APPLICATIONES MATHEMATICAE
37,4 (2010), pp. 413–427

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BOX-SPLINE HISTOGRAMS FOR MULTIVARIATE DENSITY ESTIMATION

Abstract. The uniform approach to calculation of MISE for histogram and density box-spline estimators gives us a possibility to obtain estimators of derivatives of densities and the asymptotic constant.

1. Histograms. We have two methods of bandwidth selection for the Rosenblatt–Parzen estimator: cross-validation (unbiased and biased) and plug-in (see for instance [16]). In our paper we present higher order point estimators to obtain plug-in estimates for the bandwidth in the case of histograms. An excellent introduction to histograms is given in the book by Scott [17].

In Section 1 we give a simple introduction to box-spline operators and box-spline histograms based on these operators. From the point of view of estimation of density, two properties of approximation are crucial: the rate of convergence and the so called saturation property (Theorem 3.1). These properties divide the box-spline estimators into three classes. These classes are represented by a histogram, a linear histogram, and a Zwart–Powell histogram (ZP histogram for short). This is the reason why we fix our attention on these three histograms. The basic results are recalled in Section 2. In Section 3 we show how to use the saturation property to estimate derivatives. The presented method is a version of the method from [13], and it is applicable only to box-spline estimators of the type of the ZP histogram. In Section 4 we present a method of estimating the asymptotic constant (see (11)). This method is more general and is applicable to all cases. We present it for the histogram. It seems to be a version of the "no diagonals" estimator [18].

2010 *Mathematics Subject Classification*: 41A35, 41A60, 62G07, 62G20.
Key words and phrases: histogram, linear histogram, spline-estimator, MISE, bandwidth selection.

DOI: 10.4064/am37-4-2

We consider only dimension $d = 2$ just for simplicity. It is also not complicated to introduce a nonhomogeneous scaling [9], so we omit it. Spline estimators were introduced by Ciesielski [5]. There are a large number of papers concerning methods of bandwidth selection. Let us mention some of them: [1], [11], [14].

We consider a pair of functions (F, G) which are nonnegative, piecewise polynomials with compact support

$$F, G : \mathbb{R}^2 \to \mathbb{R}.$$

The additional assumptions are given below. A box-spline operator under consideration is defined by

$$Qf(x) = \int_{\mathbb{R}^2} K(x, y) f(y)\, dy, \tag{1}$$

with the kernel depending on F, G,

$$K(x, y) = \sum_{\alpha \in \mathbb{Z}^2} F(y - \alpha) G(x - \alpha). \tag{2}$$

The operator Q defines a family of operators Q_h for $h > 0$,

$$Q_h = \sigma_h \circ Q \circ \sigma_{1/h}, \tag{3}$$

where

$$\sigma_h f(x) = f(x_1/h, x_2/h), \qquad x = (x_1, x_2).$$

Remarks. Since $F, G \geq 0$, it follows that the operators Q_h are positive, i.e. if $f \geq 0$ then $Q_h f \geq 0$. Moreover, we assume that our functions satisfy

$$\sum_{\alpha \in \mathbb{Z}^2} F(\cdot - \alpha) = \frac{1}{\int_{\mathbb{R}^2} G} \qquad \text{a.e.}$$

By this assumption the operators Q_h map densities to densities, i.e. if f is a density, then $\int_{\mathbb{R}^2} Q_h f = 1$. To ensure a good approximation we assume that the Q_h reproduce at least constant polynomials, $Q_h(1) = 1$ (here 1 is the function $1(x) = 1$), or equivalently

$$\sum_{\alpha \in Z^2} G(x - \alpha) = \frac{1}{\int_{\mathbb{R}^2} F} \qquad \text{a.e.}$$

Remark. In the definition of the kernel K, instead of $\mathbb{Z}^2$ we can take another lattice, for instance $A\mathbb{Z}^2$, where

$$A = \begin{bmatrix} 1 & \sin \pi/6 \\ 0 & \cos \pi/6 \end{bmatrix}. \tag{4}$$

The definition so modified includes for instance the histograms and the linear histogram based on the regular hexagon considered in [17].

Let $X_1, \ldots, X_n$ be a random sample from a distribution with density f. We define a density estimator based on the kernel K by

$$f_{h,n}(x) = \frac{1}{nh^2} \sum_{k=1}^{n} K(x/h, X_k/h). \tag{5}$$

Note that

$$Ef_{h,n} = Q_h f. \tag{6}$$

Now we introduce three examples of box-spline estimators. Let H be the characteristic function of the square $[0,1]^2$, i.e.

$$H(x) = I_{[0,1]^2}(x) = \begin{cases} 1, & x \in [0,1]^2, \\ 0, & x \notin [0,1]^2. \end{cases}$$

In this paper we will consider three examples of pairs (F_i, G_i), $i = 1, 2, 3$.

EXAMPLE 1. *The histogram* corresponds to the choice

$$F_1 = G_1 = H.$$

EXAMPLE 2. *The linear histogram* corresponds to the choice

$$F_2(x_1, x_2) = H(x_1 - 0.5, x_2 - 0.5)$$

and G_2 is the hat function given by

$$G_2(x_1, x_2) = \int_0^1 G_1(x_1 - t, x_2 - t)\, dt.$$

EXAMPLE 3. *The Zwart–Powell histogram* (for short ZP histogram) corresponds to the choice

$$F_3(x_1, x_2) = H(x_1, x_2 - 1)$$

and G_3 is the Zwart–Powell function given by

$$G_3(x_1, x_2) = \int_0^1 G_2(x_1 + t, x_2 - t)\, dt.$$

See [3] for the definition of box-splines and [7] for the definition of box-spline estimators.

2. Asymptotic formulas for MISE. We say that the box-spline operator Q *reproduces the polynomials* of degree less than ϱ if $Q(P) = P$ for all polynomials P with $\deg P < \varrho$. We then say that Q has *polynomial order* ϱ. For a pair of functions (F_j, G_j) introduced in the previous section we will add the superscript j to the operator, i.e. Q^j, and to the kernel i.e. K^j, $j = 1, 2, 3$. Note that the operator Q^1 reproduces only constant polynomials, i.e. $\varrho_1 = 1$, and the operators Q^j, $j = 2, 3$, reproduce the linear and constant polynomials, i.e. $\varrho_j = 2$. The parameter ϱ gives the rate of approximation.

We may check [8] that if Q has polynomial order ϱ, then there is $C > 0$ such that for functions f from the Sobolev space W_2^ϱ,

$$\|Q_h f - f\|_2 \le Ch^\varrho |f|_{\varrho,2}, \tag{7}$$

where

$$|f|_{\varrho,2} = \sum_{|\beta|=\varrho} \|D^\beta f\|_2, \qquad \|f\|_2 = \Big(\int_{\mathbb{R}^d} |f|^2\Big)^{1/2}.$$

$$D^\beta f = \frac{\partial^{|\beta|} f}{\partial x_1^{\beta_1} \partial x_2^{\beta_2}}, \qquad \beta = (\beta_1, \beta_2), \qquad |\beta| = \beta_1 + \beta_2.$$

Recall that the Sobolev space is defined by

$$W_2^\varrho = \Big\{ f \in L^2 : \sum_{|\beta|=\varrho} \|D^\beta f\|_2 < \infty \Big\}.$$

A monomial of degree $|\beta|$ will be denoted by $[]^\beta$, i.e. for $x = (x_1, x_2)$,

$$[]^\beta(x) = x^\beta = x_1^{\beta_1} x_2^{\beta_2}.$$

We assume that $f \in L^2$ to consider the mean integrated square error, given by

$$\mathrm{MISE}(f,h) = E\Big[\int_{\mathbb{R}^2} [f_{h,n} - f]^2 \Big]. \tag{8}$$

Consequently,

$$\mathrm{MISE}(f,h) = E\Big[\int_{\mathbb{R}^2} [f_{h,n} - Q_h f]^2 \Big] + \int_{\mathbb{R}^2} [Q_h f - f]^2. \tag{9}$$

The deterministic part is considered in [8].

THEOREM 2.1. *Assume that Q has polynomial order ϱ. Let $f \in W_2^\varrho(\mathbb{R}^2)$. Then*

$$\begin{aligned} &\lim_{h\to 0^+} \Big\| \frac{Q_h f - f}{h^\varrho} \Big\|_2 \qquad (10)\\ &= \bigg(\int_{\mathbb{R}^2} \bigg(\int_{[0,1]^2} \Big| \sum_{|\beta|=\varrho} \frac{1}{\beta!} D^\beta f(t) (Q([]^\beta)(x) - []^\beta(x)) \Big|^2 dx \bigg) dt \bigg)^{1/2}. \end{aligned}$$

Let us define the asymptotic constant depending on f and the box-spline histogram ($j = 1, 2, 3$) by

$$\begin{aligned} \theta_j &= (\mathrm{Asym}(f,j))^2 \qquad (11)\\ &= \int_{\mathbb{R}^2} \bigg(\int_{[0,1]^2} \Big| \sum_{|\beta|=\varrho_j} \frac{1}{\beta!} D^\beta f(t) (Q^j([]^\beta)(x) - []^\beta(x)) \Big|^2 dx \bigg) dt. \end{aligned}$$

$\mathrm{Asym}(f,1)$ is known (see for instance [17]):

$$\theta_1 = (\mathrm{Asym}(f,1))^2 = \frac{1}{12}\int_{\mathbb{R}^2}\bigg(\Big(\frac{\partial f}{\partial x_1}\Big)^2 + \Big(\frac{\partial f}{\partial x_2}\Big)^2\bigg). \tag{12}$$

An easy calculation shows that

$$\begin{aligned}\theta_2 &= (\mathrm{Asym}(f,2))^2 \\ &= \int_{\mathbb{R}^2}\bigg\{\Big(\frac{\partial^2 f}{\partial x_1^2}\Big)^2\cdot\frac{49}{2880} + \Big(\frac{\partial^2 f}{\partial x_2^2}\Big)^2\cdot\frac{49}{2880} + \Big(\frac{\partial^2 f}{\partial x_1\partial x_2}\Big)^2\cdot\frac{1}{90} \\ &\quad + \Big(\frac{\partial^2 f}{\partial x_1^2}\frac{\partial^2 f}{\partial x_2^2}\Big)\cdot\frac{1}{32} + \Big(\frac{\partial^2 f}{\partial x_1^2}\frac{\partial^2 f}{\partial x_1\partial x_2}\Big)\cdot\frac{17}{720} + \Big(\frac{\partial^2 f}{\partial x_2^2}\frac{\partial^2 f}{\partial x_1\partial x_2}\Big)\cdot\frac{17}{720}\bigg\},\end{aligned} \tag{13}$$

$$\theta_3 = (\mathrm{Asym}(f,3))^2 = \int_{\mathbb{R}^2}\bigg\{\frac{1}{6}\Big(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_1^2}\Big)\bigg\}^2. \tag{14}$$

Let us consider the first term of (9). We have the following result (compare [8, Theorem 1.4]).

THEOREM 2.2. *Let the density f be in $W_2^{\varrho}(\mathbb{R}^2)$. If $nh^2 \to \infty$ and $h \to 0$ then*

$$\lim_{nh^2\to\infty} nh^2 E\Big[\int_{\mathbb{R}^2}[f_{h,n} - Q_h f]^2\Big] = \int_{\mathbb{R}^2}\Big[\int_{[0,1]^2}(K(x,y))^2\,dy\Big]\,dx. \tag{15}$$

REMARK 1. By (9), (10) and (15) we get

$$\mathrm{MISE}(f,h) \sim \mathrm{AMISE}(f,h)$$

where for the box-spline histograms

$$\mathrm{AMISE}(f,h) = \frac{1}{nh^2}\int_{\mathbb{R}^2}\Big[\int_{[0,1]^2}(K^j(x,y))^2\,dy\Big]\,dx + h^{2\varrho_j}(\mathrm{Asym}(f,j))^2. \tag{16}$$

So the best choice of the parameter $h > 0$ to minimize (16) is

$$h = \bigg(\frac{\int_{\mathbb{R}^2}[\int_{[0,1]^2}(K^j(x,y))^2\,dy]\,dx}{\varrho_j n(\mathrm{Asym}(f,j))^2}\bigg)^{-1/(2\varrho_j+2)}. \tag{17}$$

Now we have another estimation problem of $\theta_j = (\mathrm{Asym}(f,j))^2$ with a different bandwidth denoted by a. As for the density estimation, the choice of a is crucial to the performance of the estimator $\widehat{\theta}_j(a)$. We use here the notation from [15]. In the next section we construct an estimator g_{an} of the derivatives $D_{Q_3}f$, where (compare (14))

$$D_{Q_3}f = \frac{1}{6}\Big(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_1^2}\Big).$$

Hence an estimator of θ_3 is given by

$$\widehat{\theta}_3(a) = \int_{\mathbb{R}^2} (g_{an})^2.$$

In Section 4 we estimate θ_j directly.

3. Choice of bandwidth for estimation of derivatives of density: ZP histogram. The problem of estimation of derivatives in the multivariate case is rather ambiguous. We look for estimators of derivatives which appear in the asymptotic formula. The following theorem ([10, Theorem 2.5]) is important. Let us denote $\breve{F}(x) = F(-x)$.

THEOREM 3.1. *Let $f \in W_2^{\varrho_j}$. If $a \to 0$ then*

$$\frac{Q_a^j f - f}{a^{\varrho_j}} \to D_{Q^j} f \tag{18}$$

weakly in L^2 for $j = 1, 2, 3$, where

$$D_{Q^j} f = \frac{1}{(2\pi i)^{\varrho_j}} \sum_{|\beta| = \varrho_j} \frac{D^\beta f}{\beta!} D^\beta(\widehat{G_j}\widehat{\breve{F}_j})(0).$$

It is crucial for our construction that for $j = 3$ in (18) we have L^2 convergence, but not for $j = 1, 2$ in general. Hence

$$(\mathrm{Asym}(f, 3))^2 = \int_{\mathbb{R}^2} (D_{Q^3} f)^2.$$

It is not difficult to prove (Theorem 3.2 below) that if $a \to 0$, then also

$$\frac{Q_a^3(Q_a^3 f) - Q_a^3 f}{a^2} \to D_{Q^3} f = \frac{1}{6}\left(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_1^2}\right), \tag{19}$$

in L^2 norm. The property (19) helps us construct an estimator of $D_{Q^3} f$. It leads us to the operator

$$T := Q^3 \circ Q^3 - Q^3.$$

Note that the operator T has the same structure as Q, i.e.

$$Tf(x) = \int_{\mathbb{R}^2} \kappa(x, y) f(y)\, dy,$$

where

$$\kappa(x, y) = \sum_{\alpha \in \mathbb{Z}^2} F_3(y - \alpha)(Q^3(G_3) - G_3)(x - \alpha). \tag{20}$$

We define as above a family of operators T_a for $a > 0$. Now we are ready to define an estimator of the derivatives $D_{Q^3} f$. Let $X_1, \ldots, X_n$ be a random sample from a distribution with density f. Then we define an estimator of $D_{Q^3}f$ by

$$g_{an}(x) = \frac{1}{na^4}\sum_{k=1}^{n}\kappa(x/a, X_k/a). \tag{21}$$

Note that

$$Eg_{an} = \frac{T_a(f)}{a^2}$$

and

$$E\int_{\mathbb{R}^2}|g_{an} - D_{Q^3}f|^2 = E\int_{\mathbb{R}^2}\left|g_{an} - \frac{T_a(f)}{a^2}\right|^2 + \int_{\mathbb{R}^2}\left|\frac{T_a(f)}{a^2} - D_{Q^3}f\right|^2.$$

THEOREM 3.2. *Let* $na^6 \to \infty$ *and* $a \to 0$ *and* $f \in W_2^4$. *Then*

$$\left(\int_{\mathbb{R}^2}\left|\frac{T_a(f)}{a^2} - D_{Q^3}f\right|^2\right)^{1/2} \le C(a|f|_{3,2} + a^2|f|_{4,2}) \tag{22}$$

and

$$\lim_{na^6\to\infty} na^6 E\int_{\mathbb{R}^2}\left|g_{an} - \frac{T_a(f)}{a^2}\right|^2 = \int_{\mathbb{R}^2}\Big\{\int_{[0,1]^2}\kappa^2(x,y)\,dy\Big\}\,dx.$$

Proof. If we modify slightly the end of the proof of Theorem 2.23 with $\varrho = 0$ in [6] and use Lemma 1.1 of [8], we get

$$\left\|\frac{Q_a^3 f - f}{a^2} - D_{Q^3}f\right\|_2 \le Ca|f|_{3,2}. \tag{23}$$

Now the triangle inequality implies that

$$\begin{aligned}\left\|\frac{T_a(f)}{a^2} - D_{Q^3}f\right\|_2 &= \left\|\frac{Q_a^3Q_a^3 f - Q_a^3 f}{a^2} - D_{Q^3}f\right\|_2 \\ &\le \left\|\frac{Q_a^3Q_a^3 f - Q_a^3 f}{a^2} - Q_a^3 D_{Q^3}f\right\|_2 + \|Q_a^3 D_{Q^3}f - D_{Q^3}f\|_2.\end{aligned} \tag{24}$$

Since the operators Q_a^3 are uniformly bounded, applying (23) we get

$$\left\|\frac{Q_a^3Q_a^3 f - Q_a^3 f}{a^2} - Q_a^3 D_{Q^3}f\right\|_2 \le C\left\|\frac{Q_a^3 f - f}{a^2} - D_{Q^3}f\right\|_2 \le Ca|f|_{3,2}.$$

We now turn to the second term of (24). Applying (7) we get

$$\|Q_a^3 D_{Q^3}f - D_{Q^3}f\|_2 \le Ca^2|D_{Q^3}f|_{2,2}.$$

This finishes the proof of the first inequality.

The proof of the second formula is rather similar to that of [8, Theorem 1.4]. ∎

Now the choice of the estimator of θ_3 is obvious:

$$\widehat{\theta}_3(a) = \int_{\mathbb{R}^2} (g_{an})^2.$$

We can turn to the second strategy of estimating θ_3. Note that

$$(g_{an})^2(x) = \Big(\frac{1}{na^4}\Big)^2 \Big(\sum_{k\neq l}^{n} \kappa(x/a, X_k/a)\kappa(x/a, X_l/a) + \sum_{k=1}^{n}(\kappa(x/a, X_k/a))^2\Big) \tag{25}$$

and

$$E(g_{an}(x))^2 = \frac{n^2-n}{n^2}\Big(\frac{T_a(f)(x)}{a^2}\Big)^2 + \frac{1}{a^8}\,\frac{1}{n}\int_{\mathbb{R}^2} (\kappa(x/a, y/a))^2 f(y)\,dy.$$

Now another estimator ("no diagonals") of θ_3 can be given by the formula

$$\widehat{\theta}_3(a) = \Big(\frac{1}{na^4}\Big)^2 \int_{\mathbb{R}^2} \sum_{k\neq l}^{n} \kappa(x/a, X_k/a)\kappa(x/a, X_l/a)\,dx.$$

To avoid tedious calculations we propose the following simpler estimator for an even size of a sample:

$$\widehat{\theta}_3(a) = \frac{1}{(n/2)a^8} \int_{\mathbb{R}^2} \sum_{k=1}^{n/2} \kappa(x/a, X_k/a)\kappa(x/a, X_{n-k}/a)\,dx. \tag{26}$$

This approach with minor changes is applicable to the histogram and the linear histogram. We will see it in the next section for the histogram, i.e. we will construct $\widehat{\theta}_1$.

4. Choice of bandwidth for estimation of the asymptotic constant: histogram. We will explain the estimation of the asymptotic constant in the case of the histogram.

First we construct an operator Q^5 reproducing the polynomials of degree less than or equal to two by the formula

$$Q^5(f) = \sum_{|\gamma|\leq 1} a_\gamma Q^3(f(\cdot - \gamma)).$$

Applying (10) and (14) we obtain, for $|\beta| = 2$,

$$Q^3([]^\beta)(x) - x^\beta = A_\beta,$$

where $A_{(1,1)} = 0$, $A_{(2,0)} = 1/3$, $A_{(0,2)} = 1/3$. Consequently, to find the coefficients a_γ we need to solve the system of equations, for all $|\beta| \leq 2$,

$$Q^5([]^\beta) = \sum_{|\gamma|\leq 1} a_\gamma Q^3((\cdot - \gamma)^\beta) = []^\beta.$$

One of the solutions is $a_{(0,0)} = 4/3$ and $a_{(\gamma_1,\gamma_2)} = -1/12$ for all $|\gamma_1| = |\gamma_2| = 1$ and the other a_γ are zero. Since Q_3 reproduces polynomials of degree less than or equal to two by (7), there is $C > 0$ such that for all $f \in W_2^3$,

$$\|Q_h^5 f - f\|_2 \le Ch^3 |f|_{3,2}.$$

By definition,

$$Q^5(f)(x) = \int_{\mathbb{R}^2} K^5(x,y) f(y)\, dy,$$

where

$$K^5(x,y) = \sum_{\alpha\in\mathbb{Z}^2} F_3(y-\alpha) G_5(x-\alpha), \qquad G_5(x) = \sum_{|\gamma|\le 1} a_\gamma G_3(x-\gamma).$$

Now we consider the operator defined as follows:

$$T^1 := Q^1 \circ Q^5 - Q^5.$$

Using this operator we construct an estimator of θ_1. We can write

$$T^1(f)(x) = \int_{\mathbb{R}^2} \kappa^1(x,y) f(y)\, dy$$

with

$$\kappa^1(x,y) = \sum_{\alpha\in\mathbb{Z}^2} F_3(y-\alpha) K(x-\alpha), \qquad K(x) = Q^1(G_5)(x) - G_5(x).$$

Let $X_1,\dots,X_n$ be a random sample from a distribution with density f. For simplicity let n be even. To avoid tedious calculations let

$$\widehat{\theta}_1(a) = \frac{1}{(n/2)a^6} \int_{\mathbb{R}^2} \sum_{k=1}^{n/2} \kappa^1(x/a, X_k/a)\kappa^1(x/a, X_{n-k}/a)\, dx, \tag{27}$$

for short $\widehat{\theta}_1 = \widehat{\theta}_1(a)$. By definition,

$$E\widehat{\theta}_1(a) = \int_{\mathbb{R}^2} \left(\frac{T_a^1 f}{a}\right)^2.$$

We have

$$E[\widehat{\theta}_1 - \theta_1]^2 = E[\widehat{\theta}_1 - E\widehat{\theta}_1]^2 + [E\widehat{\theta}_1 - \theta_1]^2.$$

The asymptotic behavior of the deterministic part follows from Theorem 4.1 and the equality

$$[E\widehat{\theta}_1 - \theta_1]^2 = \left| \left\| \frac{T_a^1 f}{a} \right\|_2 - \operatorname{Asym}(f,1) \right|^2 \left| \left\| \frac{T_a^1 f}{a} \right\|_2 + \operatorname{Asym}(f,1) \right|^2.$$

THEOREM 4.1. *Let $f \in W_2^3$. Then*

$$\left| \left\| \frac{T_a^1 f}{a} \right\|_2 - \operatorname{Asym}(f,1) \right| \le C(a|f|_{2,2} + a^2 |f|_{3,2}).$$

Proof. From Theorem 8 and Lemma 11 of [9] we infer that there is $C>0$ such that for $g\in W_2^2$,

$$\left|\left\|\frac{Q_a^1 g-g}{a}\right\|_2-\mathrm{Asym}(g,1)\right|\le Ca|g|_{2,2}.$$

Put $g=Q_a^5 f$. Consequently,

$$\left|\left\|\frac{Q_a^1 Q_a^5 f-Q_a^5 f}{a}\right\|_2-\mathrm{Asym}(Q_a^5 f,1)\right|\le Ch|Q_a^5 f|_{2,2}.$$

From Corollary 2.1 of [10] we obtain, for $|\beta|=2$,

$$\|D^\beta Q_a^5 f-D^\beta f\|_2\le Ca|f|_{3,2}.$$

Then

$$|Q_a^5 f|_{2,2}\le C(|f|_{2,2}+a|f|_{3,2}).$$

Consequently,

$$\left|\left\|\frac{Q_a^1 Q_a^5 f-Q_a^5 f}{a}\right\|_2-\mathrm{Asym}(Q_a^5 f,1)\right|\le C(a|f|_{2,2}+a^2|f|_{3,2}). \tag{28}$$

From the triangle inequality

$$|\mathrm{Asym}(Q_a^5 f,1)-\mathrm{Asym}(f,1)|$$
$$\le\bigg(\int_{\mathbb{R}^2}\bigg(\int_{[0,1]^2}\bigg|\sum_{|\beta|=1}\frac{1}{\beta!}|D^\beta f(t)-D^\beta Q_a^5 f(t)|(Q^1([]^\beta)(x)-[]^\beta(x))\bigg|^2\,dx\bigg)\,dt\bigg)^{1/2}.$$

By the above mentioned Corollary 2.1 of [10] with $|\beta|=1$ we have

$$|\mathrm{Asym}(Q_a^5 f,1)-\mathrm{Asym}(f,1)|\le Ca^2|f|_{2,2}. \tag{29}$$

Combining (28) and (29) we finish the proof. ∎

We need the following lemma.

LEMMA 4.1. *Let $I:=[0,1]\times[1,2]$. Let f be a bounded density such that $f\in L^1(\mathbb{R}^2)\cap L^2(\mathbb{R}^2)$. Then for fixed $\alpha\in\mathbb{Z}^2$,*

$$\lim_{h\to0}\frac{1}{h^2}\sum_{\alpha_1\in\mathbb{Z}^2}\int_{Ih+\alpha_1 h} f(u)\,du\int_{Ih+(\alpha_1+\alpha)h} f(u)\,du=\int_{\mathbb{R}^2} f^2.$$

The proof is left to the reader. We can reformulate the lemma to obtain the following statement. Let f be a density such that $f\in L^2(\mathbb{R}^2)$. Let $\alpha\in\mathbb{Z}^2$ be fixed. Then for a.e. $x_1,x_2\in[0,1]^2$,

$$\lim_{h\to0}\sum_{\alpha_1\in\mathbb{Z}^2} f(hx_1+\alpha_1 h)f(hx_2+\alpha_1 h+\alpha h)h^2=\int_{\mathbb{R}^2} f^2.$$

We mention this because the convergence of the Riemann sums was observed for Lebesgue-integrable functions in the papers [4] and [12].

Let us note that the support of the function F_3 is equal to I.

THEOREM 4.2. *Let f be a density such that $f \in W_2^2$. If $na^6 \to \infty$ and $a \to 0$ then*

$$\lim na^6 E(\widehat{\theta}_1 - E\widehat{\theta}_1)^2 = 2 \int_{\mathbb{R}^2} f^2 \sum_{\alpha\in\mathbb{Z}^2} b_\alpha^2, \tag{30}$$

where

$$b_\alpha = \int_{\mathbb{R}^2} K(x)K(x-\alpha)\,dx.$$

Proof. Write

$$\begin{aligned}
&E(\widehat{\theta}_1 - E\widehat{\theta}_1)^2 \\
&\quad = E\bigg(\frac{1}{(n/2)a^6}\int_{\mathbb{R}^2}\sum_{k=1}^{n/2}\kappa^1(x/a, X_k/a)\kappa^1(x/a, X_{n-k}/a)\,dx - \int_{\mathbb{R}^2}\bigg(\frac{T_a^1 f}{a}\bigg)^2\bigg)^2 \\
&\quad = \frac{4}{n^2a^4}E\bigg(\sum_{k=1}^{n/2}\int_{\mathbb{R}^2}\bigg(\frac{1}{a^4}\kappa^1(x/a, X_k/a)\kappa^1(x/a, X_{n-k}/a) - (T_a^1 f(x))^2\bigg)\,dx\bigg)^2 \\
&\quad = \frac{2}{na^4}E\bigg(\int_{\mathbb{R}^2}\bigg(\frac{1}{a^4}\kappa^1(x/a, X_1/a)\kappa^1(x/a, X_2/a) - (T_a^1 f(x))^2\bigg)\,dx\bigg)^2 \\
&\quad = \frac{2}{na^4}E\bigg(\int_{\mathbb{R}^2}\frac{1}{a^4}\kappa^1(x/a, X_1/a)\kappa^1(x/a, X_2/a)\,dx\bigg)^2 - \frac{2}{na^4}\bigg(\int_{\mathbb{R}^2}(T_a^1 f)^2\bigg)^2.
\end{aligned}$$

Only the first term of the last formula is important (let us denote it by P). Using the assumption $f \in W_2^2$ we find that the second term is negligible. Using the kernel representation we get

$$\begin{aligned}
P &= \frac{2}{na^4}E\bigg(\int_{\mathbb{R}^2}\frac{1}{a^4}\kappa^1(x/a, X_1/a)\kappa^1(x/a, X_2/a)\,dx\bigg)^2 \\
&= \frac{2}{na^4}E\bigg(\int_{\mathbb{R}^2}\frac{1}{a^4}\sum_{\alpha_1\in\mathbb{Z}^2}\sum_{\alpha_2\in\mathbb{Z}^2}F_3(X_1/a-\alpha_1)F_3(X_2/a-\alpha_2) \\
&\qquad\qquad \times K(x/a-\alpha_1)K(x/a-\alpha_2)\,dx\bigg)^2 \\
&= \frac{2}{na^4}E\bigg(\frac{1}{a^2}\sum_{\alpha_1\in\mathbb{Z}^2}\sum_{\alpha_2\in\mathbb{Z}^2}F_3(X_1/a-\alpha_1)F_3(X_2/a-\alpha_2)b_{\alpha_1-\alpha_2}\bigg)^2 \\
&= \frac{2}{na^8}\sum_{\alpha_1\in\mathbb{Z}^2}\sum_{\alpha_2\in\mathbb{Z}^2}\sum_{\alpha_3\in\mathbb{Z}^2}\sum_{\alpha_4\in\mathbb{Z}^2}E(F_3(X_1/a-\alpha_1)F_3(X_1/a-\alpha_3)) \\
&\qquad\qquad \times E(F_3(X_2/a-\alpha_2)F_3(X_2/a-\alpha_4))b_{\alpha_1-\alpha_2}b_{\alpha_3-\alpha_4}.
\end{aligned}$$

Observe that since F_3 is the characteristic function of I, if $\alpha_1 \neq \alpha_3$ we have

$$E(F_3(X_1/a - \alpha_1)F_3(X_1/a - \alpha_3)) = 0,$$

while if $\alpha_1 = \alpha_3$,

$$\begin{aligned} E(F_3(X_1/a - \alpha_1))^2 &= \int_{\mathbb{R}^2} (F_3(u/a - \alpha_1)) f(u)\, du \\ &= \int_{Ia+\alpha_1 a} f(u)\, du, \end{aligned}$$

where (recall) $I = [0,1] \times [1,2]$. Consequently,

$$P = \frac{2}{na^8} \sum_{\alpha_1 \in \mathbb{Z}^2} \sum_{\alpha_2 \in \mathbb{Z}^2} (b_{\alpha_1 - \alpha_2})^2 \int_{Ia+\alpha_1 a} f(u)\, du \int_{Ia+\alpha_2 a} f(u)\, du.$$

Using Lemma 4.1 finishes the proof since $b_\alpha = 0$ for $|\alpha| > 4$. ∎

Note that applying the two last theorems we deduce that to estimate the asymptotic constant the bandwidth is $a_{\mathrm{MISE}} \sim (1/n)^{1/8}$.

5. Simulation results. We show an accuracy of the estimation of the asymptotic constant for the histogram. We take the dimension $d = 1$ and 1000 samples from the distribution of random variables

$$X = \sigma Z + 3\sigma Y,$$

where Z is standard normal $N(0,1)$. The random variable Y is independent of Z and has binomial distribution with $p = 0.5$. We estimate

$$\theta_1 = \frac{1}{12} \int_{\mathbb{R}} (f')^2.$$

In the case of $d = 1$ the formula (27) can be written as

$$\widehat{\theta}_1(a) = \frac{2}{na^3} \sum_{k=1}^{n/2} \sum_{j \in Z} \sum_{|l| \le 4} A_l I_{[1,2]}(X_n/a - j) I_{[1,2]}(X_{n-k}/a - j - l),$$

where $I_{[1,2]}$ is the characteristic function of $[1,2]$,

$$\begin{aligned} A_l &= \int_{\mathbb{R}} K(x+l)K(x)\, dx, \\ K(x) &= -\frac{1}{6}(Q_1(G_3) - G_3)(x-1) \\ &\quad + \frac{4}{3}(Q_1(G_3) - G_3)(x) - \frac{1}{6}(Q_1(G_3) - G_3)(x+1) \end{aligned}$$

and G_3 is the B-spline, i.e.

$$G_3(x) = \frac{1}{2}\sum_{j=0}^{3}(-1)^{r-j}\binom{r}{j}(j-x)_+^2.$$

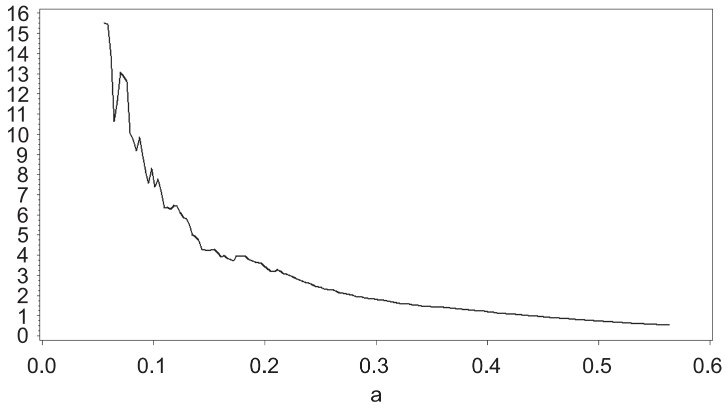
In this case, Q_1 is the orthogonal projection

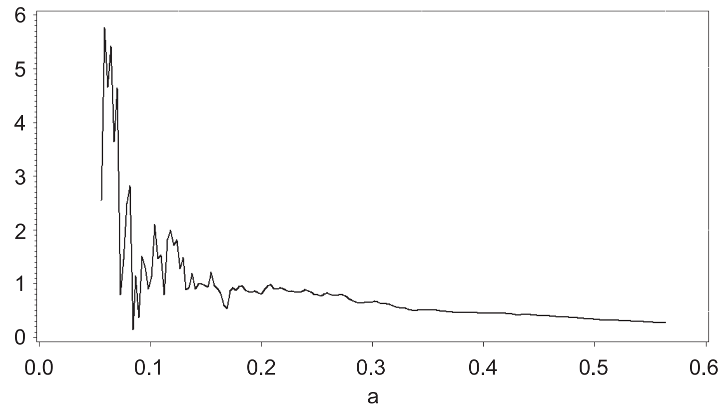
$$Q_1 f(x) = \sum_{k\in Z}\int_k^{k+1} f(u)\,du\, I_{[k,k+1]}(x).$$

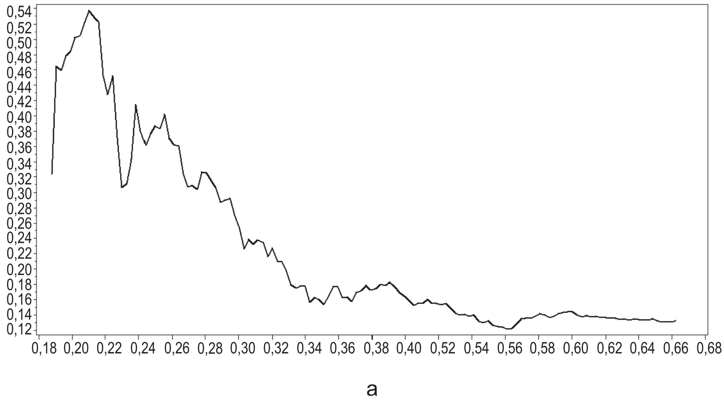
We have

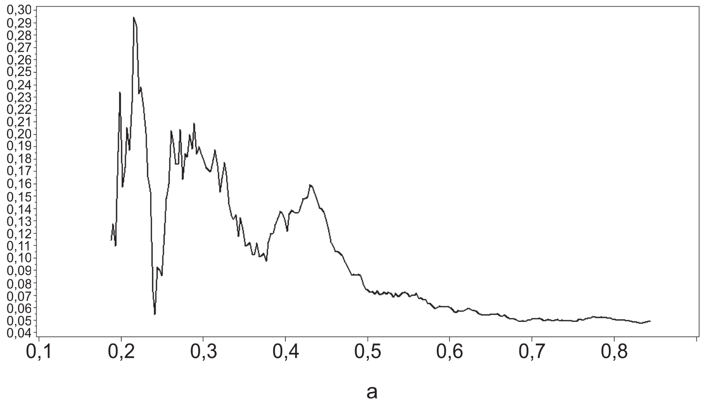
σ	0.1	0.2	0.3	0.4
θ_1	3.709	0.464	0.137	0.058

We show the four functions $\widehat{\theta}_1(a)$ (SAS 9) with respect to different σ from 0.1 to 0.4. The simulations show that a for which $\widehat{\theta}_1(a)$ gives a good estimation of θ_1 lies in the region where the oscillations diminish. It would be interesting to prove it.









Acknowledgments. This research is supported in part by the grant "The exploitation of white cabbage for phytoremediation and biofumigation of soils (AGROBIOKAP)" co-financed by European Union from European Regional Development Fund in a framework of the Innovative Economy Operational Programme 2007-2013.

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Received on 12.10.2009;
revised version on 14.9.2010 (2020)