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Nonparametric Smooth Estimation of Probability Density Function and Other Related Functionals: Some New Developments*

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Abstract **-** In this paper, I will highlight some recent developments in the area of nonparametric functional estimation with emphasis on nonparametric density estimation. A lemma attributed to Hille, and its generalization [see Lemma 1, Feller [26], §VII.1)] has been used to propose estimators in the context of *i.i.d.* observations in Chaubey and Sen [15] and Chaubey *et al.* [13]. The generality of the technique is illustrated to non-standard situations such as biased data and circular data. A review of recent results and contrasting various techniques is also given.

Keywords**:** Hazard function, Multivariate distribution, Mean residual life, Non-parametric smoothing, Survival function.

1. Introduction

Nonparametric estimation of probability density function in particular, and that of functionals of a distribution function in general, presents an important area of statistics in the modern era of data analysis (see Fan and Gijbels [25], Scott[34], Prakasa Rao [36] and Sylvapulle and Sen [35]).

The adequacy of nonparametric density estimation in contrast to the parametric modelling lies in the fact that parametric inference procedures are efficient as long as the assumed and true distributions are the same, however, any discrepancy between the assumed and true distributions, may grossly affect parametric procedures, providing inefficient or inconsistent procedures. For example, if the underlying density is gamma with shape parameter $p(>> 1)$ while we assume it to be exponential (for which $p = 1$), then the true and assumed pdf may differ drastically at the lower end point (0) as well as in the upper tail ($x \to \infty$).

Among many nonparametric density estimation procedures the basic kernel method developed by Rosenblatt [32], and popularized by Parzen [30] still remains to be one of the most popular methods (see Härdle [28]). Based on a random sample $(X_1,X_2,...,X_n)$, from a univariate distribution with density $f(.)$, the kernel estimator of f is given by

$$\hat{f}_n(x) = (nh_n)^{-1}\sum_{i=1}^{n} k((X_i - x)/h_n) \tag{1.1}$$

where $h_n(> 0)$, known as the band-width is so chosen that $h_n \to 0$ but $nh_n \to \infty$, as $n \to \infty$. $k(.)$ is termed, the kernel function, and it is typically taken to be symmetric. Rosenblatt[32] motivated it by generalizing the histogram estimator

$$f_n(x) = \frac{F_n(x+h) - F_n(x-h)}{2h}, \tag{1.2}$$

where

$$F_n(x) = \frac{1}{n}\sum_{i=1}^{n} I(X_i \le x). \tag{1.3}$$

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The inherent problem of the possibility of assigning positive probability to the zero-probability region, in this context, was noted by Silverman [36]. He suggested using kernel estimator on log-transformed data.

In addition, an alternative proposal to use exponential kernel was studied by Bagai and Prakasa Rao [2]. On the other hand, Chaubey and Sen [15] considered the problem of estimating the survival function and the corresponding density for survival data where the density is typically supported on the non-negative half of the real line.

The approach taken in this paper is to smooth the distribution (survival) function based on Poisson weights, and consider the density estimator as its derivative. According to this approach, essentially, a smooth estimator of $F(x)$ is given by

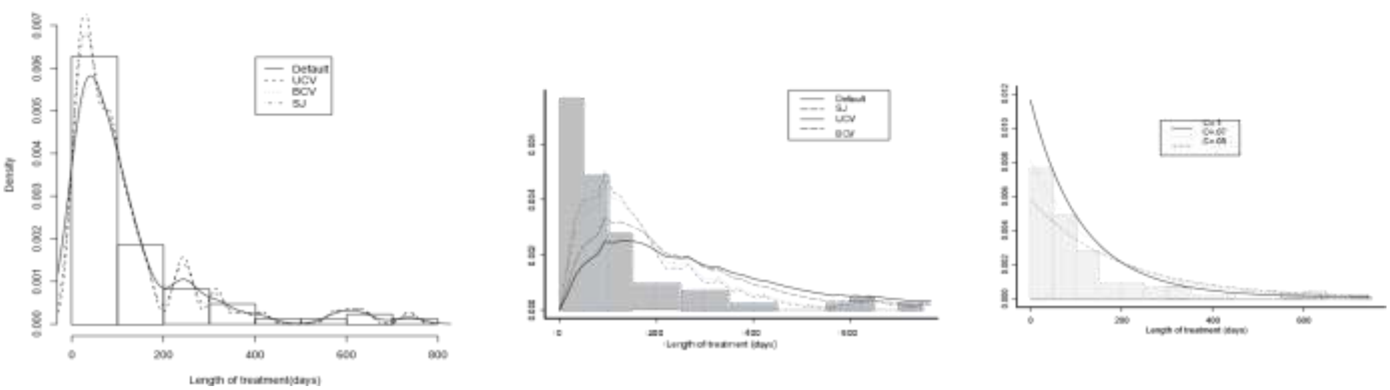
$$\tilde{F}_n(x) = \sum_{k=0}^{\infty} F_n\left(\frac{k}{\lambda_n}\right) p_k(\lambda_n x) \tag{1.4}$$

where $p_k(\mu) = e^{-\mu}\mu^k/k!$, $k = 0,1,2,...,$ and $\lambda_n \to \infty$ as $n \to \infty$. The derived smooth estimator of $f(x)$ is then given by

$$\tilde{f}_n(x) = \lambda_n \sum_{k=0}^{\infty} \left[F_n\left(\frac{k+1}{\lambda_n}\right) - F_n\left(\frac{k}{\lambda_n}\right)\right] p_k(\lambda_n x) \tag{1.5}$$

It may be noted that the estimator in Chaubey and Sen [15], in contrast to that of Bagai and Prakasa Rao [2], uses the whole data and naturally provides consistent estimate of $f(0)$, in case $f(0) > 0$. Also, the log-transformation may provide a sharp spike at zero that may be undesirable is some cases.

Figure 1a gives kernel estimators for different choices of bandwidths using the Gaussian kernel for the *Suicide Data* given in Silverman (page 8) [36] consisting of lengths of 86 spells of psychiatric treatment undergone by patients used as controls in a study of the relationship between suicide risk and time under treatment. The reader may refer to Venebles and Ripley [37](§5.5) for a description of these choices. The bandwidth choices given by the *default* option and BCV criterion produce smoother estimates as compared to the other two choices. However, all the bandwidth choices produce non-negative estimates of the density below zero where it should be definitely zero.



(a) Kernel estimators (b) BP Kernel estimators (c) CS Kernel estimators

Fig. 1: Smooth density estimators for suicide study data (Silverman, 1986).

In Figure 1b, we produce the estimators due to Bagai and Prakasa Rao [2] using a standard exponential kernel with the same bandwidths as used for producing Figure 1a. Here, we see that the density is necessarily zero at zero, which may not be desirable. We may also note that some boundary correction methods (see Karunamuni and Alberts [29]) produce density estimators for this data with positive mass at zero. Figure 1c gives smooth density estimators for the same data as in Figure 1a for different values of *c*, obtained from the expression in Eq. (1.5) based on the Poisson weights. Here, we note that a quite different picture emerges. The motivation for the estimator in Chaubey and Sen [15] is the following lemma attributed to Hille as given in Feller [26] (see Lemma 1 in §VII.1).

Lemma 1.1 *Let u(x) be bounded, continuous function on* **R**$^+$*. Then*

$$e^{-\lambda x}\sum_{k\geq 0} u(k/\lambda)(\lambda x)^k/k! \to u(x), \quad \text{as } \lambda\to\infty, \tag{1.6}$$

uniformly in any finite interval **J** *contained in* **R**$^+$*.*

Adapting this lemma for estimation of $F(x)$, replacing $u(x)$ by the empirical distribution function $F_n(x)$ provides the estimator given in equation (1.4). In studying the properties of the resulting estimator of the distribution function, the following results are worth a mention.

Theorem 1.1 *If* $S(t)$ *is continuous (a.e.),* $\lambda_n \to \infty$ *and* $n^{-1}\lambda_n \to 0$ *then*

$$\|\tilde{S}_n - S\| = \sup\{|\tilde{S}_n(t) - S(t)| : t\in \mathbf{R}^+\} \to 0 \ \ a.s., \ \ as \ n\to\infty. \tag{1.7}$$

The closeness of the smooth estimator of survival function to the true survival function as given in the following theorem implies also the same asymptotic normality for the smooth as well as the empirical estimator of the survival function.

Theorem 1.2 *Under the hypothesis on* λ_n *in the previous theorem, whenever* $f(t)$ *is absolutely continuous with a bounded derivative a.e. on* **R**$^+$*,*

$$\|\tilde{S}_n - S_n\| = O(n^{-3/4}(\log n)^{1+\delta}) \ \ \text{a.s.}, \ \ \text{as } n\to\infty, \tag{1.8}$$

where $\delta(>0)$ *is arbitrary.*

Asymptotic properties for the derived density functions were also established in Chaubey and Sen [15].

Here I will highlight a generalization of Lemma 1.1 that yields new nonparametric estimators of density but alleviates the problems by classical kernel estimator, such as providing inconsistent estimator at the boundaries as well as assigning positive mass in the non-positive region. This generalisation has been used in [13] to provide alternative kernel estimators for non-negative data. This has been detailed in §2, and smooth estimation of functionals of a survival function are outlined in \S 3. Section 4 provides other applications and Section 5 presents newer developments to length biased data, directional data, dependent data, quantile estimation and smooth estimation of density of a function of observations and §6 gives some conclusions.

2. The Generalized Approximation Lemma and Applications

Chaubey *et al.* [13] used the following generalization of Hille's lemma in proposing alternative estimators of density and distribution functions.

Lemma 2.1 (Lemma 1, §VII.1, Feller [26]) *Let u be any bounded and continuous function. Let* $G_{x,n}$*,* $n = 1,2,\ldots$ *be a family of distributions with mean x and variance* $h_n^2(x)$ *then we have for* $h_n(x)\to 0$

$$\tilde{u}(x) = \int_{-\infty}^{\infty} u(t)dG_{x,n}(t) \to u(x) \tag{2.1}$$

The convergence is uniform in every subinterval in which $h_n(x)\to 0$ *and u is uniformly continuous.*

Hille's lemma is obtained by choosing $G_{x,n}$ generated by attaching probabilities $p_k(\lambda_n x)$ to (k/λ_n), thus $G_{x,n}$ having mean x and variance $h_n^2(x) = x/\lambda_n$, in case the support of F is $[0,\infty)$.

This generalization may be easily adapted for smooth estimation of the distribution (survival) function as given below;

$$\tilde{F}_n(x) = \int_{-\infty}^{\infty} F_n(t) dG_{x,n}(t) \tag{2.2}$$

Strong convergence of $\tilde{F}_n(x)$and other properties parallel to those of the estimator using the Hille's lemma were studied in [14]. Technically, $G_{x,n}$ can have any support but it may be prudent to choose it so that it has the same support as the random variable under consideration; because this will get rid of the problem of the estimator assigning positive mass to undesired region.

The estimator $\tilde{F}_n(x)$ can be explicitly written as

$$\tilde{F}_n(x) = 1 - \int_{-\infty}^{\infty} G_{x,n}(u) dF_n(u) = 1 - \frac{1}{n}\sum_{i=1}^{n} G_{x,n}(X_i) \tag{2.3}$$

Thus, for $\tilde{F}_n(x)$ to be a proper distribution function, $G_{x,n}(t)$ must be decreasing function of x. This can be shown using an alternative form of $\tilde{F}_n(x)$. In addition to being computationally attractive, this form provides an insight into the usual kernel estimator for distributions with infinite support. This also leads us to propose a smooth estimator of the density as

$$\tilde{f}_n(x) = \frac{d\tilde{F}_n(x)}{dx} = -\frac{1}{n}\sum_{i=1}^{n} \frac{d}{dx} G_{x,n}(X_i), \tag{2.4}$$

The representation given by Eq. (2.4) can also be used to derive the kernel estimator given by Eq. (1.1) as follows. Let $G_{x,n}(.)$ be given by

$$G_{x,n}(t) = K\left(\frac{t-x}{h}\right), \tag{2.5}$$

which has mean x and variance h^2, where $K(.)$ is a distribution function with mean zero and variance 1. Note also that symmetry of K is not required as is usually required in kernel estimation. The condition that $h \equiv h_n(x) \to 0$, which is enough to guarantee the almost sure convergence of $\tilde{F}_n(x)$, may not be enough for consistency of $f_n(x)$.

The general smoothing lemma may also be used directly for proposing motivating the kernel estimator. Replacing $u(x)$ by $f(x)$, we see that a close approximation to $f(x)$ is given by

$$\tilde{f}_n(x) = E(g_{x,n}(X)) \tag{2.6}$$

which can be estimated for an *i.i.d.* sample by

$$\tilde{f}_n(x) = \frac{1}{n}\sum_{i=1}^{n} g_{x,n}(X_i). \tag{2.7}$$

Choosing $g_{x,n}$ as an appropriate symmetric density gives the usual kernel estimator; however, it also suggests alternative estimators in the case of restricted support for the distribution. Chen[24] chose Gamma kernels for non-negative random variables and Beta kernels for distributions centered on the unit interval, which can be motivated from the above approach, although no such motivation is provided in Chen [24]. Similar estimators for the density function are also given by Scaillet [33] using inverse Gaussian and reciprocal inverse Gaussian kernels. One of the major drawback of these estimators is that the resulting estimate of the density is always zero at $x = 0$. Also note that in general the two estimators given by Eqs. (2.4) and (2.7) may be different. Bouezmarni and Scaillet [3] have considered the use of Chaubey and Sen [15] and Chen [24] estimators for estimation of the density of a time series with $\alpha-$ mixing.

For the data concentrated on [0,1], the use of Lemma 2.1 provides Bernstein-polynomial estimator for the density function by using an appropriate binomial distribution. Such an estimator was originally proposed by Vitale [38] and it was later investigated by Babu *et al.* [1] from the point of view of the Hille's lemma. Chaubey and Sen [20] generalised Lemma 2.1 to the multivariate case and studied the properties of the corresponding smooth estimators of multivariate survival and density functions (see also the review article by Chaubey [4]).

3. Functionals of the Survival Function

The paper by Chaubey and Sen [16] investigated the asymptotic properties of the derived functionals of *distribution function* (d.f.) $F(\cdot)$,such as the *hazard function* $h(t) = f(t)/S(t) = -(d/dt)\log S(t)$ and, the *cumulative hazard function* (c.h.f.) $H(t)$,

$$H(t) = \int_0^t h(y)dy = -\log S(t),\ t \geq 0 \quad (3.1)$$

In [18], Chaubey and Sen considered estimating the *mean residual life function* $m(t) = \int_t^\infty S(u)du/S(t)$ using the plugging in $\tilde{S}_n(t)$ for $S(t)$. They established almost sure convergence and asymptotic normality of the resulting smooth estimator of $m(t)$.

Chaubey and Sen [17] investigated the properties of the smooth estimator of survival, density, hazard and cumulative hazard functions in the case of randomly censored data establishing results similar to the uncensored case. The role of $S_n = 1 - F_n$ is played by the Kaplan-Meier product-limit estimator (PLE). These results have been extended in Chaubey and Sen [14] in the context of estimating the *mean residual life function*.

4. Other Applications

Chaubey and Sen [19] noted that if $u(x)$ is monotone then so is $\tilde{u}(x)$. This fact is used in proposing nonparametric smooth estimators of monotone hazard rate, monotone density and monotone mean residual life functions. Chaubey and Kochar [9, 10] have also used this fact for estimating the survival function subject to stochastic ordering and uniform stochastic ordering constraints. More recently, Chaubey and Xu [23] have considered the use of smoothing given by the Hille's lemma for estimating survival functions under mean residual life ordering.

5. Further Developments

5.1. Length Biased Data

For the biased data, the observations have density g given by

$$g(x) = \frac{w(x)f(x)}{\mu_w},\quad x > 0 \quad (4.1)$$

where $w(x)$ is a given biasing function and $\mu_w = \int w(x)f(x)dx$ is assumed to be finite. The object of interest is the density f. For the length biased data case $w(x) = x$ and the observations are typically non-negative. Chaubey *et al.* [22] and Chaubey and Li [12] considered generalized kernel smoothing and Poisson smoothing of the empirical distribution function in this case given by

$$F_n(x) = \frac{\sum_{i=1}^n \frac{1}{X_i} I\{X_i \leq x\}}{\sum_{i=1}^n \frac{1}{X_i}} \quad (4.2)$$

They also compared it with the corresponding version of smooth versions of $G_n(x)$ along with the study of the asymptotic properties of the resulting estimators of the density and distribution functions.

5.2. Directional Data: Circular Kernel Density Estimator

For the densities defined on the points on a unit circle the density function $f(\theta)$, $\theta \in [-\pi,\pi]$, is 2π−periodic, *i.e.*

$$f(\theta) \geq 0 \text{ for } \theta \in \mathbb{R} \text{ and } \int_{-\pi}^{\pi} f(\theta)d\theta = 1. \tag{4.3}$$

Given a random sample $\{\theta_1,\ldots\theta_n\}$ from the above density, the kernel density estimator may be written as

$$\bar{f}(\theta;h) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{\theta-\theta_i}{h}\right). \tag{4.4}$$

However, this estimator is not periodic, if linear kernels are used. However, if we replace the kernel k by a circular distribution with location θ and concentration parameter approaching to zero as $n \to \infty$, it is possible to remove this difficulty. Thus replacing the kernel k by the wrapped Cauchy-density with location parameter μ and concentration parameter ρ as given by

$$K_{WC}(\theta;\mu,\rho) = \frac{1}{2\pi}\frac{1-\rho^2}{1+\rho^2-2\rho\cos(\theta-\mu)}\ , -\pi \leq \theta < \pi, \tag{4.5}$$

that becomes degenerate at $\theta = \mu$ as $\rho \to 1$. The smooth estimator of $f(\theta)$ is now given by

$$\hat{f}_{WC}(\theta;\rho) = \frac{1}{n}\sum_{i=1}^{n} K_{WC}(\theta;\theta_j,\rho) \tag{4.6}$$

Note that taking the sequence of concentration coefficients $\rho \equiv \rho_n$ such that $\rho_n \to 1$, the density function of the Wrapped Cauchy will satisfy the conditions in the definition in place of K_n. In general K_n, appearing in the above theorem may be replaced by a sequence of periodic densities on $[-\pi,\pi]$, that converge to a degenerate distribution at $\theta = 0$. Indeed the wrapped Cauchy kernel may be replaced by any other circular distribution that converges to the point mass θ, however the wrapped Cauchy kernel appears in a natural way with connection to Fourier series density estimation (see Chaubey [5]).

5.3. Dependent observations

It is of interest to consider the generalization of the estimator in Eq. (2.4) to the multivariate case, especially to the case of restricted support and/or dependent observations. This was explored by Chaubey *et al.* [11] for non-negative stationary ergodic observations and by Chaubey *et al.* [10] for dependent size biased data. On the other hand, Chaubey *et al.* ([6], [7]) considered smooth density estimation for non-negative stationary associated sequences based on Poisson smoothing and general asymmetric kernels.

5.4. Quantile Estimation

The quantile function is defined by $Q(t) = \sup\{x : S(x) \geq 1 - t\}$, $0 \leq t \leq 1$, along with its empirical function given by $Q_n(t) = \sup\{x : S_n(x) \geq 1 - t\}$. Its smooth vcersion may be defined by

$$\tilde{Q}_n(t) = sup\{x : \tilde{S}_n(x) \geq 1 - t\}, 0 \leq t \leq 1, \tag{4.7}$$

This basically requires numerical inversion of $\tilde{S}_n(x)$. An alternative to this may be to use the Bernstein polynomial smoothing (studied by Babu et al. [1] for smoothing distributions functions defined on the interval [0,1]) of the empirical quantile function given by

$$Q_n(u) = inf\,\{x : F_n(x) \geq u\} = X_{([nu]+1)}, \tag{4.8}$$

where $[nu]$ represents the integer part of nu and $X_{(i)}$; $i = 1,2,...,n$ denotes the i^{th} order statistic. The Bernstein polynomial estimator of $Q(u)$ is then given by

$$\tilde{Q}_{n,m}(u) = \sum_{j=1}^{m} b(j;m,u) Q_n\left(\frac{j}{m}\right) \tag{4.9}$$

where m is to be obtained by some cross-validation method, and, $b(j;m,u) = \binom{m}{j} u^j (1-u)^{m-j}$; $j=0,1,2,...,m,$ as in the case of kernel smoothing. Properties of this estimator are under investigation.

5.5. Distribution of a Non-negative Function of Observations

Let $\{X_1,...,X_n\}$ be a random sample from a continuous distribution F defined on the $k-$dimensional Euclidean space $\mathbf{R}^k$, for some $k \geq 1$. In many statistical applications we are interested in statistical properties of a function $h(X_1,...,X_m)$ of $m \geq 1$ observations. Frees [30] considered estimating the density function g associated with the distribution function

$$G(t) = P\big(h(X_1, ..., X_m) \leq t\big) \tag{4.10}$$

using the kernel method. In many applications, though, the functions of interest are non-negative where the usual symmetric kernels applied in the kernel density estimation are not appropriate. Chaubey and Sen [21] considered smooth estimation of $G(t)$ for a non-negative adapted the alternative density estimator developed in Chaubey and Sen [15] by smoothing the so called *empirical kernel distribution function*:

$$G_n(t) = \binom{n}{m}^{-1} \sum_{(n,m)} \mathbf{1}\big(h(X_{i_1}, X_{i_2}, ..., X_{i_m}) \leq t\big) \tag{4.11}$$

where $\mathbf{1}(A)$ denotes the indicator of A and $\sum_{(n,m)}$ denotes the sum over all possible $\binom{n}{m}$ combinations.

6. Conclusions

This paper presents an extensive review of the applications of the generalized smoothing lemma for motivating the smooth estimators of density and other distribution functionals in a variety of contexts. It is seen that where the usual kernel method may not be appropriate, the smooth estimators obtained by using this lemma may provide appropriate alternatives. It has opened an important area of smooth nonparametric estimation in various nonstandard situations.

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