Neural Network Interest Group

Título/Title:<br>Nonparametric Density and Entropy Estimation (with a Focus on the Parzen Window Method)<br>Autor(es)/Author(s):<br>J. P. Marques de Sá<br>Relatório Técnico/Technical Report No. 3 /2006

Título/Title:
Nonparametric Density and Entropy Estimation (with a Focus on the Parzen Window Method)
Autor(es)/Author(s):
J.P. Marques de Sá

Relatório Técnico/Technical Report No. 3 /2006
Publicado por/Published by: NNIG. http://paginas.fe.up.pt/~nnig/
Julho 2006
© INEB: FEUP/INEB, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal

## Contents

1 Nonparametric Density Estimators ..... 5
1.1 Estimability of Functionals ..... 5
1.2 Histogram-Based Density Estimator ..... 5
1.3 Rosenblatt's Kernel Estimator ..... 7
1.4 Parzen Window Estimator ..... 9
2 Entropy Estimation Based on Parzen Windows ..... 13
2.1 Plug-in Estimates ..... 13
3 Appendix ..... 15
3.1 Asymptotic Notation ..... 15
3.2 Convolution properties ..... 16
3.3 Proof of the convergence of $E\left[f_{n}\right]$ to $f$ ..... 16
3.4 Proof of the Result on the Perturbed Density Estimate ..... 17
References ..... 17

## 1 Nonparametric Density Estimators

### 1.1 Estimability of Functionals

The first question to be addressed is whether or not a given functional $q(F)$, where $F$ belongs to a family of distributions $F$, is estimable based on a sequence of i.i.d. random variables $X_{1}, \ldots, X_{n}$.
Reference [15] defines estimability in the following way: $q(F)$ is estimable with $n$ observations if there exists a statistic $\delta\left(X_{1}, \ldots, X_{n}\right)$ such that

$$
E_{F}\left[\delta\left(X_{1}, \ldots, X_{n}\right)\right]=q(F)
$$

Therefore, estimability means the existence of unbiased estimators.
Reference [15] explains the necessary and sufficient conditions of estimability for a convex family ${ }^{1}$ of distribution functions and presents examples of estimable and nonestimable functionals. Here are some of them:

Examples of estimable functionals:

- The variance: $q(F)=\sigma^{2}(F)$.
- $q(F)=F\left(x_{0}\right)$ for some fixed $x_{0} \in \mathfrak{R}$.
- $q(F)=\int_{\mathfrak{R}} \exp \left(i t_{0} x\right) F(d x)$

Examples of non-estimable functionals:

- $q(F)=f\left(x_{0}\right)$ for some fixed $x_{0} \in \mathfrak{R}$.
- The regression function of $Y$ on $X: q(F)=\int_{R} y f(x, y) d y / \int_{R} f(x, y) d y$
- The conditional density of $Y$ given $x: q(F)=f(x, y) / \int_{R} f(x, y) d y$

Although unbiased estimators do not exist in general for $f$, it is possible to define sequences of density estimators, $\hat{f}_{n}$, asymptotically unbiased:

$$
\lim _{n \rightarrow \infty} E_{F}\left[\hat{f}_{n}(x)\right]=f(x)
$$

### 1.2 Histogram-Based Density Estimator

We are given a random sample $\left\{x_{1}, \ldots, x_{k}, \ldots, x_{n}\right\}$ observations of i.i.d. r.v. from an unknown absolutely continuous pdf.

We restrict ourselves to the univariate case.

[^0]If the unknown pdf, $g(x)$, has an infinite support we content ourselves with estimating the truncated density

$$
f(x)=\left\{\begin{array}{lc}
g(x) / \int_{a}^{b} g(t) d t & x \in[a, b] \\
0 & \text { otherwise }
\end{array}\right.
$$

Let us partition the interval by $a=t_{0}<t_{1}<\ldots<t_{i}<\ldots<t_{m}=b$. (We use " $t_{i}$ " for no confusion with the $x_{k}$.)

Let us denote:

$$
\begin{aligned}
& T_{i}=\left[t_{i}, t_{i+1}[;\right. \\
& q_{i}=\sum_{k=1}^{n} I_{x_{k} \in T_{i}}, \quad t \in T_{i}\left(\# \text { cases falling in } T_{i}\right) ; \\
& l\left(T_{i}\right)=t_{i+1}-t_{i} .
\end{aligned}
$$

## Histogram:

$$
p(t)= \begin{cases}q_{i} / n & t \in T_{i} \\ q_{m-1} / n & t=b \\ 0 & t \notin[a, b]\end{cases}
$$



Histogram-based density estimator:

$$
\hat{f}_{H}(t)= \begin{cases}p(t) / l\left(T_{i}\right) & t \in T_{i} \\ p(t) / l\left(T_{m-1}\right) & t=b \\ 0 & t \notin[a, b]\end{cases}
$$



Rationale: The variable $q_{i}$ is a multinomial r.v. Thus, $q_{i} / n$ estimates $\int_{T_{i}} f(t) d t$. If $f$ is absolutely continuous and $T_{i}$ is small, then $f(t) \approx f\left(t_{i}\right)$ for $t \in T_{i}$. Hence, $q_{i} /\left(n \times l\left(T_{i}\right)\right)$ estimates $f(t)$.
Properties (for details, see [9]):

- Let us assume an estimator based on assigning quantities $c_{i}$ to the $T_{i}$ intervals. Among all such estimators $\hat{f}_{H}$ uniquely maximizes the likelihood $L\left(c_{0}, \ldots, c_{m-1}\right)$.
- Theorem: Suppose that $f$ is bounded and has continuous derivatives up to order three except at the endpoints of $[a, b]$. Suppose equal spacing, $t_{i+1}-t_{i}=2 h(n) \equiv$ $2 h_{n}$. Then, if $n \rightarrow \infty$ and $h_{n} \rightarrow 0$ such that $n h_{n} \rightarrow \infty$, for $x \in[a, b]$

$$
\operatorname{MSE}\left(\hat{f}_{H}(x)\right)=E\left[\left(\hat{f}_{H}(x)-f(x)\right)^{2}\right] \rightarrow 0
$$

i.e., $\hat{f}_{H}$ is a consistent estimator for $f(x)$.

- The proof of the above Theorem leads to the results ${ }^{2}$

$$
\begin{aligned}
& \operatorname{MSE}\left(\hat{f}_{H}\left(x^{\prime}\right)\right)=\frac{f\left(x^{\prime}\right)}{2 n h_{n}}+\frac{h_{n}^{4}}{36}\left|f^{\prime \prime}\left(x^{\prime}\right)\right|^{2}+O(1 / n)+O\left(h_{n}^{5}\right) \\
& \operatorname{MSE}\left(\hat{f}_{H}(x)\right) \leq \frac{f\left(x^{\prime}\right)}{n h_{n}}+2\left|f^{\prime}\left(x^{\prime}\right)\right|^{2} h_{n}^{2}+O(1 / n)+O\left(h_{n}^{3}\right),
\end{aligned}
$$

is based on a Taylor series development around the midpoint $x^{\prime}$ of the interval containing $x$ and uses the well-known result ${ }^{3}$ :

$$
E\left[\left(\hat{f}_{H}\left(x^{\prime}\right)-f\left(x^{\prime}\right)\right)^{2}\right]=\operatorname{Bias}^{2}\left(\hat{f}_{H}\left(x^{\prime}\right)\right)+\operatorname{Var}\left(\hat{f}_{H}\left(x^{\prime}\right)\right)
$$

- From the formula of $\operatorname{MSE}\left(\hat{f}_{H}(x)\right)$ one may select $h_{n}=\left[\frac{f\left(x^{\prime}\right)}{4\left(f^{\prime}\left(x^{\prime}\right)\right)^{2}}\right]^{1 / 3} n^{-1 / 3}$ to obtain convergence throughout the $k$ th interval of order $n^{-2 / 3}$.
- The integrated mean square error is minimized by selecting

$$
h_{n}=\left[\frac{1}{4 \int\left(f^{\prime}(x)\right)^{2} d x}\right]^{1 / 3} n^{-1 / 3}
$$

to obtain

$$
\int \operatorname{MSE}\left(\hat{f}_{H}(x)\right)=I M S E \leq 3\left[\frac{1}{2} \int\left(f^{\prime}(x)\right)^{2} d x\right]^{1 / 3} n^{-2 / 3}+O\left(\frac{1}{n}+h_{n}^{3}\right)
$$

### 1.3 Rosenblatt's Kernel Estimator

Rosenblatt's estimator (introduced in 1956) is an extension of the histogram-based estimator:

$$
\hat{f}_{n}(x)=\frac{\text { \# sample points in } \left.] x-h_{n}, x+h_{n}\right]}{2 n h_{n}}, \quad h_{n}=0.2 ; 2 n h_{n}=0.25
$$

i.e., we shift the interval such as to center it at $x$.


[^1]The estimate can also be written as:

$$
\hat{f}_{n}(x)=\frac{F_{n}\left(x+h_{n}\right)-F_{n}\left(x-h_{n}\right)}{2 h_{n}}
$$

where $F_{n}(x)$ is the empirical distribution (also called empirical measure in the previous tutorial).


The shifted histogram estimator of Rosenblatt can be represented as:

$$
\hat{f}_{n}(x)=\frac{1}{n} \sum_{i=1}^{n} \frac{1}{h_{n}} w\left(\frac{x-x_{i}}{h_{n}}\right)
$$

where $w(u)=\left\{\begin{array}{cc}1 / 2 \quad|u|<1 \\ 0 & \text { otherwise }\end{array}\right.$ is the kernel (rectangular).
Properties (for details, see [9]):

- In the same conditions as above:

$$
\operatorname{MSE}\left(\hat{f}_{H}(x)\right)=\frac{f(x)}{2 n h_{n}}+\frac{h_{n}^{4}}{36}\left|f^{\prime \prime}(x)\right|^{2}+o\left(\frac{1}{n h_{n}}+h_{n}^{4}\right)
$$

- One may minimize the first two terms in the above formula, selecting $h_{n}=\left[\frac{9 f(x)}{2\left(f^{\prime \prime}(x)\right)^{2}}\right]^{1 / 5} n^{-1 / 5}$ to obtain an MSE of order $n^{-4 / 5}$. Therefore the MSE of Rosenblatt's estimator decreases faster than the fixed grid histogram estimator (order of $n^{-2 / 3}$ ).
- The integrated mean square error is minimized by selecting $h_{n}=\left[\frac{9}{2 \int\left(f^{\prime \prime}(x)\right)^{2} d x}\right]^{1 / 5} n^{-1 / 5}$, yielding $I M S E \sim n^{-4 / 5}$.


### 1.4 Parzen Window Estimator

The Parzen window estimator is a generalization of the shifted-histogram estimator, introduced by Parzen in 1962 [1]:

$$
\hat{f}_{n}(x)=\frac{1}{n} \sum_{i=1}^{n} \frac{1}{h_{n}} K\left(\frac{x-x_{i}}{h_{n}}\right),
$$

where $K(x)$, the kernel function, is any Borel function ${ }^{4}$ satisfying:
i. Boundedness: $\sup |K|<\infty$
ii. $\quad K \in L_{1}: \int|K|<\infty$
iii. Decreasing faster than $1 / x: \lim _{x \rightarrow \infty}|x K(x)|=0$
iv. $\int K=1$.

The Parzen window estimator can also be written as a convolution of the window with the (derivative of the) empirical distribution:

$$
\hat{f}_{n}(x)=\int \frac{1}{h_{n}} K\left(\frac{x-y}{h_{n}}\right) d F_{n}(y)=\int K_{h_{n}}(x-y) d F_{n}(y),
$$

where $K_{h_{n}}(x)=\frac{1}{h_{n}} K\left(\frac{x}{h_{n}}\right)$. The positive constants $h_{n}$ are the bandwidths. Note that $\int\left|K_{h_{n}}\right|=\int|K|$.

Convolutions enjoy a series of properties given in Appendix. Particularly note the smoothing imposed by convolutions with a large class of kernels (Fourier Transform property). For a large class of kernels $\hat{f}_{n}(x)$ is a blurred, smoothed, version of $f(x)$.

In the following we often use, for simplicity reasons, the notation $h, K_{h}$ and $f_{n}$ instead of $h_{n}, K_{h_{n}}$ and $\hat{f}_{n}$, respectively.

A central role in the consistency of this estimator is played by the following:
Lemma (Bochner, 1960): Let $K$ be a Borel function satisfying i, ii and iii. Let $g \in L_{1}$ and

$$
g_{n}(x)=\int K_{h}(x-y) g(y) d y=K_{h} \otimes g
$$

If $h_{n}$ is a sequence of positive constants having $\lim _{n \rightarrow \infty} h=0$ the following holds (at every continuity point of $g$ ):

[^2]$$
\lim _{n \rightarrow \infty} g_{n}(x)=g(x) \int K(y) d y
$$

In [2] (Devroye, 2001) this Lemma is stated as an equivalent Theorem, stating:

$$
\lim _{h \rightarrow 0}| | g \otimes K_{h}-g \int K \mid=0
$$

Sometimes the Parzen window estimator is written as

$$
f_{n}(x)=\frac{1}{n h} \sum_{i=1}^{n} K\left(\frac{x-X_{i}}{h}\right)
$$

to stress the fact that $f_{n}(x)$ is a r.v.
The $r$ derivative of $f(x)$ is estimated by [6]

$$
f_{n}^{(r)}(x)=\frac{1}{n h^{r+1}} \sum_{i=1}^{n} K^{(r)}\left(\frac{x-X_{i}}{h}\right)
$$

## Properties (for details see [1], [2], [9], [11], [14-16]):

- If $K$ is an even function we have:

$$
\mu_{n}=\bar{x} ; \quad \sigma_{n}^{2}=s^{2}+h^{2} \int x^{2} K(x) d x
$$

The proofs are in [9].

- The estimate is unbiased: $\lim _{n \rightarrow \infty} E\left[f_{n}(x)\right]=f(x)$. A direct corollary of the above Lemma. The proof is in Appendix.
- If in addition to $\lim _{n \rightarrow \infty} h=0$ the bandwidths satisfy $n h_{n} \rightarrow \infty$ (they decrease less than $1 / n$ ) the estimate verifies:

$$
\lim _{n \rightarrow \infty} n h \mathrm{~V}\left[f_{n}(x)\right]=f(x) \int K^{2}(y) d y
$$

For a Gaussian kernel: $\quad \lim _{n \rightarrow \infty} \mathrm{~V}\left[f_{n}(x)\right]=\frac{f(x)}{2 n h \sqrt{\pi}}$

- From the two preceding results follows that the estimate is consistent:

$$
\operatorname{MSE}\left(f_{n}(x)\right) \rightarrow 0
$$

- The consistent estimate, for a density having $r$ derivatives, verifies:

$$
\operatorname{MSE}\left(f_{n}(x)\right) \sim \frac{f(x)}{n h_{n}} \int_{-\infty}^{\infty} K^{2}(y) d y+h_{n}^{2 r} k_{r}^{2}\left|f^{(r)}(x)\right|^{2}
$$

where $k_{r}$ is the characteristic exponent of the Fourier transform of $K(x)$, that we denote $k(u)$, defined as:

$$
k_{r}=\lim _{u \rightarrow 0}\left[\frac{1-k(u)}{|u|^{r}}\right]
$$

For the Gaussian kernel:

$$
\begin{gathered}
K(x)=\frac{1}{\sqrt{2 \pi}} e^{-x^{2} / 2} \Leftrightarrow \quad \Leftrightarrow(u)=e^{-u^{2} / 2} \\
k(u)=1+\sum_{i=1}^{\infty} \frac{\left(-u^{2} / 2\right)^{i}}{i!}=1-\frac{u^{2}}{2}+O\left(u^{4}\right)
\end{gathered}
$$

Thus: $k_{r}=1 / 2$, for $r=2$.
Any even kernel having $x^{2} K(x) \in L_{1}$ has a nonzero finite $k_{r}$ for $r=2$.

- The optimal MSE is given by:

$$
\operatorname{MSE}_{\text {opt }}\left(f_{n}(x)\right) \sim(2 r+1)\left\{\frac{f(x)}{2 n r} \int_{-\infty}^{\infty} K^{2}(y) d y\right\}^{2 r /(2 r+1)}\left|k_{r} f^{(r)}(x)\right|^{2 r /(2 r+1)}
$$

Thus, the decrease of the MSE is of order $n^{-2 r /(2 r+1)}$. Therefore, for symmetric $x^{2} K(x) \in L_{1}$ kernels the decrease obtainable is of order $n^{-4 / 5}$ as good as for the shifted histogram.

- The optimal integrated mean square error of the consistent estimate in the above conditions is obtained for:

$$
h_{n}=n^{-1 /(2 r+1)} \alpha(K) \beta(f)
$$

with

$$
\begin{aligned}
& \alpha(K)=\left[\frac{\int K^{2}(y) d y}{2 r\left(\int y^{r} K(y) d y / r!\right)^{2}}\right]^{1 /(2 r+1)} \\
& \beta(f)=\left[\int\left|f^{(r)}(y)\right|^{2} d y\right]^{-1 /(2 r+1)}
\end{aligned}
$$

For symmetric $x^{2} K(x) \in L_{1}$ kernels we have:

$$
h_{n}=n^{-1 / 5} \alpha(K) \beta(f)
$$

with
$\alpha(K)=\left[\frac{\int K^{2}(y) d y}{\left(\int y^{2} K(y) d y\right)^{2}}\right]^{1 / 5}$
$\beta(f)=\left[\int\left|f^{\prime \prime}(y)\right|^{2} d y\right]^{-1 / 5}$

Some values for $\alpha(K)$ :

| $K$ | $\alpha(K)$ |  |
| :---: | :---: | :---: |
| $K(y)=1 / 2$ | $\|y\| \leq 1$ | 1.3510 |
| $K(y)=1-\|y\|$ | $\|y\| \leq 1$ | 1.8882 |
| $K(y)=\frac{15}{16}\left(1-y^{2}\right)^{2}$ | $\|y\| \leq 1$ | 2.0362 |
| $K(y)=\frac{1}{\sqrt{2 \pi}} e^{-y^{2} / 2}$ | $\|y\|<\infty$ | 0.7764 |

The difficulty lies in the fact that $\beta(f)$ is generally unknown. One could consider iteratively improving an estimate of $\beta(f)$.
For the Gaussian density with standard deviation $\sigma$, we have:

$$
\int\left|f^{\prime \prime}(y)\right|^{2} d y \approx 0.212 \sigma^{-5} \Rightarrow \beta(f) \approx 1.3637 \sigma \Rightarrow h_{n} \approx 1.06 \sigma n^{-1 / 5}
$$

Some values of optimal $h_{100}$ using a Gaussian kernel:

| Density | $\beta(f)$ | $h_{100}$ |
| :---: | :---: | :---: |
| $N(0,1)$ | 1.3637 | 0.42 |
| $.5 N(-1.5,1)+.5 N(1.5,1)$ | 1.6177 | 0.50 |
| $t_{5}$ | 1.0029 | 0.31 |
| $F_{10,10}$ | 0.4853 | 0.15 |

Quoting reference [9]: "kernel estimators are not in general robust against poor choices of $h_{n}{ }^{\prime \prime}$.

Reference [11] mentions the use of $h_{n}=0.79 R n^{-1 / 5}$, where $R$ is the interquartile range, for skew distributions.

- The optimal IMSE for symmetric $x^{2} K(x) \in L_{1}$ kernels is given by:

$$
I M S E=\frac{5}{4} C(K) \beta^{-1}(f) n^{-4 / 5}
$$

The quantity $C(K)$ is minimized for the Epanechnikov kernel:

$$
K_{e}(t)=\left\{\begin{array}{cc}
\frac{3}{4 \sqrt{5}}\left(1-\frac{1}{5} t^{2}\right) & -\sqrt{5} \leq t \leq \sqrt{5} \\
0 & \text { otherwise }
\end{array}\right.
$$

Reference [11] indicates the efficiencies (IMSE or $C(k)$ ratios) of other kernels compared to $K_{e}$. The efficiency of the Gaussian kernel is $\approx 0.9512$.

- The errors of the consistent estimate are asymptotically normal:

$$
\lim _{n \rightarrow \infty} P\left\{\frac{f_{n}(x)-E\left[f_{n}(x)\right]}{\sigma\left[f_{n}(x)\right]} \leq c\right\}=N_{0,1}(c)
$$

- By the bounded difference inequality:

$$
P\left(\left|\int\right| f_{n}-f \mid-E\left[\int\left|f_{n}-f\right|\right] \geq t\right) \leq 2 e^{-t^{2} / 2 n\left(\int|K|\right)^{2}}
$$

- Schuster's Lemma [6]: If $f$ and its $r+1$ derivatives are bounded and if $\left\{\varepsilon_{n}\right\}$ is a sequence of positive numbers such that $h_{n}=o\left(\varepsilon_{n}\right)$, then there exist positive constants $C_{1}$ and $C_{2}$ such that

$$
P\left\{\sup \left|f_{n}^{(r)}-f^{(r)}\right|>\varepsilon_{n}\right\} \leq C_{1} \exp \left(-C_{2} n \varepsilon_{n}^{2} h_{n}^{2 r+2}\right)
$$

for sufficiently large $n$.

- Suppose that one of the $X_{i}$ changes value while the other $n$ - 1 data points remain fixed. Let $f_{n}^{*}$ denote the new perturbed estimate. Then: $\int\left|f_{n}-f_{n}^{*}\right| \leq \frac{2}{n} \int|K|$ (Parzen window estimates are stable). See proof in Appendix.
- The Parzen window estimator is a regularized estimate of the density ([3]).


## 2 Entropy Estimation Based on Parzen Windows

### 2.1 Plug-in Estimates

We only consider the Shannon functional: $H(f)=-\int f(x) \ln f(x) d x$.
Plug-in estimates [5] are based on using a density estimate $f_{n}$ obtained from the data. There are four types of plug-in estimators:

- Integral estimator
- Resubstitution estimator
- Splitting data estimator
- Cross-validation estimator

We'll only consider the first two:

1. Integral estimator: $H_{n}(f)=-\int_{A_{n}} f_{n}(x) \ln f_{n}(x) d x$

This estimator requires numerical integration. $A_{n}$ typically excludes tail values of the distribution.

Theorem (strong consistency; Dmitriev and Tarasenko, 1973: [6]): Assume that a function $M$ exists such that

$$
\sup _{|y| \leq x} \frac{1}{f(y)} \leq M(x) \quad \forall x
$$

If $h(n)=n^{-1 / 4}$ and $A_{n}=\left[-k_{n}, k_{n}\right]$ with $k_{n}=M^{-1}\left(n^{1 / 10}\right)$, then $H_{n}(f)$ converges to $H(f)$ a.s.
2. Resubstitution estimator: $H_{n}(f)=-\frac{1}{n} \sum_{i=1}^{n} \ln f_{n}\left(X_{i}\right)$
(This estimator seems to have been first proposed by I.A. Ahmad and P-E Lin in 1976; [8].)

## Properties for discrete distributions [7]:

- The resubstitution estimate is strongly universally consistent (also consistent in $L_{2}$ ).
- $\mathrm{E}\left[H_{n}\right] \leq H ; \mathrm{V}\left[H_{n}\right] \leq \ln ^{2} n / n$
- $P\left\{\mid H_{n}-\mathrm{E}\left[H_{n}\right]>\varepsilon\right\} \leq 2 e^{-n \varepsilon^{2} / 2 \ln ^{2} n}$
- There is no universal convergence rate of $\left|H_{n}-H\right|$. In other words, the convergence of $H_{n}$ to $H$ can be arbitrarily slow.

For continuous distributions [8], [12]:

- $L_{1}$ consistency [8]: If $n h_{n} \rightarrow \infty$ as $n \rightarrow \infty, \int[\ln f]^{2} f<\infty, f^{\prime}$ is continuous and $\sup \left|f^{\prime}\right|<\infty, \int|u| K(u) d u<\infty$ then $\mathrm{E}\left[H_{n}-H \mid\right] \underset{n \rightarrow \infty}{\rightarrow} 0$.
- $L_{2}$ consistency [8]: If, in addition, $\int\left(f^{\prime}(x) / f(x)\right)^{2} f(x)<\infty$ (finite Fisher information number) then $\mathrm{E}\left[\left|H_{n}-H\right|^{2}\right] \underset{n \rightarrow \infty}{\rightarrow} 0$

Refernce [8] states that the above conditions are mild and are satisfied by the following distributions: Gamma distribution with $\alpha=1$ and $\beta=0$ or $\alpha>2$ and $\beta>0$; Weibull distribution with parameters $\alpha>0$ and $\beta>2$; normal distribution.

- Almost sure consistency: $H_{n} \rightarrow$ n $H$ a.s., under certain mild conditions stated in [13] (the multivariate case is studied).
- Reference [13] presents upper bounds for the moments of $\left|H_{n}-H\right|$. The formulas are complex, dependent on the support limits (stated above as $[a, b]$; denoted $\left[-K_{n}, K_{n}\right]$ in [13], since they vary with $n$ ) and applicable only when $\varphi(u)=\inf \{f(x) ;|x| \leq u\}>0$ (analogous for the multivariate case). Therefore, their formulas do not apply to densities with restricted support.
Here is the formula for the first order moment (univariate case):

$$
E\left[H_{n}-H\right] \leq\left(\varepsilon_{n}+\frac{K(0)}{n h_{n}}\right) \varphi^{-1}\left(K_{n}\right)+c_{1}(1) \exp \left(-\frac{1}{2} c_{2} n \varepsilon_{n}^{2} h_{n}^{2}\right)+c_{2}(1) n^{-1 / 2}\left|\ln \varphi\left(K_{n}\right)\right|+c_{3}(1) \ln K_{n} / K_{n}^{\rho-1}
$$

## 3 Appendix

### 3.1 Asymptotic Notation

- $f(x)=O(g(x))$ if there are constants $c, x_{0}>0$ such that $|f(x)| \leq c|g(x)|, \quad \forall x \geq x_{0}$. In other words, an $O(g(x))$ term (an asymptotic upper bound; "order of $g(x)$ ") deviates in absolute value less than $c|g(x)|$ after a given $x_{0}$.
- $f(x)=o(g(x))$ if $\lim _{x \rightarrow \infty} f(x) / g(x)=0$. In other words, an $o(g(x))$ term converges to zero faster than $g(x)$.
- $\quad f(x)=o(g(x))$ implies $f(x)=O(g(x))$, but not vice-versa.
- $f(x) \sim g(x)$ if $\lim _{x \rightarrow \infty} f(x) / g(x)=1$ (" $f$ goes asymptotically to $g$ ").
- $f(x)=\Theta(g(x))$ if $f(x)=O(g(x))$ and $g(x)=O(f(x))$ ("asymptotic tight bound").


## Examples:

- $\sin x=O(1)$
- $x \sin x=O(x)$. However, $x \sin x \neq o(x)$.
- $e^{x}=1+x+\frac{x^{2}}{2}+O\left(x^{3}\right)$
- $\int k x^{3} d x=O\left(x^{4}\right)$
- $x=o\left(x^{2}\right)$. Also $x=O\left(x^{2}\right)$.
- In the calculation of $\operatorname{MSE}\left(\hat{f}_{H}\left(x^{\prime}\right)\right)$ for the histogram-based density estimator, the expression of the variance is:

$$
\operatorname{Var}\left(\hat{f}_{H}\left(x^{\prime}\right)\right)=\frac{1}{2 n h_{n}}\left[f\left(x^{\prime}\right)-2 h_{n} f^{2}\left(x^{\prime}\right)+\frac{h_{n}^{2}}{6} f^{\prime \prime}\left(x^{\prime}\right)+O\left(h_{n}^{3}\right)\right]
$$

Hence:

$$
\operatorname{Var}\left(\hat{f}_{H}\left(x^{\prime}\right)\right)=\frac{f\left(x^{\prime}\right)}{2 n h_{n}}+\frac{1}{2 n}\left[-2 f^{2}\left(x^{\prime}\right)+\frac{h_{n}}{6} f^{\prime \prime}\left(x^{\prime}\right)+O\left(h_{n}^{2}\right)\right],
$$

since $O\left(h_{n}^{3}\right) / h_{n}=O\left(h_{n}^{2}\right)$. Moreover, since $h_{n} \rightarrow 0$, we have:

$$
\frac{1}{2 n}\left[-2 f^{2}\left(x^{\prime}\right)+\frac{h_{n}}{6} f^{\prime \prime}\left(x^{\prime}\right)+O\left(h_{n}^{2}\right)\right]=O\left(\frac{1}{n}\right)
$$

Finally:

$$
\operatorname{Var}\left(\hat{f}_{H}\left(x^{\prime}\right)\right)=\frac{f\left(x^{\prime}\right)}{2 n h_{n}}+O\left(\frac{1}{n}\right)
$$

Link: http://en.wikipedia.org/wiki/Big_O_notation

### 3.2 Convolution properties

- $f \otimes g=g \otimes f$
- $f \otimes(g \otimes h)=(f \otimes g) \otimes h$
- $(f+g) \otimes K=f \otimes K+g \otimes K$
- $\quad(a f) \otimes K=a(f \otimes K), \quad a \in \mathfrak{R}$
- $\frac{d}{d x}(f \otimes g)=\frac{d f}{d x} \otimes g=f \otimes \frac{d g}{d x}$
- $\quad F(g \otimes K)=F(g) \times F(K), \quad F \equiv$ Fourier transform
- $\int|f \otimes K| \leq \int|f| \times \int|K| \quad$ (Young's inequality)
- $\int|f \otimes K-g \otimes K| \leq \int|K| \int|f-g| \quad$ (convolution lowers total variation; the proof is based on Young's inequality)


### 3.3 Proof of the convergence of $E\left[f_{n}\right]$ to $f$

We have:

$$
E\left[f_{n}(x)\right]=E\left[K_{h}(x-X)\right]=\int_{-\infty}^{\infty} K_{h}(x-y) f(y) d y
$$

Applying Bochner's Lemma (if the respective conditions are satisfied):

$$
\lim _{n \rightarrow \infty} E\left[f_{n}(x)\right]=f(x) \int_{-\infty}^{\infty} K(y) d y=f(x)
$$

The original justification ([10]) for this result ran like this: Consider:

$$
\hat{f}_{n}(x)=\frac{F_{n}\left(x+h_{n}\right)-F_{n}\left(x-h_{n}\right)}{2 h_{n}} \text { where } F_{n}(x)=\frac{\# \text { sample points } \leq x}{n}
$$

Partition the real line into three intervals: ]- $\left.\left.\left.\left.\infty, x_{1}\right],\right] x_{1}, x_{2}\right],\right] x_{2},+\infty[$. Denote:

$$
Y_{1}=F_{n}\left(x_{1}\right) ; \quad Y_{2}=F_{n}\left(x_{2}\right)-F_{n}\left(x_{1}\right) ; \quad Y_{3}=1-F_{n}\left(x_{2}\right)
$$



Then, $\left(n Y_{1}, n Y_{2}, n Y_{3}\right)$ is a trinomial r.v. with probabilities $\left(F\left(x_{1}\right), F\left(x_{2}\right)-F\left(x_{1}\right), 1-F\left(x_{2}\right)\right)$. Thus, we have $E\left[F_{n}(x)\right]=F(x)$.

### 3.4 Proof of the Result on the Perturbed Density Estimate

Assume w.l.o.g. that is the value of $X_{1}$ that changes. We have:

$$
\left|f_{n}-f_{n}^{*}\right|=\frac{1}{n}\left|\left(K_{h}\left(x-x_{1}\right)-K_{h}\left(x-x_{1}^{\prime}\right)\right)\right| \leq \frac{1}{n}\left(K_{h}\left(x-x_{1}\right)+K_{h}\left(x-x_{1}^{\prime}\right)\right)
$$

Therefore:

$$
\int\left|f_{n}-f_{n}^{*}\right| \leq \frac{1}{n} \int\left(K_{h}\left(x-x_{1}\right)+K_{h}\left(x-x_{1}^{\prime}\right)\right) d x=\frac{2}{n} \int|K|
$$

If $\int|K|=1: \int\left|f_{n}-f_{n}^{*}\right| \leq \frac{2}{n}$

## References

[1] - Emanuel Parzen (1962) On Estimation of a Probability Density Function and Mode. Annals Math. Stat., 33:1065-1076.
[2] - Luc Devroye, Gábor Lugosi (2001). Combinatorial Methods in Density Estimation. Springer-Verlag
[3] - Vladimir Vapnik (1998) Statistical Learning Theory. John Wiley \& Sons, Inc.
[4] - A. Kolmogorov, S. Fomin (1999) Elements of the Theory of Functions and Functional Analysis. Dover Pub. Inc.
[5] - J. Beirlant, EJ Dudewicz, L Györfi, EC van der Meulen (1997) Nonparametric Entropy Estimation: An Overview. Int. J. Math. Stat. Sci., 6(1):17-39.
[6] - Yu. G. Dmitriev, F.P. Tarasenko (1973) On the Estimation of Functionals of the Probability Density and its Derivatives. Theory of Probability and its Applications, 18:628-633.
[7] - András Antos, Iannis Kontoyiannis (2001) Convergence Properties of Functional Estimates for Discrete Distributions. Random Structures \& Algorithms, 19: 163193.
[8] - I.A. Ahmad, P-E Lin (1976) A Nonparametric Estimation of the Entropy for Absolutely Continuous Distributions. IEEE Tr. IT, pp. 372-375.
[9] - Richard A. Tapia, James R. Thompson (1978) Nonparametric Probability Density Estimation. The John Hopkins University Press.
[10] - Murray Rosenblatt (1956) Remarks on some nonparametric estimates of a density function. Annals of Math. Statistics, 27:832-835. (Not available.)
[11] - B.W. Silveman (1986) Density Estimation for Statistics and Data Analysis, Chapman and Hall Ltd.
[12] - Abdelkader Mokkadem (1989) Estimation of the Entropy and Information of Absolutely Continuous Random Variables. IEEE Tr. IT, 35 (1): 193-196.
[13] - A.V. Ivanov, M.N. Rozhkova (1982) Properties of the Statistical Estimate of the Entropy of a Random Vector with a Probability Density. Problems Inform. Transmission, 17: 171-178.
[14] - R.O. Duda, P.E. Hart, D.G. Stork (2001) Pattern Classification. John Wiley \& Sons, Inc.
[15] - B.L.S. Prakasa Rao (1983) Nonparametric Functional Estimation. Academic Press Inc.
[16] - M. P. Wand, M. C. Jones (1995) Kernel Smoothing. Chapman \& Hall.


[^0]:    ${ }^{1} F$ is a convex family if for every $F, G \in \mathcal{F}$ and $0 \leq \alpha \leq 1, \alpha F+(1-\alpha) G \in \mathcal{F}$.

[^1]:    ${ }^{2}$ Note that $\hat{f}_{H}(x)$ is a r.v. (dependent on $\left\{X_{1}, \ldots, X_{k}, \ldots, X_{n}\right\}$ ); $f(x)$ is a constant.
    ${ }^{3}$ Therefore a convergence in the MSE sense is equivalent to a convergence of the mean $\left(E\left[\hat{f}_{H}\right] \underset{\mathrm{n} \rightarrow \infty}{\rightarrow} f\right)$ together with a convergence of the variance towards zero $\left(\operatorname{Var}\left[\hat{f}_{H}\right] \underset{\mathrm{n} \rightarrow \infty}{\rightarrow} 0\right)$.

[^2]:    ${ }^{4} \mathrm{~A}$ Borel function is a measurable function. A continuous function is a Borel function.

