adaptive weight kernel density estimator and boundary problems are also studied. Monte Carlo simulations were conducted to demonstrate the performance of the proposed bandwidth selection methods. Finally, the performance of wKDE is illustrated via an application to biased sampling problem and a real data application.

Keywords and phrases: Biased Sampling, Informative Censoring, Right Censoring.

1. Introduction

Kernel-type density estimators are widely used due to their simple forms and smoothness. In survival analysis, weighted kernel estimation is an important method of estimating the density of the survival times and the hazard function for censoring data[11]. Let X_1, X_2, \dots, X_n be a set of data. A general class of density estimators can be defined as reweighted weight function estimators,

$$\hat{f}(x) = \sum_{i=1}^n w(X_i)W(x, X_i), \quad (1)$$

where $W(\cdot)$ is a weight function, which is usually taken to be a (symmetric) density function, and $w(\cdot)$ is a re-weighting function which can be adjusted to

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control the roles of different data points in the sample. If we take

$$W(x, y) = \frac{1}{h}K\left(\frac{y-x}{h}\right) = K_h(y-x) \quad \text{and} \quad w(x) = \frac{1}{n},$$

we get a standard kernel density estimator,

$$\hat{f}(x) = \sum_{i=1}^n \frac{1}{nh}K\left(\frac{x-X_i}{h}\right) = \sum_{i=1}^n \frac{1}{n}K_h(x-X_i), \quad (2)$$

where $K(\cdot)$ is a kernel function and h is the bandwidth which controls the smooth of the estimate. Often the re-weighting function $w(\cdot)$ is required to be non-negative and sum up to 1. It can be a function of X itself and/or a vector of covariates. For example, Gisbert used a function of the population of each country to reweight the kernel density estimate of per capita GDP[8]. Marron and Padgett used a weighting function s , which is defined to be the jump sizes at X of the product-limit (PL) estimator by Kaplan and Meier[10], to correct the random right-censoring bias (MP estimator hereafter)[15]. In the MP estimator, s is a function of both X and the censoring variable Δ , which is defined to be

$$\Delta(X_i) = \begin{cases} 0, & \text{if } X_i \text{ is censored,} \\ 1, & \text{if } X_i \text{ is not censored.} \end{cases}$$

Thus, the bias induced by the random right-censoring can be corrected by the following MP estimator,

$$\hat{f}_{mp}(x) = \sum_{i=1}^n s_i K_h(x-X_i). \quad (3)$$

Throughout this paper, the following general form of weighted kernel density estimator will be used,

$$\hat{f}(x) = \sum_{i=1}^n w(X_i, Z_i)K_h(x-X_i), \quad (4)$$

where Z is the covariate(s). We simply choose $K(\cdot)$ to be a Gaussian kernel. For computational considerations, the Epanechnikov kernel can be used for large samples. Literature shows that there is very little to choose between various kernels on the basis of mean integrated square error. In this study, will focus on data with small or moderate sizes, so computation burden will not be a big issue.

The bandwidth selection problem has been well studied and documented for the unweighted kernel density estimation. In Section 2 we will discuss the bandwidth selection problem for wKDE. Two rough estimators and a plug-in estimator of the optimal bandwidth are proposed. The least-squares cross-validation method will also be discussed to refine the three estimates from Section 2 and

to automatically select the bandwidth. The adaptive wKDE and the boundary problem will be discussed in Session 3 and Section 4 respectively. The performance of the proposed methods will be illustrated via simulation studies in Section 5. Section 6 consists of two applications: an application of estimating densities from biased sampling by wKDE and a real data application showing how to estimate from survival data subject to informative censoring. Section 7 concludes the paper with a brief summary.

2. Bandwidth Selection

2.1. Two rough approaches

Bandwidth selection is one of the most important issues in kernel density estimation. In this paper, we consider selecting bandwidths based on the *mean integrated squared error* (MISE) criteria. The MISE criteria was first proposed by Rosenblatt[20] and has been widely used for automatic bandwidth selection. The MISE of \hat{f} can be decomposed into a sum of an integrated square bias term and an integrated variance term as below,

$$MISE(\hat{f}) = \int \{E\hat{f}(x) - f(x)\}^2 dx + \int var\hat{f}(x)dx. \quad (5)$$

If we take equal weights for all data points such that $w(\cdot) = 1/n$ in (4), the optimal bandwidth minimizing the MISE is

$$h_{opt} = k_2^{-2/5} \left\{ \int K(t)^2 dt \right\}^{1/5} \left\{ \int f''(x)^2 dx \right\}^{-1/5} n^{-1/5}, \quad (6)$$

where $k_2 = \int t^2 K(t)dt$ [24]. However, with unequal weights, the expectation of $\hat{f}(x)$ for each x is

$$E\hat{f}(x) = \sum E[w(X_i, Z_i)K_h(x - X_i)]. \quad (7)$$

The bias in (5), $E\hat{f}(x) - f(x)$, can be rewritten as

$$\begin{aligned} bias_h(x) &= \int w(y, z) \frac{n}{h} K\left(\frac{x-y}{h}\right) f(y) dy - f(x) \\ &\stackrel{y=x-ht}{=} \int nw(x-ht, z) K(t) f(x-ht) dt - f(x) \\ &= \int K(t) [n \cdot w(x-ht, z) f(x) - f(x)] dt \\ &\quad - nhf'(x) \int w(x-ht, z) t K(t) dt \\ &\quad + \frac{nh^2}{2} f''(x) \int t^2 w(x-ht, z) K(t) dt \\ &\quad + O(h^3). \end{aligned} \quad (8)$$

If $w(\cdot) \neq 1/n$, $n \cdot w(x - ht, z)f(x) - f(x) \neq 0$, and the first term to the right hand side (RHS) of (8) won't be zero. Also, although the Gaussian kernel is used such that $\int tK(t)dt = 0$, after the Taylor series expansion, the integral part in the second term to the RHS of (8) won't be zero either, even if $w(\cdot)$ is free of Z . Therefore, we can not rewrite the bias of \hat{f} in form of the sum of a term of order h^2 and higher order terms as in [29, 24].

An easy and rough approximation is to expand and view the weighted sample as an new unweighted sample. For instance, let $X = \{X_1, X_2, \dots, X_n\}$ be the observed survival data with random right-censoring. If X_i is censored, the true survival time of the i th individual is $T_i \geq X_i$. Thus, we can view the censored survival data as a data set consists of observed event times and latent true survival times, with the same size and all data points have equal weights. Thus, we can continue to use h_{opt} in (6) to select the optimal bandwidth. We can find that k_2 and $K(t)$ in (6) do not depend on the data. If n is kept unchanged, we need only figure out how to compute $\int f''^2$ based on the weighted sample in computing h_{opt} . For complete weighted data, n may be hard to determine, we will leave this problem for future studies. With additional assumptions, we propose the following two rough approach of h_{opt} .

Rough approach 1: In the same spirit of Parzen (1962) and Silverman (1986), we use a normal reference density to compute $\int f''^2$ and approximate the optimal bandwidth roughly by

$$h_n = 0.9An^{-1/5}, \quad (9)$$

where

$$A = \min(s_w, IQR_w/1.34),$$

where s_w and IQR_w are the sample standard deviation and sample inter-quartile range. We compute the weighted sample mean and sample variance by

$$\begin{aligned} \mu_w &= \sum_{i=1}^n w(X_i, Z_i)X_i, \\ s_w^2 &= \sum_{i=1}^n w(X_i, Z_i)(X_i - \mu_w)^2. \end{aligned}$$

Let $X_{(1)}, X_{(2)}, \dots, X_{(n)}$ be the order statistics of X_1, X_2, \dots, X_n and w_1, w_2, \dots, w_n be the corresponding weights of the order statistics. We find two integers q_1 and q_2 such that

$$\begin{aligned} \sum_{i=1}^{q_1} w_i \leq .25 \quad \text{and} \quad \sum_{i=1}^{q_1+1} w_i > .25, \\ \sum_{i=1}^{q_2} w_i \leq .75 \quad \text{and} \quad \sum_{i=1}^{q_2+1} w_i > .75. \end{aligned}$$

Let

$$p_1 = .25 - \sum_{i=1}^{q_1} w_i \quad \text{and} \quad p_2 = .75 - \sum_{i=1}^{q_2} w_i.$$

Based on the weighted sample, we can compute the first and third quartiles and IQR_w by

$$\begin{aligned} Q_{1w} &= X_{(q_1)} + p_1(X_{(q_1+1)} - X_{(q_1)}), \\ Q_{3w} &= X_{(q_2)} + p_2(X_{(q_2+1)} - X_{(q_2)}), \end{aligned}$$

and

$$IQR_w = Q_{3w} - Q_{1w}.$$

Rough approach 2: In survival data analysis, the exponential reference density is widely used in estimating $\int f''^2$. Let

$$f(x) = 1/\lambda \cdot \exp(-x/\lambda),$$

We have

$$\int f''(x)^2 dx = \frac{1}{\lambda^6} \int e^{-2x/\lambda} dx = \frac{1}{2\lambda^5}. \quad (10)$$

Plug-in (10) to (6), we get

$$h_{opt} = \pi^{-1/10} \lambda n^{-1/5} = .892 \lambda n^{-1/5}. \quad (11)$$

The coefficient in (11) is close to 0.9 as in (9). We then get another rough estimate of the optimal bandwidth, h_e , by keeping the form of (9),

$$h_e = 0.9 B n^{-1/5}, \quad (12)$$

where

$$B = \min(\hat{\lambda}, IQR_w/1.34),$$

and λ can be estimated by a maximum likelihood estimate $\hat{\lambda} = \sum X_i / \sum \Delta_i$ for the right-censored data and $\hat{\lambda} = \bar{X}$ for the complete data.

2.2. Plug-in estimator

For complete equal weighted data, in stead of using normal or exponential reference densities, a plug-in method can be used to automatically select the bandwidth by estimating $\int f''^2$ in (6) with another kernel based estimate as in [18, 22]. However, for weighted samples or incomplete data such as the right-censored data, we won't be able to get a close form of the bandwidth h by minimizing the first two terms of the usual asymptotic expansion of its mean integrated squared error,

$$AMISE(h) = (h)^{-1} R(K) + h^4 \sigma_k^4 R(f'')/4.$$

So the direct plug-in method won't work here. Even we can view the right-censored data as a data set of the same size with invisible data points, we will have trouble to compute the $\hat{S}_D(\cdot)$ and $\hat{T}_D(\cdot)$ in Sheather and Jones (1991) (page 689) [22].

In this study, we compute h_p by using the direct plug-in method bandwidth selector for un-weighted data and plug-in it to (4). The performance of h_n and h_e will be compared to h_p in Section 5. Simulation results show that h_p works well for right-censored data although the plug-in method does not applicable for weighted samples.

2.3. Least-squares cross-validation

To select the bandwidth completely automatically, we apply the least-squares cross-validation (LSCV) method after we computed the bandwidth by (9) or (12). The LSCV optimal bandwidth will be found by finding an h in the nearby regions of the rough estimate(s) that minimizes the intergrated square error (ISE) of \hat{f} ,

$$ISE(\hat{f}) = \int (\hat{f} - f)^2 = \int \hat{f}^2 - 2 \int \hat{f}f + \int f^2. \quad (13)$$

Note that the third term to the right-hand-side does not depend on the data. So minimizing ISE in (13) is equivalent to minimizing the sum of the first two terms. The first term can be computed by using \hat{f} in (4). For simplicity, we denote $w(X_i, Z_i)$ as w_i and we have

$$\begin{aligned} \int \hat{f}(x)^2 dx &= \int \sum_i \frac{w_i}{h} K\left(\frac{x - X_i}{h}\right) \times \sum_j \frac{w_j}{h} K\left(\frac{x - X_j}{h}\right) dx \\ &\stackrel{t=x/h}{=} \frac{1}{h} \sum_i \sum_j w_i w_j \int K\left(\frac{X_i}{h} - t\right) K\left(t - \frac{X_j}{h}\right) dt. \end{aligned}$$

The integral part is convolution of the kernel with itself. Due to the fact that the convolution of two Gaussians is another Gaussian, by elementary manipulations, we obtain

$$\begin{aligned} \int \hat{f}(x)^2 dx &= \frac{1}{\sqrt{2}h} \sum_i \sum_j w_i w_j K\left(\frac{X_i - X_j}{\sqrt{2}h}\right) \\ &= \sum_i \sum_j w_i w_j K_{\sqrt{2}h}(X_i - X_j). \end{aligned}$$

The second term in (13) can be estimated by $-2/n \sum \hat{f}_{-i}(X_i)$, where \hat{f}_{-i} is a Jackknife estimate which is constructed based on the data set by leaving the i -th point out of computing,

$$\hat{f}_{-i}(x) = \frac{\sum_{j \neq i} w_j K_h(x - X_j)}{\sum_{j \neq i} w_j}. \quad (14)$$

We can further simplify the second term by,

$$\begin{aligned} \frac{1}{n} \sum_i \hat{f}_{-i}(X_i) &= \frac{1}{n} \sum_i \left[\frac{\sum_{j \neq i} w_j K_h(x - X_j)}{\sum_{j \neq i} w_j} \right] \\ &= \frac{1}{n} \sum_i \left[\frac{\hat{f}(X_i) - w_i K_h(0)}{\sum_{j \neq i} w_j} \right] \\ &= \frac{1}{n} \sum_i \left[\frac{\hat{f}(X_i) - w_i/\sqrt{2\pi}}{\sum_{j \neq i} w_j} \right]. \end{aligned}$$

If all weights sum up to 1, we can compute $\sum_{j \neq i} w_j$ by $1 - w_i$. However, for censored survival data, the weights may not necessary be sum up to one. Here we simply leave the denominator as is.

Thus, the LSCV optimal bandwidth, h_{lscv} , can be found by minimizing

$$\sum_i \sum_j w_i w_j K_{\sqrt{2}h}(X_i - X_j) - \frac{2}{n} \sum_i \left[\frac{\hat{f}(X_i) - w_i/\sqrt{2\pi}}{1 - w_i} \right]. \quad (15)$$

Algorithm 2.1 To find h_{lscv} , we do the following grid search,

Step 1: First search on $[h_l, h_u]$, where $h_l = 0.25h$ and $h_u = 1.5h$, and h is computed by either (9) or (12).

Step 2: Second, expand the searching as below:

- a. If the minimum occurred at the left edge, let $h'_l = h_l + \delta$ and $h'_u = 0.2h'_u$ and repeat the grid search in Step 1 over $[h'_l, h'_u]$. The δ is an increment in each step of searching. It should not be too small when the sample size is reasonably large due to that it will tremendously slow down the algorithm.
- b. If the minimum occurred at the right edge, let $h'_l = h_u - \delta$ and $h'_u = 5h'_l$ and repeat the grid search in Step 1.
- c. If the minimum occurred not at the edge, let $h'_l = (h_l + h_{min})/2$ and $h'_u = (h_u + h_{min})/2$ and repeat the grid search in Step 1.

Step 3: Repeat Step 1 and Step 2 for k times.

When we expand the searching in Step 2, we prefer that the new searching range, $[h'_l, h'_u]$, has a small overlap with the old one, $[h_l, h_u]$, in case that h_{lscv} stays within $[h_l, h_l + \epsilon]$ or $[h_u - \epsilon, h_u]$ for small ϵ . As for how to select k , it depends on the value of δ . We suggest a large k such as 5 or 6 and a large δ , say, $\delta = (h_u - h_l)/20$. We need also take the sample size into consideration. If the sample size is large, the optimal bandwidth tends to be small and we will prefer to adjust the coefficients in Step 2a and Step 2b such that the searching will be focused on the left side of the intervals; otherwise, on the right side.

3. Adaptive Weighted Kernel Density Estimator

One of the drawbacks of using a fixed bandwidth over the whole range of the sample data is that for long-tailed distributions that either the details where the data are dense will be masked or spurious noise will show in the tails. For weighted samples, the shape of the estimated density will be greatly affected by the weighting function. For example, the MP estimator will correct the estimation bias in the following way: (1) all censored survival times will finally be excluded from constructing the density estimate. (2) starting from the smallest observed time, the weight of a censored data point t_i will be equally re-distributed to the data points with $t > t_i$. As a result, the largest uncensored data point will gain more weight from the censored data points and could cause bump at the right tail of the estimated density.

To illustrate the above assertion, we assume the true survival times are

$$16, 17, 19, 20, 21, 22, 24, 25, 28, 35.$$

A standard kernel density estimate was computed based on the above data by using the Gaussian kernel and the bandwidth was selected with the direct plug-in method (built-in R package *KernSmooth 2.22* [27]). The estimated curve was shown as the solid curve in Figure 1. Now, if the 9th observation ($T = 28$) was

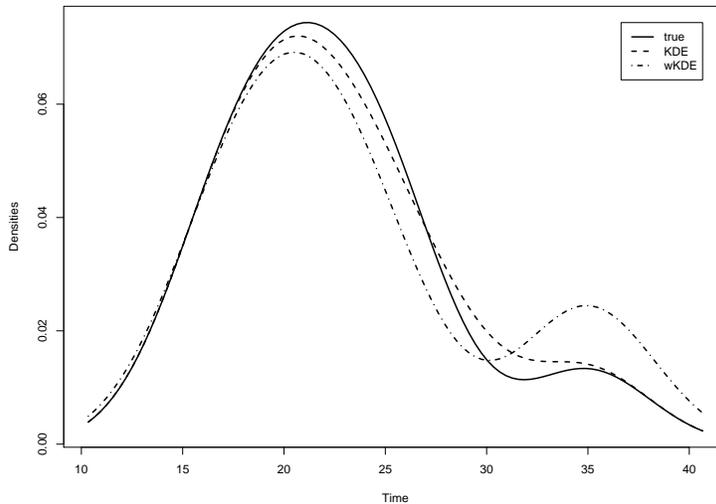


FIG 1. Density estimate of righted-censored data

censored and the censored value is, say, $X = 26$. The estimated density curve by the MP estimator shows an obvious bimodal pattern (dash-dotted curve). The dashed curve in Figure 1 is the estimated density curve by using the standard

kernel density estimator as in (2), which treats the censored time as the true survival time. If the survival times follow distributions with long tails such as exponential or Weibull distribution, the uncensored observations in regions near the right tail will gain extra weights from the censored data points with small values and more likely spurious noise will show up in the estimated density curve. Following the idea of the conventional adaptive kernel estimator from [24], we propose an adaptive weighted kernel density estimator (awKDE). The key idea of the adaptive method is to use shorter bandwidth in regions where the data are dense and use wider bandwidth in regions with sparse data.

Algorithm 3.1 *The following algorithm shows how to construct the adaptive estimates:*

Step 1: Find a pilot estimate \hat{f} by (4) with bandwidth h_n , h_e or h_p .

Step 2: Define local bandwidth factor λ_i by

$$\lambda_i = \{\hat{f}(X_i)/g\}^{-\alpha}, \quad (16)$$

where

$$\log g = n^{-1} \sum \log \hat{f}(X_i)$$

and the sensitivity parameter α satisfies $0 \leq \alpha \leq 1$.

Step 3: Define the adaptive kernel estimate \tilde{f} by

$$\tilde{f}(t) = \sum_{i=1}^n w(X_i, Z_i) \frac{1}{h\lambda_i} K\left(\frac{t - X_i}{h\lambda_i}\right). \quad (17)$$

Literature shows that the pilot estimate in Step 1 is not that crucial [4, 1, 24]. The performance of the awKDE and the choice of α will be studied via Monte-Carlo method in Section 5.

4. Boundary Problem

It is often the case that the natural domain of definition of a density to be estimated is an interval bounded on one or two sides. In [8], the per capita GDP mentioned above are measurements of positive quantities. In survival data analysis, the survival times will never be negative. There could also exist an upper bound in some other cases.

If there are not many observations near zero, one possible solution is to calculate the estimate as if there is no restriction and then set $\hat{f}(x)$ to zero for negative x . Normalizing can also be done to ensure the estimate integrate to unity. Another remedy is to do the log-transformation to the data on the half-line and compute the estimate, then transform back to the original scale. This method could be useful, but the smoothness could be a potential problem: the smoothness is guaranteed for the transformed data by selecting an appropriate bandwidth, but not for the data at the original scale. Sun and Wang [25] showed

that the transformation based kernel density estimate sometimes is less smooth for the transformation $X_t = g(X) = X^{\theta+1}$, where $\theta > 0$.

Asymmetric kernels, such as inverse Gaussian, reciprocal inverse Gaussian and gamma-type kernels, were also considered to eliminate the difficulty of the kernel density estimation around the origin for censored data[5, 21, 13]. Muller and Wang (1994) defined a class of boundary kernels and proposed to reduce the boundary effects by using boundary kernels in the boundary regions and varying bandwidth under minimum mean squared errors criteria[17].

In this study, the reflection method and replication method is adopted to solve the boundary problem[3]. By adding reflections of all points in the data, we get a new data set $\{X_1, -X_1, X_2, -X_2, \dots, X_n, -X_n\}$. Let \hat{f}' be the kernel density estimate constructed based on the new data set. We can show that the density of the original data set can be computed by

$$\hat{f}(x) = \begin{cases} 2\hat{f}'(x), & \text{for } x \geq 0, \\ 0, & \text{for } x < 0. \end{cases}$$

Of course we need not reflect all data points. Because a point stays 4σ away from x will contribute very little to the density at x , we reflect points $X_i \in [0, 4h)$ for $i = 1, 2, \dots, n$. The new weighted density estimator can be rewritten as

$$\hat{f}(x) = \sum_{i=1}^n w(X_i, Z_i) [K_h(x - X_i) + K_h(x + X_i) \cdot I_{0 \leq x < 4h}], \quad (18)$$

where $I(\cdot)$ is an indication function.

5. Simulation

Simulation results will be presented in two parts. In part 1, we will illustrate the performance of h_{lscv} and the adaptive bandwidths. In part 2, we will show the performance of h_n , h_e and h_p .

5.1. Part 1: LSCV and awKDE

Experiments were done to illustrate the performance of h_{lscv} and the adaptive bandwidth. The following algorithm was used.

- Step 1:** draw a random sample from the targeted population;
- Step 2:** compute h_n and h_p based on the sample;
- Step 3:** search h_{lscv} based on h_n ;
- Step 4:** compute the wKDEs with h_n , h_p and h_{lscv} respectively and the corresponding L_1 distances.
- Step 5:** take sensitivity parameter $\alpha = 0.3, 0.4, 0.5, 0.6, 0.7$ and compute the pilot estimates of f by wKDE with h_n , h_{lscv} and h_p respectively; compute the corresponding L_1 distances.

We used two different population distributions: $N(13, 3^2)$ and $Weibull(2, 1)$ and took different sample sizes $n = 20, 30, 50, 100, 300$. For each pair of n and f , the above procedure was repeated for 10000 times and the mean and standard error of the L_1 distances were computed.

5.1.1. Complete Data

Simple random samples were drawn from $N(13, 3^2)$. All data points in the samples were equally weighted, under which all wKDE estimates reduce to the standard kernel density estimate.

Table 1 shows the simulation results. The two values to the left are the mean

TABLE 1
Complete data from Normal distribution

| Size | h_p | awKDE | h_n | awKDE | h_{lscv} | awKDE |
|-------|-------------|-------------|-------------|-------|------------|-------|
| 20 | <u>.274</u> | .277 | .281 | .288 | .320 | .315 |
| (e-3) | 1.143 | 1.180 | 1.111 | 1.142 | 1.611 | 1.664 |
| 30 | .235 | .236 | <u>.232</u> | .238 | .273 | .267 |
| (e-3) | .923 | .955 | .866 | .892 | 1.276 | 1.335 |
| 50 | .194 | .193 | <u>.192</u> | .197 | .225 | .219 |
| (e-3) | .729 | .746 | .676 | .692 | .997 | 1.054 |
| 100 | .148 | <u>.147</u> | <u>.147</u> | .151 | .170 | .166 |
| (e-3) | .523 | .528 | .484 | .492 | .710 | .754 |
| 300 | .097 | <u>.095</u> | .097 | .099 | .108 | .105 |
| (e-3) | .306 | .298 | .282 | .281 | .403 | .425 |

L_1 distance of the wKDE by using either h_p or h_n or h_{lscv} respectively (top) and its standard error (bottom). While the values to the right are those of the awKDE by using the corresponding bandwidth estimates. For each setting, only the best result for different α is displayed. In all cases, simulation results suggest $\alpha = 0.3$.

From Table 1, we find that the mean L_1 distances and the standard errors decrease as n increases. The performance of h_n and h_p is similar: both outperform h_{lscv} . The awKDE improves the estimate for h_{lscv} . For h_n and h_p , the awKDE does not improve the estimates. It improves the estimate for h_p a little bit when n is large, and makes the estimate worse for h_n .

5.1.2. Incomplete Data

We drew random samples from both $N(13, 3^2)$ and $Weibull(2, 1)$, with 30% of the data points randomly right-censored. The weighting function $w(\cdot)$ is taken to be the jump sizes of the Kaplan-Meier estimator as MP estimator. Simulation results are listed in Table 2 and Table 3. The sample sizes in the two tables are the sizes of the original data before censoring. We took larger sample sizes such that we had approximately the same amount of uncensored data points, as in Table 1, in computing the kernel density estimates. We can find that h_{lscv} does

TABLE 2
Incomplete data from Normal population

| Size | h_p | awKDE | h_n | awKDE | h_{lscv} | awKDE |
|-------|-------------|-------------|-------------|-------|------------|-------|
| 30 | .269 | .271 | <u>.265</u> | .272 | .312 | .306 |
| (e-3) | 1.112 | 1.156 | 1.048 | 1.084 | 1.535 | 1.593 |
| 40 | .240 | .242 | <u>.239</u> | .245 | .278 | .272 |
| (e-3) | .964 | 1.005 | .908 | .942 | 1.320 | 1.382 |
| 70 | .197 | .198 | <u>.196</u> | .202 | .226 | .221 |
| (e-3) | .742 | .763 | .694 | .716 | 1.004 | 1.055 |
| 140 | .156 | <u>.155</u> | .156 | .160 | .177 | .173 |
| (e-3) | .551 | .563 | .517 | .530 | .717 | .759 |
| 300 | <u>.120</u> | .121 | .121 | .125 | .134 | .132 |
| (e-3) | .394 | .399 | .374 | .379 | .491 | .522 |

TABLE 3
Incomplete data from Weibull population

| Size | h_p | awKDE | h_n | awKDE | h_{lscv} | awKDE |
|-------|-------|-------|-------------|-------|------------|-------|
| 30 | .297 | .301 | <u>.296</u> | .302 | .413 | .414 |
| (e-3) | 1.149 | 1.190 | 1.124 | 1.158 | 1.134 | 1.324 |
| 40 | .269 | .272 | <u>.268</u> | .273 | .398 | .397 |
| (e-3) | .993 | 1.025 | .985 | 1.011 | 1.298 | 1.262 |
| 70 | .230 | .231 | <u>.229</u> | .232 | .373 | .371 |
| (e-3) | .797 | .811 | .790 | .800 | 1.266 | 1.212 |
| 140 | .194 | .194 | <u>.193</u> | .194 | .353 | .347 |
| (e-3) | .606 | .609 | .603 | .605 | 1.339 | 1.280 |
| 300 | .168 | .168 | <u>.166</u> | .167 | .330 | .323 |
| (e-3) | .465 | .460 | .462 | .459 | 1.471 | 1.413 |

not work as well as h_n and h_p for data from both populations. The adaptive method improves the estimate with h_{lscv} , but not those with h_p and h_n .

Remarks: (a) The h_{lscv} does not work well. This is consistent to the conclusion in [2], where Altman and Léger suggested plug-in estimator instead of using leave-one-out or leave-some-out method to seek optimal bandwidth. For right-censored data, the reweighting scheme will compromise the sparseness of data at the right tail and the adaptive method won't work as well as expected. (b) The rough approach h_n outperforms the other two methods (in some settings, its performance is very similar to h_p).

5.2. Part 2: Performance of h_n , h_e and h_p

In this part, we studied the performance of h_n , h_e and h_p by comparing with an existing estimator by Kuhn and Padgett (1997, KP estimator hereafter)[12]. The KP estimator is an estimator proposed for survival data subject to random right-censoring which selects the bandwidth locally by minimizing a mean absolute error, which is supposed to be more nature than the mean squared error criteria [6]. The optimal bandwidth used by KP estimator is

$$h_{kp}(x) = \left\{ \frac{4\alpha^2 f(x)R(K)}{n\mu_2^2 f''(x)^2 H^*(x)} \right\}^{1/5}, \tag{19}$$

where $\alpha = 0.4809489$. When a Gaussian kernel is used, we have $R(K) = (2\sqrt{\pi})^{-1}$ and $\mu_2^2 = 1$. The censoring survival function, $H^*(x)$, is estimated by the product-limit (PL) estimator, $H^*(x) = 1 - \hat{H}(x)$, where

$$\hat{H}(x) = \begin{cases} 1, & 0 \leq x \leq X_{(1)}, \\ \prod_{i=1}^{k-1} \left(\frac{n-i}{n-i+1} \right)^{1-\Delta_i}, & X_{(k-1)} < x \leq X_{(k)}, k = 2, \dots, n, \\ 0, & x > X_{(n)}. \end{cases}$$

Here $X_{(1)}, \dots, X_{(n)}$ are the order statistics of X_1, \dots, X_n . An exponential reference density, $f_R(x) = \lambda^{-1} \exp(-x/\lambda)$, is preferred, where λ is estimated by the maximum likelihood estimate

$$\hat{\lambda} = \frac{\sum_{i=1}^n X_i}{\sum_{i=1}^n \Delta_i}.$$

Thus we have

$$h_{kp}(x) = 0.7644174 \cdot \hat{\lambda} H^*(x)^{-1/5} e^{x/5\hat{\lambda}} n^{-1/5} \tag{20}$$

and we can express the KP estimate by

$$\hat{f}_{kp}(x) = \sum_{i=1}^n \frac{\Delta_i}{nH^*(X_i)} K_{h_{kp}(X_i)} \left(\frac{x - X_i}{h_{kp}(X_i)} \right). \tag{21}$$

Random samples were drawn from three different distributions: (a) normal distribution with mean 13 and variance 9, (b) exponential distribution with mean 1, and (c) Weibull distribution with shape parameter 2 and scale parameter 1. For each sample, approximately 30% of the data points were randomly right-censored. Based on the censored data together with the censoring information (Δ), we estimated the density by wKDE with different bandwidths h_n , h_e , h_p and h_{kp} respectively. The L_1 distances were computed and shown in Table 4 through Table 6 together with the corresponding standard errors.

TABLE 4
 $N(13, 3^2)$

| Size | h_{kp} | h_n | h_e | h_p |
|-------|----------|-------|-------|-------------|
| 30 | .741 | .283 | .276 | <u>.267</u> |
| (e-3) | .590 | 1.076 | 1.105 | 1.095 |
| 50 | .710 | .234 | .230 | <u>.224</u> |
| (e-3) | .501 | .828 | .845 | .887 |
| 100 | .654 | .180 | .178 | <u>.175</u> |
| (e-3) | .381 | .601 | .607 | .665 |
| 200 | .586 | .143 | .142 | <u>.139</u> |
| (e-3) | .284 | .442 | .445 | .492 |

From Table 4, it can be found that h_n , h_e and h_p all work well for censored data from the normal population, while h_p outperforms the other three methods.

TABLE 5
Exponential(1)

| Size | h_{kp} | h_n | h_e | h_p |
|-------|-------------|-------|-------|-------|
| 30 | <u>.263</u> | .335 | .334 | .382 |
| (e-3) | 1.200 | 1.287 | 1.291 | 1.207 |
| 50 | <u>.243</u> | .301 | .301 | .345 |
| (e-3) | 1.004 | 1.032 | 1.037 | .941 |
| 100 | <u>.223</u> | .264 | .264 | .302 |
| (e-3) | .793 | .777 | .779 | .704 |
| 200 | <u>.207</u> | .236 | .237 | .267 |
| (e-3) | .614 | .592 | .590 | .532 |

TABLE 6
Weibull(2, 1)

| Size | h_{kp} | h_n | h_e | h_p |
|-------|----------|-------|-------|-------------|
| 30 | .344 | .299 | .296 | <u>.289</u> |
| (e-3) | .843 | 1.128 | 1.142 | 1.104 |
| 50 | .321 | .257 | .257 | <u>.251</u> |
| (e-3) | .740 | .905 | .919 | .890 |
| 100 | .284 | .212 | .213 | <u>.210</u> |
| (e-3) | .603 | .676 | .688 | .676 |
| 200 | .248 | .181 | .182 | <u>.180</u> |
| (e-3) | .476 | .524 | .531 | .524 |

The estimator h_n has a relatively larger mean L_1 distances and the smallest standard errors. The KP estimator does not work well. This may be due to the fact that we used a normal density while KP estimator assume an exponential reference density. Though, the performance of h_e was not affected much because we took the minimum of s_w and $IQR_w/1.34$ in (12). As shown in Table 5, when f is actually an exponential p.d.f., the KP estimator outperforms the other three methods as expected. This is not surprising because it uses more (correct) information than the others. The performance of h_n and h_e are alike, both outperform h_p . In Table 6, when a Weibull population was used, h_p is the winner. Both h_n and h_e also work well. When n increases, their performance becomes very similar.

6. Applications

6.1. Density Estimation from Biased Sampling

The wKDE can be used to estimate the densities based on biased samples. In biased sampling, if whether an element with $X = x$ will be observed depends on its true value x , we obtain a biased sample. Let's assume that $X_i = x_i$, will be sampled with probability $b(x_i)$. Let $f(x)$ be the population density, we can show that the density of the biased sample is a weighted version of $f(x)$,

$$f_s(x) = b(x)f(x)/\kappa, \tag{22}$$

where κ is a normalizing constant such that

$$\kappa = \int b(x)f(x)dx.$$

Both $b(\cdot)$ and $f(\cdot)$ in (22) are non-parametrically identifiable if two or more random samples with overlaps are available [28]. However, based on just one sample, we need further restrictions on either $b(\cdot)$ or $f(\cdot)$ or both to ensure the identifiability [26, 7]. Throughout this paper, we assume $b(\cdot)$ and further $w(\cdot)$ to be parametrically known.

We can estimate $f_s(x)$ by a standard kernel density estimator as in (2) and therefore obtain a natural estimate of $f(x)$,

$$\hat{f}_b(x) = \kappa \hat{f}_s(x)/b(x) = \frac{\kappa}{n \cdot b(x)} \sum_{i=1}^n K_h(x - X_i). \quad (23)$$

Wu (1997) proposed to estimate $f(x)$ for s -dimension data by a kernel density estimator [30]. We simply take $s = 1$ and get its univariate version estimate,

$$\hat{f}_{wu}(x) = \kappa' \sum_{i=1}^n b^{-1}(X_i)K_h(x - X_i), \quad (24)$$

where $\kappa' = 1/\sum b(X_i)$.

Which estimate is better, $\hat{f}_b(x)$ or $\hat{f}_{wu}(x)$? In (23), if the biasing function $b(x)$ is coarse or not continuous, the estimate in (23) may also be coarse. While in (24), the estimate is smooth. A Monte Carlo study was carried out to compare their performance in density estimation based on biased samples. We first drew a random sample, X , of size 200 from a targeted population; second, we mimicked the biased sampling scheme by keeping observation $X = x$ in the data set with probability $b(x)$; finally, we computed \hat{f}_b and \hat{f}_{wu} based on the biased samples. To evaluate the performance, the L_1 distance between f and \hat{f} is computed,

$$\hat{L}_1(f, \hat{f}) = \int |\hat{f} - f| \approx \sum_{i=1}^m |\hat{f}(y_i) - f(y_i)| \cdot d_i, \quad (25)$$

where $0 \leq y_1 < y_2 < \dots < y_m$ and $d_i = (y_{i+1} - y_{i-1})/2$ for $i = 2, 3, \dots, m - 1$ and $d_1 = y_2 - y_1$, $d_m = y_m - y_{m-1}$.

We took two targeted populations: (a) Weibull distribution with shape parameter 2 and scale parameter 1; and (b) normal distribution with mean 10 and standard deviation 2. Two different biasing function were used for biased sampling,

$$b_1(x) \propto x$$

$$b_2(x) = \begin{cases} 0.2 & \text{if } x \leq \mu - 1.2\sigma, \\ 0.4 & \text{if } \mu - 1.2\sigma < x \leq \mu - 0.4\sigma, \\ 0.6 & \text{if } \mu - 0.4\sigma < x \leq \mu + 0.4\sigma, \\ 0.8 & \text{if } \mu + 0.4\sigma < x \leq \mu + 1.2\sigma, \\ 1.0 & \text{if } x > \mu + 1.2\sigma. \end{cases}$$

We repeated the above procedure for 10000 times for each setting and approximate the mean L_1 distance and the standard error. The results are shown in Table 7. We find in all the four scenarios, \hat{f}_{wu} outperforms \hat{f}_b .

TABLE 7
Performance of $wKDE$ and KDE for biased samples

| $b(\cdot)$ | \hat{f} | N(10,2) | | Weibull(2,1) | |
|--------------|----------------|---------|---------|--------------|---------|
| | | mean | se | mean | se |
| $b_1(\cdot)$ | \hat{f}_b | .130 | 4.37e-4 | .167 | 6.51e-4 |
| | \hat{f}_{wu} | .127 | 4.33e-4 | .150 | 6.41e-4 |
| $b_2(\cdot)$ | \hat{f}_b | .194 | 4.43e-4 | .221 | 5.80e-4 |
| | \hat{f}_{wu} | .145 | 5.36e-4 | .167 | 5.76e-4 |

In Figure 2, the Weibull distribution was used in plot (a) and (c), and the

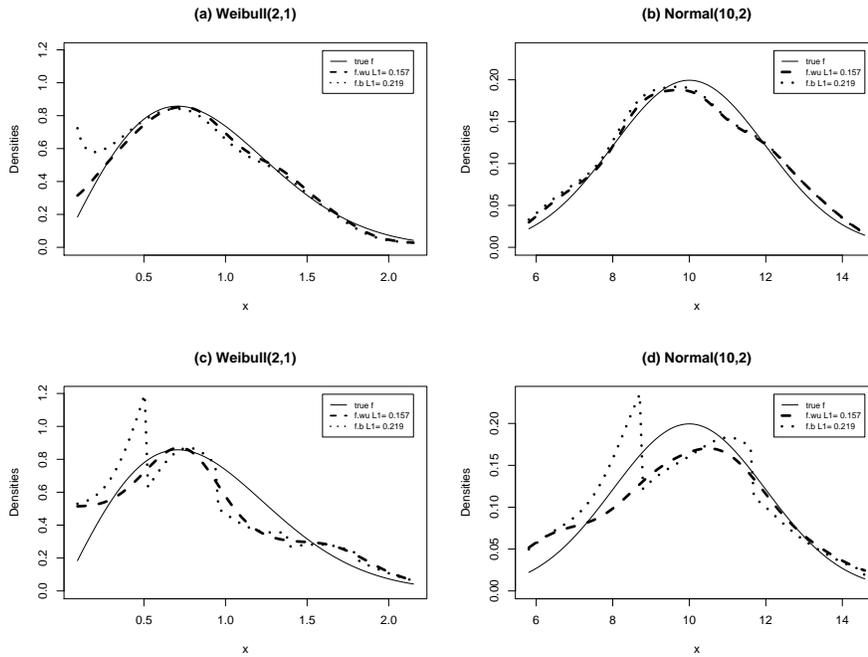


FIG 2. Kernel density estimate of length biased data

normal distribution was used in plot (b) and (d). In Figure 2, the solid curves show the true density curves of f . The dashed curves and dotted curves represent the estimated density curves by \hat{f}_{wu} and \hat{f}_b respectively. In plot (a) and (b), we find that when $b(x)$ is smooth, both \hat{f}_b and \hat{f}_{wu} are smooth. The two estimators work similarly well except that \hat{f}_b has a boundary problem due to that $b(x) \rightarrow 0$ when $x \rightarrow 0$. The results in Table 7 also demonstrate that the difference between the two mean L_1 -distances of \hat{f}_b and \hat{f}_{wu} is not very large. However, in plot (c)

and (d), we can find that when the biasing function is a step function, \hat{f}_{wu} is still smooth, but \hat{f}_b is not. The difference between the two mean L_1 -distances also becomes larger. In conclusion, \hat{f}_{wu} has better performance than \hat{f}_b .

6.2. Density Estimation from Informative Censoring

In a clinical trial by the Eastern Cooperative Oncology Group, the survival times of 61 patients with inoperable carcinoma of the lung, progressions of which are usually associated with shortened residual lifetime, who were treated with the drug cyclophosphamide were collected [14]. Among the 61 patients, 33 died and their survival times were observed and listed in Table 8. Table 9 lists the other 28 censored observations representing patients whose treatment was terminated, at the times indicated, because of the appearance of metastatic disease or a significant increase in the size of their primary lesion. The eventually failure times of the 28 censored patients were also collected (in parentheses) by a follow-up study. These 28 failure times were contaminated due to that those patients received other therapies thought to be more beneficial than cyclophosphamide after they were removed from the study and their ultimate survival times are possibly slightly better than what they would have been if they were kept on study and continued on cyclophosphamide.

TABLE 8
Observed deaths

0.43, 2.86, 3.14, 3.14, 3.43, 3.43, 3.71, 3.86, 6.14, 6.86, 9.00, 9.43, 10.71, 10.86, 11.14, 13.00, 14.43, 15.71, 18.43, 18.57, 20.71, 29.14, 29.71, 40.57, 48.57, 49.43, 53.86, 61.86, 66.57, 68.71, 68.96, 72.86, 72.86

TABLE 9
Observed Censored times (ultimate survival times)

0.14(3.00), 0.14(12.43), 0.29(1.14), 0.43(17.14), 0.57(4.43), 0.57(5.43), 1.86(12.14), 3.00(7.86), 3.00(13.86), 3.29(10.57), 3.29(34.43), 6.00(7.86), 6.00(38.00), 6.14(9.29), 8.17(20.43), 10.57(25.00), 11.86(17.29), 15.57(51.57), 16.57(45.00), 17.29(24.14), 18.71(29.43), 21.29(26.71), 23.86(29.00), 26.00(53.86), 27.57(49.71), 32.14(63.86), 33.14(99.00), 47.29(48.71)

Let T be the true survival times, T^c be the censored times and T^u be the ultimate survival times. We compute the observed residual lifetime of the 28 patients by $T^r = T^u - T^c$. The T^r s contain the carry-over effects by treatments other than cyclophosphamide. Plot (a) of Figure 3 shows the relationship between $\log(T^r/T^c)$ and T^c . The point marked with “X” is a potential outlier and we leave it out. A smoothed curve was fitted to the data shown in plot (a) by the following model,

$$\log(T^{r1}/T^c) = S(T^c) + \epsilon, \tag{26}$$

where $S(\cdot)$ is a smooth function to be estimated. The fitted curve (solid line) shows a curvilinear pattern: the ratio of T^r and T^c was large for removed patients who stayed in the system for either shorter or longer period of times. The upper

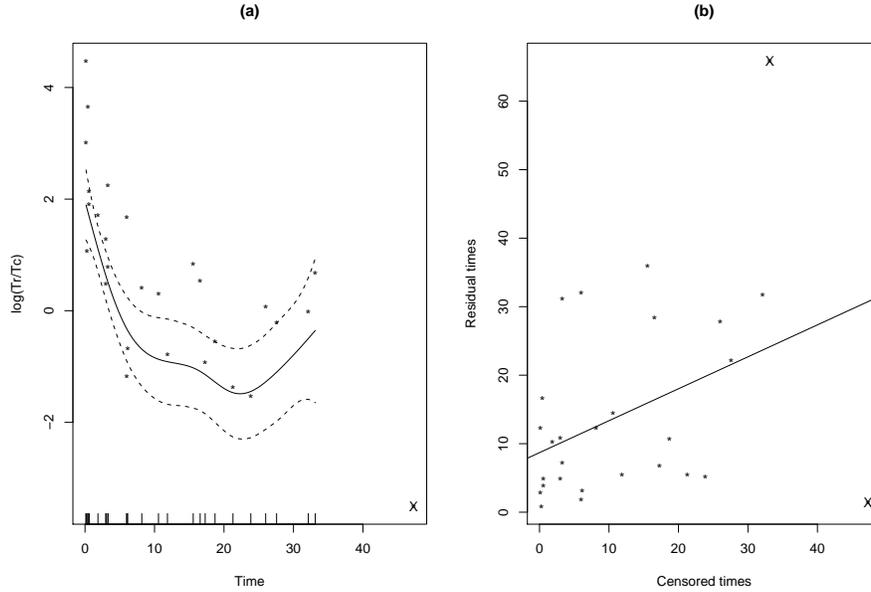


FIG 3. Lung data

and lower dotted curves were added at 2 standard errors above and below the estimate of the smooth. Plot (b) gives a scatter plot of T^r on T^c . A least squares line was added to the plot by fitting a simple linear regression model,

$$T^{r2} = \beta_0 + \beta_1 T^c + \epsilon. \quad (27)$$

The slope was computed to be $\beta_1 = .4662$, which is significantly different from zero with p-value= 0.03478. Two potential outliers were marked and excluded from computation. From the above two plots, we can see there do exist some relationship pattern between T^r and T^c .

Although \hat{T}^r can not be used to replace the true residual times, it could provide useful information about the true survival times. This type of information can be used to adjust the weighting function in wKDE to improve the estimate. Due to that the other therapies were thought to be more beneficial than cyclophosphamide, it is reasonable for us to believe that a removed patient was more likely to die no later than the observed ultimate survival time, $T \leq T^u$. In stead of reassigning the weight belongs to a censored data point X_i equally to all points thereafter, we can assign its weight to all points fall between T_i^c and $T_i^c + \hat{T}_i^r$. If no observation lies inside the above range, we assign the weight of T_i to the observation which stays the closest to the upper boundary. The MP estimator will not work because we know that the true residual times were less likely to be larger than $T^u - T^c$. In this study, the two \hat{T}^r 's by (26) and (27) lead to exactly the same kernel density estimate, which is shown as the

solid curve in Figure 4 (labeled as “lm/gam”). In Figure 4, the dashed curve is

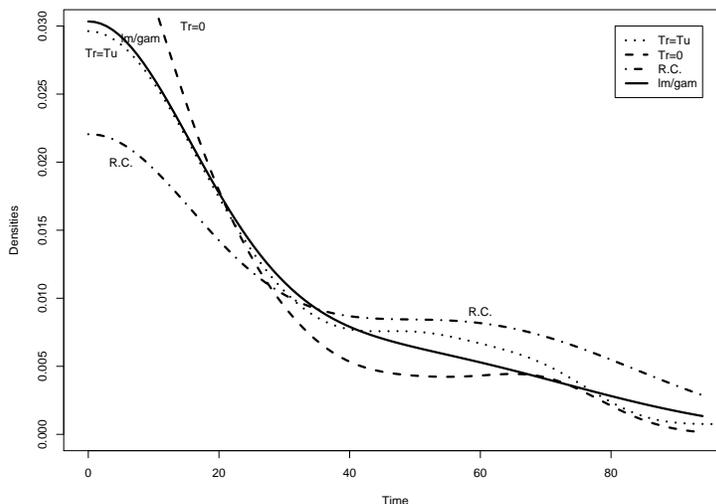
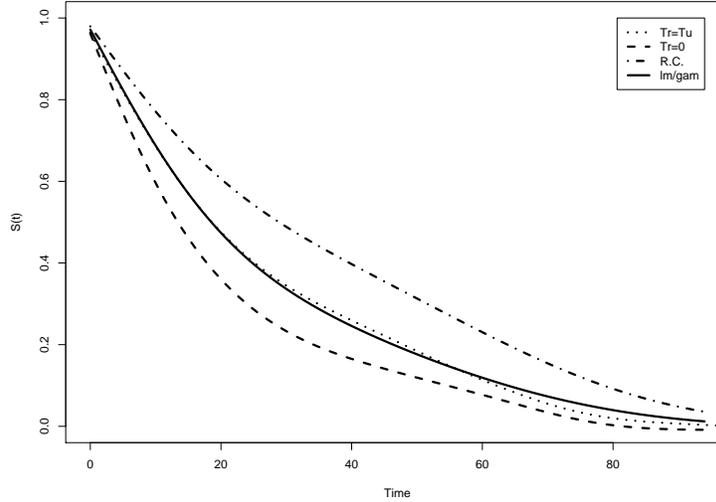


FIG 4. *Density estimates*

the estimated density curve by taking $T^r = 0$, where all removed patients were assumed to die right after T^c given no other therapies were provided. While the dotted curve is the one by assuming the residual times are exactly the ultimate observed survival times. The dash-dotted curve was estimated by assuming random right censoring and computed by MP estimator. The survival functions were also computed and plotted in figure 5 based on the above different estimates of f . Obviously, the MP estimate is too optimistic and under-estimates the risk (dash-dotted curve). The dashed curve provides an estimate of the survival function by assuming the dropout patients die right after the censored times. It over-estimates the risk and seems to be too pessimistic. By reassigning the weights to points in a neighborhood of the censored data points, we obtain the survival function as the solid curve in figure 5. This curve is very close to the one by assuming the true survival times are the ultimate survival times.

7. Summary

In summary, the two rough approaches and the plug-in method work well in bandwidth selection for wKDE. If the target distribution is a exponential-like distribution, the KP estimator is also a good choice. The LSCV method and the adaptive estimator won't improve the estimate for wKDE. For large samples, Fourier transform or fast Fourier transform and kernels such as Epanechnikov kernel can be considered, which could remarkably improve the computational speed [16, 23, 9].

FIG 5. *Survival Function Estimates*

By choosing an appropriate weighting function, the wKDE can be used to robustly and efficiently estimate the densities from survival data subject to random censoring. The situation for data subject to informative censoring is much complicated, because the it's hard to model the sampling scheme. A possible solution is try to classify the censored data points into several categories and use the prior information we have to define different weight-redistribution schemes, and finally apply wKDE to estimate the density. Alternatively, instead of assigning weights to values after the censoring times equally or only to points in certain neighborhoods, we can also consider impute the censored times and re-assign weights to points in the nearby regions. When covariates are available, a parametric model or quantile regression could be more efficient. Further studies will be carried out and the results will be presented in another research paper.

All algorithms have been implemented in R and C, and are available on request.

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