The Discrepancy Principle for Choosing Bandwidths in Kernel Density Estimation

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Abstract

We investigate the discrepancy principle for choosing smoothing parameters for kernel density estimation. The method is based on the distance between the empirical and estimated distribution functions. We prove some new positive and negative results on $L_1$-consistency of kernel estimators with bandwidths chosen using the discrepancy principle. Consistency crucially depends on a rather weak Hölder condition on the distribution function. We also unify and extend previous results on the behavior of the chosen bandwidth under more strict smoothness assumptions. Furthermore, we compare the discrepancy principle to standard methods in a simulation study. Surprisingly, some of the proposals work reasonably well over a large set of different densities and sample sizes, and the performance of the methods at least up to $n = 2500$ can be quite different from their asymptotic behavior.

1 Introduction

We investigate the discrepancy principle, a simple method for choosing the bandwidth in kernel density estimation which – unlike most other methods like cross-validation or plug-in estimates – does not directly aim at minimizing the risk.

In the following, let $X_1, \ldots, X_n$ denote iid random variables having a distribution with Lebesgue density $f$ and distribution function $F$. We denote the empirical distribution function by $F_n$.

A function $K : \mathbb{R} \rightarrow \mathbb{R}$ is called a kernel of order $\ell$ for $\ell \in \mathbb{N}$, if $u^j K(u) \in L_1(\mathbb{R})$ for $j = 0, \ldots, \ell$ and

$$
\int u^j K(u) du = \begin{cases} 1 & (j = 0) \\ 0 & (j = 1, \ldots, \ell - 1) \\ k_\ell & (j = \ell) \end{cases}, \quad k_\ell \in \mathbb{R} \setminus \{0\}.
$$

For a kernel $K$ and $h > 0$ we define $K_h(u) := h^{-1} K(h^{-1}u)$. We denote the distribution function associated with $K$ (which is not necessarily monotone if $K$ is not a probability density) by $F$. For iid random variables $X_1, \ldots, X_n$, a kernel $K$ of order $\ell \in \mathbb{N}$ and a bandwidth $h > 0$ the function $x \rightarrow \hat{f}_h(x)$ given by

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

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is called the kernel density estimator. A corresponding kernel estimator of the distribution function is given by

$$
\hat{F}_n^h(x) := \int_{-\infty}^{x} \hat{f}_h(t)dt = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\left(\frac{x-X_i}{h}\right) = (F_n * K_h)(x).
$$

(1)

More important than the choice of the kernel is the choice of the bandwidth $h$. Depending on the risk function and on additional assumptions on $f$, often an explicit expression for the (at least asymptotically) optimal value can be derived. However, it necessarily depends on some functionals of the unknown true density $f$. Most parameter choice strategies used in practice aim at minimizing the risk. In contrast, the strategies considered here are based on a measure of distance between the empirical and estimated distribution functions, i.e. a direct comparison of the estimate with the data.

In the following, by the discrepancy principle for choosing the bandwidth for kernel density estimators we mean that $h$ is chosen such that

$$
d(F_n, \hat{F}_n^h) = s(n).
$$

(2)

The threshold function $s : \mathbb{N} \rightarrow \mathbb{R}^+$ depends on $n$ only and fulfills $s(n) = o(1)$ for $n \rightarrow \infty$. For the distance $d$ between distribution functions we will always take the Kolmogorov or (generalized) Kuiper distances although, in principle, other metrics could be used. The different suggestions in the previous literature differ in their choices of $s(n)$ and $d$ and possibly in their prescriptions for the selection of a solution of (2) in case there are multiple solutions.

The discrepancy principle was first introduced by Morozov (1966) in the context of (deterministic) inverse problem theory, where it is one of the most widely known methods for choosing a regularization parameter. In Statistical Learning Theory, the connection between nonparametric statistics and ill-posed problems is strongly emphasized, and already in the seventies density estimation was recognized as being closely related to the problem of numerical differentiation, which is an ill-posed problem. Methods adapted from deterministic inverse problem theory as well as using the discrepancy principle for choosing their smoothing parameters have been suggested by Vapnik and Stefanyuk (1978) and Aidu and Vapnik (1989), see also Chapter 7 in Vapnik (1998) and Chapter 7 in Vapnik (2000) for detailed accounts.

Variants of the discrepancy principle (but under different names) have also independently been proposed in the context of the so-called Data Features or Data Approximation approach (Davies 1995, 2008) which has its roots in robust statistics and exploratory data analysis. The main idea is to choose the simplest estimate (with simplicity e.g. measured by smoothness) that is sufficiently close to the data. Several procedures for density estimation based on these ideas have been proposed, including methods based on kernel density estimators (Davies 1995), regular histograms (Davies et al., 2009) and the taut-string estimator (Davies and Kovac, 2004).

The discrepancy principle has also been used in a few other approaches to density estimation. Eggermont and LaRiccia (1996) suggest a version for kernel density estimation that chooses a bandwidth of the optimal order under standard assumptions; see also Eggermont and LaRiccia (2001) Ch. 7.6. The same authors also use their method for choosing a penalty parameter in a penalized-likelihood approach (Eggermont and LaRiccia 2001 Ch. 7.7) and in a density deconvolution method (Eggermont and LaRiccia 1997).

The different variants of the discrepancy principle for density estimation mentioned above have largely been suggested independently of each other, and to our knowledge, there has never been a systematic investigation of this approach.

In Section 2, we show that a solution of (2) exists under very weak conditions, and we show that the almost sure $L_1$-consistency of the resulting kernel density estimate mainly depends on a rather mild Hölder condition on the distribution function $F$. This condition is, for example, fulfilled for all square-integrable densities provided that the threshold function $s$ decays slowly enough. We also give sufficient conditions for the resulting estimator to be inconsistent. In Section 3 we extend and unify some known results on the exact order of the chosen bandwidth.
Furthermore, we compare different versions of the discrepancy principle with standard methods of smoothing parameter selection in a simulation study (Section 4). The methods can behave quite differently to what is predicted by the asymptotic results even for sample sizes up to at least \( n = 2500 \). This is not so much of a surprise as the asymptotics are mostly based on the law of the iterated logarithm for the empirical distribution function. Indeed, some versions of the discrepancy principle that were previously suggested in the literature perform reasonably well over a wide range of different densities, while others suffer from oversmoothing for these sample sizes, although they are guaranteed to undersmooth asymptotically. The last section contains some concluding remarks.

2 Existence and consistency

First, we investigate the existence of a solution of (2). We measure the distance between two distribution functions \( F \) and \( G \) either by the Kolmogorov distance \( d_\infty(F, G) := \|F - G\|_\infty \) or by the \( k \)-th order Kuiper distance (for \( k \in \mathbb{N} \)) first introduced in Davies and Kovac (2004) and defined by

\[
d_{\text{kuip},k}(F, G) := \sup_{a_1 \leq b_1 \leq a_2 \leq b_2 \leq \cdots \leq a_k \leq b_k} k \sum_{i=1}^{k} |(F(b_i) - F(a_i)) - (G(b_i) - G(a_i))|.
\]

For a continuous probability distribution function \( F \) and the empirical distribution \( F_n \) of a sample of size \( n \) drawn from \( F \), the distributions of \( d_\infty(F_n, F) \) and \( d_{\text{kuip},k}(F_n, F) \) do not depend on \( F \). For \( k = 1 \) we obtain the usual Kuiper distance. All these distances are topologically equivalent and it is easy to see that

\[
d_\infty(F, G) \leq d_{\text{kuip},k}(F, G) \leq 2kd_\infty(F, G).
\]

In the following, we always have \( d = d_\infty \) or \( d = d_{\text{kuip},k} \) for some \( k \in \mathbb{N} \), and we define

\[
c_d = \begin{cases} 
1, & d = d_\infty \\
2k, & d = d_{\text{kuip},k}.
\end{cases}
\]

It should be noted that, since we allow for higher order kernels, some distribution functions do not correspond to probability measures but to signed measures.

For a kernel \( K \) with associated distribution function \( \mathbb{K} \), we define

\[
\kappa_0 := \sup_{x \in \mathbb{R}} |\mathbb{K}(x) - F_0(x)|,
\]

where \( F_0(x) := I(x \geq 0) \) is the distribution function of the Dirac measure in 0. In case \( K \) is a probability density, we have \( \kappa_0 = \max\{\mathbb{K}(0), 1 - \mathbb{K}(0)\} \). If \( K \) is also symmetric around zero, he have \( \kappa_0 = \mathbb{K}(0) = 1/2 \).

The following lemma shows that, almost surely, for fixed \( n \), the function \( h \mapsto d(F_n, \hat{F}_n^h) \) is continuous and must – under weak conditions on \( s \) – take the value \( s(n) \) for at least one \( h \) if \( n \) is large enough. An analogous statement has been proved by Eggermont and LaRiccia (1996, 2001) for the special case of a symmetric, nonnegative kernel of of order 2 and \( d = d_\infty \). The proof can be found in Mildenberger (2011), pp. 27-28.

**Lemma 2.1.** For \( F_n \) an empirical distribution function of an iid sample from a distribution with continuous distribution function and \( \hat{F}_n^h \) as in [1] we have almost surely:

1. \( d(F_n, \hat{F}_n^h) \) is continuous in \( h \).
Figure 1: Solutions of $d_\infty(F_n, \hat{F}_h^n) = s(n)$ using a standard Gaussian kernel for $X_1, \ldots, X_n \sim N(0,1)$. Top row: $n = 10$, bottom row: $n = 100$. Straight lines: $s(n) = 0.6n^{-1/2}$, broken lines: $s(n) = 0.35n^{-2/5}$.

2. $\liminf_{h \to 0} d(F_n, \hat{F}_h^n) \leq c_d \frac{s(n)}{n}$.

3. $\limsup_{h \to \infty} d(F_n, \hat{F}_h^n) \geq \kappa_0$.

Lemma 2.1 shows that if $s(n) = o(1)$ and $n^{-1} = o(s(n))$ the equation $d(F_n, \hat{F}_h^n) = s(n)$ almost surely has at least one solution $h_{s,n}$ for sufficiently large $n$. These conditions are fulfilled by the threshold functions previously proposed in the literature. Moreover, the minimum sample size that guarantees existence of at least one solution can be calculated explicitly since it depends on $s(n)$ and $\kappa_0$ only, and not on the sample or on the underlying true distribution (assuming there are no ties, which holds true almost surely). For example, if $s(n) = 0.6n^{-1/2}$ as proposed by Vapnik (1998, Ch. 7.9) or $s(n) = 0.35n^{-2/5}$ as proposed in Eggermont and LaRiccia (1996), $d = d_\infty$ and $K$ is any symmetric probability density, we have that $s(n) \in [1/2n, 1]$ for $n \geq 2$, so existence of the bandwidth can be guaranteed if there are at least two data points. As already noted by Eggermont and LaRiccia (1996), the function $h \to d(F_n, \hat{F}_h^n)$ is not necessarily monotone, so that the bandwidth chosen according to the discrepancy principle is not necessarily unique; Eggermont and LaRiccia (1996) suggest using the smallest solution while the Data Approximation approach would suggest using the largest one. However, none of the results given subsequently depends on the particular choice of the solution, and multiple solutions seem to occur only rarely in larger samples.

Figure 1 shows two realizations each for $n = 10$ and $n = 100$. The samples were drawn from a standard normal distribution and the Gaussian kernel was used. The horizontal lines correspond to the two different choices of the threshold functions mentioned above. The solution $d(F_n, \hat{F}_h^n) = s(n)$ can be computed numerically since the function $h \to d(F_n, \hat{F}_h^n)$ is continuous. In Eggermont and LaRiccia (1996), a secant method is proposed for solving this equation, but we use the related regula falsi which we found to be more stable. The possibility of using an iterative method makes selection of the bandwidth using the discrepancy quite fast in comparison to other methods (like cross-validation) where one usually has to evaluate some criterion on a grid.
of possible bandwidths. In addition, well-known formulas exist for calculating Kolmogorov- and Kuiper-distances (for \( k = 1 \)) for two distribution functions and these can be applied if \( K \) is a probability density.

In the following, we frequently need the function

\[
F_h := F \ast K_h.
\]

In case \( K_h \) is a probability density, \( F_h \) is a probability distribution function, otherwise it is the distribution function of a signed measure.

The proof of the following Lemma is based on basic properties of convolutions and the Law of the Iterated Logarithm, see [Mildenberger (2011), p. 29, for details.

**Lemma 2.2.** With probability 1,

1. \( d(F_n, F) = O\left((\log \log n/n)^{1/2}\right) \) and

2. \( d(\hat{F}_n^h, F_h) = O\left((\log \log n/n)^{1/2}\right) \) uniformly in \( h \).

The next theorem shows that bandwidths chosen using the discrepancy principle converge to 0 almost surely. This result will be needed later on for obtaining more precise statements about the behavior of the selected bandwidths. At this point, \( F \) must be continuous but does not need to have a density. As a by-product, the theorem also shows that the resulting estimator for the distribution function is always consistent w.r.t. \( d \), although our aim is to estimate the density rather than the distribution function. The proof of the second assertion is based on similar Fourier arguments as the proof of Theorem 3 in [Yamamoto (1973)]

**Theorem 2.1.** Let \( F \) be a continuous distribution function, \( F_n \) and \( \hat{F}_n^h \) as above and \( s(n) = o(1) \). For the bandwidth \( h_{s,n} \) chosen as a solution of

\[
d(F_n, \hat{F}_n^h) = s(n).
\]

we have almost surely

1. \( h_{s,n} \to 0 \)

2. \( h_{s,n} \to 0 \).

**Proof.** 1. With probability 1, we have:

\[
d(F, F_{h_{s,n}}) \leq d(F, F_n) + d(F_n, \hat{F}_{h_{s,n}}) + d(\hat{F}_{h_{s,n}}, F_{h_{s,n}})
\]

\[
= O\left((\log \log n/n)^{1/2}\right) + s(n) + O\left((\log \log n/n)^{1/2}\right)
\]

\[
= o(1),
\]

and hence

\[
d(F, \hat{F}_{h_{s,n}}) \leq d(F, F_{h_{s,n}}) + d(F_{h_{s,n}}, \hat{F}_{h_{s,n}}) = o(1).
\]

2. According to the first part, \( d_{\infty}(F, F_{h_{s,n}}) \leq d(F, F_{h_{s,n}}) \to 0 \) with probability 1; it remains to show that this implies \( h_{s,n} \to 0 \). In the following \( h_n := h_{s,n} \) denotes the sequence of bandwidths chosen, \( P \) denotes the probability measure associated with \( F \) and \( \mu_h \) the (signed) measure with Lebesgue density \( K_h \). Denote by \( P, \hat{P} \) and \( \hat{K}_h \) the Fourier transforms of \( P, K \) and \( K_h \), respectively. Observing that the sequence \((|P \ast \mu_h|)_{n \in \mathbb{N}} \) is tight ([Mildenberger [2011], pp. 30-31]) and combining Proposition 8.1.8 in [Bogachev (2007)] with a result on page 173/174 in [Katznelson (2004)], it follows that \( \hat{P}^{\hat{K}_h}(t) \to P(t) \) for all \( t \in \mathbb{R} \). Because of the continuity of the Fourier transform, we must have \( \hat{P} > 0 \) on an interval \([-\varepsilon, \varepsilon]\) for some \( \varepsilon > 0 \), which implies that \( \hat{K}_h(t) = \hat{K}(h_n t) \to 1 \) for all \( t \in [-\varepsilon, \varepsilon] \). Since \( \int u' K(u) du \neq 0 \), \( \hat{K} \) cannot be identically 1 on any interval around zero. But this implies that \( h_n \to 0 \).
While the previous results hold for any continuous distribution function $F$, for the remainder of the paper we suppose that a Lebesgue density $f$ exists.

For consistency of the kernel density estimate with bandwidth chosen by the discrepancy principle, we also need that the chosen bandwidth does not go to 0 too quickly. This can be guaranteed under rather mild conditions. For $0 < \alpha \leq 1$, let

$$C^{0,\alpha} := \left\{ F \left| F : \mathbb{R} \rightarrow \mathbb{R} \text{ and } \exists C > 0 \text{ with } \sup_{x, y \in \mathbb{R}} |F(x) - F(y)|/|x - y|^\alpha \leq C \right. \right\}$$

denote the set of all Hölder continuous functions with exponent $\alpha$. Smoothness of the distribution function follows from integrability assumptions on the density. We define for $p \in [1, \infty)$

$$L_p(\mathbb{R}) := \left\{ f \left| f : \mathbb{R} \rightarrow \mathbb{R} \text{ and } \|f\|_p := \left( \int |f|^p d\lambda \right)^{1/p} < \infty \right. \right\}$$

where $\lambda$ denotes the Lebesgue-Measure on (the Borel sets of) $\mathbb{R}$. Then we have:

**Lemma 2.3.** Let $f$ denote a probability density and $F$ the corresponding distribution function. For $p \in (1, \infty)$ we have

$$f \in L_p(\mathbb{R}) \implies F \in C^{0,(p-1)/p}.$$

**Proof.** For any $x < y \in \mathbb{R}$ and $q = \frac{p}{p-1}$ we obtain using the Hölder inequality

$$|F(y) - F(x)| \leq \|f\|_p |y - x|^{1/q}$$

and hence $F \in C^{0,(p-1)/p}$. □

This implies for example that for any square-integrable density (i.e., $f \in L_2(\mathbb{R})$) $F$ is Hölder-continuous with exponent $\alpha = \frac{1}{2}$. We also observe that, using a similar argument, for any bounded $f$ the corresponding distribution function $F$ is Hölder-continuous with exponent $\alpha = 1$.

The next theorem shows that $L_1$ consistency of a kernel density estimator with bandwidth chosen by the discrepancy principle can be guaranteed if the distribution function is Hölder continuous with an sufficiently large exponent and the threshold function goes to 0 slowly enough.

**Theorem 2.2.** Let $K$ be a kernel of order $\ell$, $\ell \geq 1$, and $f$ a density with associated distribution function $F$ such that $F \in C^{0,\alpha}$ for some $0 < \alpha \leq 1$. If the threshold function $s(n)$ is such that $\sqrt{\frac{\log \log n}{n}} = o(s(n))$ and $n^{\alpha}s(n) \rightarrow \infty$ for $n \rightarrow \infty$, then with probability 1 we have that

$$nh_{s,n} \rightarrow \infty.$$  

**Proof.** The Hölder condition $F \in C^{0,\alpha}$ implies that there is a constant $A > 0$ such that $d_{\infty}(F, F_h) \leq Ah^\alpha$, cf. Shapiro (1969), Theorem 20. With probability 1, we have that

$$n^{\alpha}s(n) = n^{\alpha}d(F_n, \hat{F}_{n,h_{s,n}})$$

$$\leq c_d n^{\alpha} \left( d_{\infty}(F_n, F) + d_{\infty}(F, F_{h_{s,n}}) + d_{\infty}(F_{h_{s,n}}, \hat{F}_{n,h_{s,n}}) \right)$$

$$\leq Ac_d n^{\alpha} h_{s,n}^\alpha + n^{\alpha}O((\log \log n/n)^{1/2})$$

which implies that

$$Ac_d n^{\alpha} h_{s,n}^\alpha \geq n^{\alpha} s(n)(1 + o(1)),$$

and hence, since $n^{\alpha}s(n) \rightarrow \infty$, that $nh_{s,n} \rightarrow \infty$. □

**Corollary 2.1.** If $K$ is a probability density and $f$ and $s$ are such that the conditions of Theorem 2.2 are fulfilled, we have

$$\lim_{n \rightarrow \infty} \int |\hat{f}_{s,n}(x) - f(x)|dx = 0$$

with probability 1.
Example 2.1. Let the sharpness of the peak:

From Corollary 2.1, we have that almost sure density and \( f \in L_2 \).

Although the conditions for consistency are rather weak, the resulting density estimate may be inconsistent if the distribution function is too rough or the threshold function vanishes too quickly:

**Theorem 2.3.** Let \( K \) be a kernel and \( 0 < \varepsilon < 1/2 \) such that \( n^s(n) = o(1) \). Let \( F_n \) denote the empirical distribution function of an iid sample drawn from a distribution with density \( f \) and distribution function \( F \). Suppose there exist constants \( c, h_0 > 0 \) such that

\[
d_{\infty}(F,F_h) \geq ch^\varepsilon
\]

for all \( 0 < h < h_0 \). Then, if \( h_{s,n} \) is a solution of \( d(F_n,F_h) = s(n) \), we have:

1. \( nh_{s,n} \rightarrow 0 \) with probability 1 and

2. if \( K \) is compactly supported and there exist \( a, b > 0 \) such that \( \lambda \{ x : f(x) \geq b \} \geq a \), where \( \lambda \) denotes Lebesgue measure on \( \mathbb{R} \), then \( \lim \inf_{n \to \infty} \| \hat{f}_{h_{s,n}} - f \|_1 \geq ab > 0 \) with probability 1.

**Proof.** 1. It follows that, with probability 1,

\[
cn^s h_{s,n}^\varepsilon \leq n^s d_{\infty}(F,F_{h_{s,n}}) \\
\leq n^s \left( d_{\infty}(F,F_n) + d(F_n,F_{h_{s,n}}) + d_{\infty}(F_{h_{s,n}},\hat{F}_{h_{s,n}}) \right) \\
= n^s O((\log \log n/n)^{1/2}) + n^s s(n) \\
= o(1),
\]

and hence \( nh_{s,n} = o(1) \).

2. If the support of \( K \) is contained within a compact interval \( I \), then, since \( \lambda \{ K_{h_{s,n}} \neq 0 \} \leq \lambda(I) \), we have almost surely

\[
\lambda \{ \hat{f}_{h_{s,n}} \neq 0 \} \leq 2nh_{s,n} \lambda(I) = o(1)
\]

because of the first assertion. It then follows almost surely that

\[
\lim \inf_{n \to \infty} \int |\hat{f}_{h_{s,n}}(x) - f(x)|dx \geq \lim \inf_{n \to \infty} \int_{\{ f \geq b \} \cap \{ \hat{f}_{h_{s,n}} = 0 \}} f(x)dx \geq ab.
\]

In the following example, we consider a family of densities with an infinite peak and see that the using the discrepancy principle can lead to consistent or inconsistent estimates depending on the sharpness of the peak:

**Example 2.1.** Let

\[
K(x) = (3/4)(1 - x^2)1(|x| \leq 1)
\]

denote the Epanechnikov kernel and choose \( s(n) \). Consider the distribution of \( X := U^\beta \) for \( \beta \in [1, \infty) \), where \( U \) is uniformly distributed on \([0, 1]\). With \( \varepsilon = \beta^{-1} \) the density of \( X \) is given by

\[
f(x) := \begin{cases} 
\varepsilon x^{-(1-\varepsilon)} & 0 < x \leq 1 \\
0 & \text{otherwise}
\end{cases}
\]
The distribution function of $X$ is given by
\[
F(x) := \begin{cases} 
0 & x \leq 0 \\
x^\varepsilon & 0 < x \leq 1 \\
1 & x > 1 
\end{cases}
\] (5)

It is easy to see that $F \in C^{0,\alpha}$ iff $\alpha \leq \varepsilon$.

First consider the case that $\sqrt{\log \log n} = o(s(n))$ and $n^\varepsilon s(n) \to \infty$. Then the conditions of Theorem 2.2 are fulfilled and the estimator will be consistent w.r.t $L_1$-distance. Note that if $\sqrt{\log \log n} = o(s(n))$ then we trivially have $n^\varepsilon s(n) \to \infty$ for all $\varepsilon > 1/2$.

Now consider the case that $0 < \varepsilon < 1/2$ and $n^\varepsilon s(n) = o(1)$. By elementary integration, we obtain
\[
|F(h) - (F * K_h)(h)| = \left(1 - \frac{3 \cdot 2^{(\varepsilon + 1)}}{\varepsilon^2 + 5\varepsilon + 6}\right) h^\varepsilon.
\]

for $h < 1$ and hence
\[
d_\infty(F, F_h) \geq c h^\varepsilon
\]
for $h < 1 =: h_0$. Since $K$ is compactly supported, inconsistency w.r.t. the $L_1$ distance directly follows from the second assertion of Theorem 2.3.

3 Rates for the bandwidths
In the following, we consider threshold functions $s(n)$ that go to 0 at different speeds:

- $s(n) = o(\sqrt{\log n/n})$ (Theorem 3.1),
- $s(n) \approx (\log n/n)^{1/2}$ (Theorem 3.2),
- $(\log n/n)^{1/2} = o(s(n))$ (Theorem 3.3).

The versions of the discrepancy principle for kernel estimators previously proposed in the literature can be obtained by choosing a threshold function that belongs to one of these classes.

To obtain more precise statements about the order of the chosen bandwidth, we need some additional assumptions of $f$ and $K$. In this section, we suppose that $f$ is in a Sobolev space defined by
\[
W^{\ell,1} := \{ f : f, f^{(1)}, \ldots, f^{(\ell)} \in L_1(\mathbb{R}) \}.
\]
where $\ell \geq 2$ is the order of the Kernel $K$.

The following Lemma is a slight generalization of a similar result by Eggermont and LaRiccia (1996, 2001), who only considered nonnegative symmetric kernels of order $\ell = 2$ and $d = d_\infty$. The proof is left out since the first part is completely analogous to Eggermont and LaRiccia (2001, Lemma 6.15 a) and the second part is easy.

Lemma 3.1. Suppose that $f \in W^{\ell,1}(\mathbb{R})$ and $K$ is a kernel of order $\ell \geq 2$. Then we have:

1. $F_h(x) - F(x) = \frac{(-1)^\ell}{n^\ell} k_{\ell} f^{(\ell-1)}(x) h^\ell (1 + o(1))$ uniformly in $x \in \mathbb{R}$.
2. $d(F_h, F) = \frac{1}{n^\ell} k_{\ell} (f^{(\ell-1)}, 0) h^\ell (1 + o(1))$.

The approximations given in Lemma 3.1 are only valid for sufficiently small $h$. Since by Theorem 2.1 for $n \to \infty$ we have that $h_{s,n} \to 0$ almost surely with $h_{s,n}$ chosen by the discrepancy principle, terms of order $o(1)$ for $h \to 0$ are also of order $o(1)$ for $n \to \infty$.
The most simple and intuitive implementation of the discrepancy principle is based on a

The second term in parentheses on the left-hand side is not only of order \( o \) 

According to Lemma 3.1, we have a.s.

Proof. According to Lemma 3.1, we have a.s.

\[
\frac{1}{f!} \| f^{(f-1)} \|_{\infty} h_{s,n} \ell (1 + o(1)) = d_{\infty}(F_{h_{s,n}}, F) 
\]

\[
\leq d_{\infty}(F, F_n) + d(F_n, \hat{F}_{h_{s,n}}) + d_{\infty}(\hat{F}_{h_{s,n}}, F_{h_{s,n}}) 
\]

\[
= O \left( (\log \log n/n)^{1/2} + s(n) \right) 
\]

\[
= O \left( (\log \log n/n)^{1/2} \right).
\]

The second term in parentheses on the left-hand side is not only of order \( o(1) \) for \( h_{s,n} \to 0 \), but also \( o(1) \) for \( n \to \infty \) since, by Theorem 2.1, \( n \to \infty \) almost surely implies \( h_{s,n} \to 0 \). Solving for \( h_{s,n} \) then proves the claim.

Theorem 3.1 shows that for \( f \in W^{\ell,1} \) and \( K \) kernel of order \( \ell \), an upper bound for the bandwidth (and hence the bandwidth itself) converges to 0 at a faster rate than the optimal bandwidths according to most criteria, which behave like \( h \approx n^{-\frac{\ell-1}{\ell+1}} \) (although this problem becomes less severe as \( \ell \) increases). The reason is that density estimation is an ill-posed problem that requires regularization. For sufficiently large \( n \), the Kolmogorov-Smirnov-test with fixed level will detect the difference between \( F \) and \( F_h \), even if \( h \) is chosen optimally. This leads to a bandwidth that is too small. The incompatibility of optimal bandwidths with confidence sets based on the Kolmogorov-Smirnov or Kuiper tests has also been observed in Davies (1995), Eggermont and LaRiccia (1996) and Hjort and Walker (2001). Asymptotically, the estimated distribution function is too close to the empirical distribution function, leading to undersmoothing.

However, the simulations in Section 4 show that discrepancy principles based on extreme quantiles of goodness-of-fit tests still oversmooth even for sample sizes as large as \( n = 2500 \), while the version proposed by Vapnik (\( c = 0.6 \)) works quite well for the sample sizes considered.

Theorem 3.1 is applicable to threshold functions of the form \( s(n) = c\log \log n/2n \), but more precise results are possible when \( c \) is large enough. A threshold of this form is motivated by the law of the iterated logarithm for \( d(F_n, F) \), and is in a sense the closest analogue to the upper bound on the error in deterministic inverse problems. Aidu and Vapnik (1989) considered the case where \( c = (1 + \tilde{k} + c) \) for kernels \( K \) of order \( \ell \), \( \tilde{k} = \| K \|_1 \) and \( d = d_{\infty} \). The next theorem is a slight extension of their theorem (Aidu and Vapnik 1989, Sec. 3) which now additionally includes the case of \( d = d_{kuip,k} \) and has essentially the same proof, see pp. 38 in Mildenberger (2011) for details.
Theorem 3.2. For \( f \in W^{\ell,1} \), \( K \) kernel of order \( \ell \geq 2 \), \( \tilde{k} = \|K\|_1 \) and \( s(n) = c_d(\tilde{k} + 1 + \varepsilon)(\log \log n / 2n)^{1/2} \), we have with probability 1:

\[
\liminf_{n \to \infty} \frac{h}{(\log \log n / 2n)^{1/2}} \geq \left( \frac{c_d \ell!}{kd(f^{(\ell-1)}, 0)} \right)^{1/\gamma}.
\]

\[
\limsup_{n \to \infty} \frac{h}{(\log \log n / 2n)^{1/2}} \leq \left( \frac{c_d(2\tilde{k} + 2 + \varepsilon)\ell!}{kd(f^{(\ell-1)}, 0)} \right)^{1/\gamma}.
\]

The theorem gives an upper and a lower bound on the selected bandwidth which are of the same order, and which again go to 0 faster than the optimal bandwidths according to most criteria.

Exact results on the limiting behavior of the bandwidth chosen by the discrepancy principle can be obtained in the case where \( s(n) \) converges to 0 at a slower rate than \( d(F_n, F) \). Noting that discrepancy principles based on fixed quantiles or the law of the iterated logarithm lead to undersmoothing, Eggermont and LaRiccia [1996, 2001] introduce a rate-corrected version. For a symmetric, nonnegative kernel, they propose to choose \( h \) as a solution of

\[
d_{\infty}(F_n, \hat{F}_n^h) = 0.35n^{-2/5}.
\]

The choice of the exponent implies that the smoothing parameter goes to 0 at the optimal rate. The next theorem is a generalization of the main result in Eggermont and LaRiccia [1996] and Chapter 7.6 of Eggermont and LaRiccia [2001]. Our version is also applicable in the case of \( d = d_{kwip,k} \) and allows for higher order kernels.

Theorem 3.3. For \( f \in W^{\ell,1} \), \( K \) kernel of order \( \ell \) and \( s(n) = cn^{-\gamma} \) for \( c > 0 \) and \( 0 < \gamma < 1/2 \) we have almost surely:

\[
h_{s,n} = \left( \frac{\ell!}{kd(f^{(\ell-1)}, 0)} \right)^{1/\gamma} n^{-\gamma} (1 + o(1)).
\]

Proof. Using the triangle inequality, we have with probability 1 that

\[
|d(F_n, \hat{F}_n^{h_{s,n}}) - d(F, F_{h_{s,n}})| \leq d(F_{h_{s,n}}, \hat{F}_n^{h_{s,n}}) + d(F, F_n) = O \left( \sqrt{\frac{\log \log n}{n}} \right).
\]

Combining this with Lemma 3.1 and again observing that, by Theorem 2.1, the \( o(1) \) term for \( h_{s,n} \to 0 \) is also of order \( o(1) \) for \( n \to \infty \), we have

\[
\frac{1}{\ell!} kd(f^{(\ell - 1)}, 0) h_{s,n} \ell (1 + o(1)) = cn^{-\gamma} + O \left( (\log \log n / n)^{1/2} \right)
\]

which implies that

\[
h_{s,n} = \left( \frac{\ell!}{kd(f^{(\ell-1)}, 0)} \right)^{1/\gamma} n^{-\gamma} (1 + o(1)).
\]

The theorem implies that for a kernel of order \( \ell \) and a threshold function of the form \( s(n) = cn^{-\gamma} \) with \( \gamma = \ell / (2\ell + 1) \) the chosen bandwidth is - for sufficiently smooth \( f \) - of the optimal order \( h = cn^{-1/(2\ell+1)} \) with respect to the \( L_1 \) or \( L_2 \) risks. The constant \( \alpha \) depends on \( c \) and the unknown true density \( f \) and is not equal to the optimal one according to any of the standard criteria. Eggermont and LaRiccia choose \( c = 0.35 \) based on simulations. Noting that \( s(n) = cn^{-2/5} = (cn^{1/10})n^{-1/2} \) we can interpret the threshold function in terms of confidence levels that depend on \( n \). For \( c = 0.35 \), the confidence level is below 0.5 up to \( n = 5624 \).

In principle, constants suitable for other classes of densities, other distances or higher order kernels can also be chosen using simulations. But Theorem 3.3 also allows for a different approach: Discrepancy principles that can be guaranteed to asymptotically choose the optimal bandwidths for a reference density. In the following example, we will sketch this approach for the normal distribution and the \( L_2 \)-optimal bandwidth.
**Example 3.1.** The asymptotically $L_2$-optimal bandwidth for a kernel of order $\ell$ is given by

$$h_{opt} = \left( \frac{\ell^2 \|K\|^2_2}{2\ell k_{\ell}^2 \|f^{(\ell)}\|^2_2} \right)^{\frac{1}{2\ell + 1}} n^{-\frac{1}{2\ell + 1}},$$

(Wand and Jones [1995, p.33]. Equating (6) and (7) yields $\gamma = \frac{\ell}{2\ell + 1}$ and

$$c = \left( \frac{\|K\|^2_2 k_{\ell}}{(2\ell)!} \right)^{\frac{1}{2\ell + 1}} \frac{d(f^{(\ell - 1)}, 0)}{\|f^{(\ell)}\|^2_2 / (2\ell + 1)}. $$

The first factor only depends on the kernel and is invariant w.r.t. rescaling of the kernel. The second factor only depends on the shape of $f$ and does not change when $f$ is translated or rescaled. For $f$ the standard normal density, we obtain $c = 0.1357$ for the Gaussian and $c = 0.1331$ for the Epanechnikov kernel (3) when using $d = d_{\infty}$. Both values are much smaller than $c = 0.35$ as suggested by Eggermont and LaRiccia (1996) independent of the kernel. This choice forces the estimate of the distribution function to lie extremely close to the empirical distribution function, causing severe undersmoothing even for very large sample sizes. For $d = d_{\text{kuip}}$, we obtain $c = 0.2715$ for the Gaussian and $c = 0.2661$ for the Epanechnikov kernel. Similar calculations can be carried out for a bandwidth minimizing an upper bound for the $L_1$ risk, but these lead to even smaller values of $c$ (Mildenberger [2011, pp. 44-45]).

## 4 Simulation Study

In this section, we explore how well different versions of the discrepancy principle work in practice. Mainly in the 1980s and 1990s, several large simulation studies on bandwidth choice methods for kernel density estimators have been conducted, of which we just mention Cao et al. (1994) (with a focus on the $L_2$-risk) and Berlinet and Devroye (1994) and Devroye (1997) in an $L_1$-context. To the best of our knowledge, there is no larger simulation study on kernel estimators that includes any version of the discrepancy principle, although in Devroye (1997) the version
proposed in [Eggermont and LaRiccia (1996)] is mentioned but not included in the study. There are some smaller simulation studies to be found in the publications in which a particular version of the discrepancy principle is suggested or directly building on these [Markovich (1989), Eggermont and LaRiccia (1996, 2001)]. Our simulation study is a replication of a part of the more extensive study described in [Mildenberger (2011)]. The aim is not to find a 'best' method but to explore whether methods based on the discrepancy principle perform reasonably well at all. Since the discrepancy principle is not designed with any specific risk in mind, we look at both the $L_1$- and $L_2$-risk (where applicable).

We use the Epanechnikov kernel as given in (3) and choose the bandwidth as a solution of $d(F_n, \hat{F}_n) = s(n)$. In [Eggermont and LaRiccia (1996)], a secant method is proposed for solving this equation, but we use the related regula falsi which we found to be more stable. Occasionally, there may be multiple solutions but we ignore this and take the first solution found.

We compare the following versions of the discrepancy principle:

- Two versions based on the 0.5 and 0.95 quantiles of the Kolmogorov-Smirnov statistic: $d = d_{\infty}$ and $s(n) = cn^{-1/2}$ with $c = 0.83$ and $c = 1.36$. These methods are denoted by $KS_{0.5}$ and $KS_{0.95}$, respectively.
- The version proposed by Vapnik: $d = d_{\infty}$ and $s(n) = 0.6n^{-1/2}$. Denoted by $V$.
- The rate-corrected version proposed by Eggermont and LaRiccia: $d = d_{\infty}$ and $s(n) = 0.35n^{-2/5}$. Denoted by $E-LR$. In contrast to the other versions considered here, this one uses a threshold function for which the assumptions in Theorem 2.2 are fulfilled.
- Two versions based on the 0.5 and 0.95 quantiles of the Kuiper statistic: $d = d_{\text{Kuip},1}$ and $s(n) = cn^{-1/2}$ with $c = 1.22$ and $c = 1.75$. Denoted by $\text{Kuip}_{0.5}$ and $\text{Kuip}_{0.95}$, respectively.
- The method based on a normal reference density as given in Example 3.1: $d = d_{\infty}$ and $s(n) = 0.1331n^{-2/5}$. Denoted by $L2NR$.

For comparison, we include $L_2$ cross-validation as described in [Celisse and Robin (2008)] (their Formula 13 with $p = 1$). This is denoted by $L2CV$. The more extensive simulations in [Mildenberger (2011)] include several more variants of the discrepancy principle, a few more standard methods for comparison, and all of the 28 densities from [Berlien and Devroye (1994)]. For the sake of brevity, here we just focus on a smaller subset but the conclusions are largely the same.

We draw 250 samples of sizes 100, 1000 and 2500 from 12 of the 28 testbed densities introduced in [Berlien and Devroye (1994)]. For this, we use the R-package benchden [Mildenberger et al., 2012, Mildenberger and Weinert, 2012]. The set of densities is depicted in Figure 2. We use the same numbering for the densities as in [Mildenberger and Devroye (1994)].

Figure 3 shows typical kernel estimates for a normal sample of size 100. In the first panel, the $L_2$-optimal bandwidth (7) was chosen. The second panel shows the result obtained using $V$, which gives a fairly good result. The bandwidth chosen using $KS_{0.95}$ is obviously too large, although it will be too small asymptotically. The bandwidth in the fourth panel has been chosen using $L2NR$. Although this will asymptotically result in the optimal bandwidth, the estimate is severely undersmoothed.

The estimated $L_1$ and (squared) $L_2$ risks and the arithmetic means of the chosen bandwidths for all densities and sample sizes considered here are given in Tables 1, 2 and 3 respectively. The smallest risk for each scenario has been highlighted. Note that Table 2 omits densities 8 and 19, since these are not in $L_2$.

In most cases, either $L2CV$ or one of $V$ and $E-LR$, which perform very similarly, is the best method with respect to the $L_2$-risk. Although $L2CV$ usually selects smaller bandwidths than $V$ and $E-LR$, the resulting risks are close in most cases. The methods based on quantiles of the Kolmogorov or Kuiper statistics ($KS_{0.5}$, $KS_{0.95}$, $Kuip_{0.5}$ and $Kuip_{0.95}$) choose larger bandwidths, which results in oversmoothing in most cases (although, by Theorem 3.1, these methods asymptotically suffer from undersmoothing). The methods based on the Kuiper statistic are usually better than those based on the corresponding quantiles of the Kolmogorov-Smirnov statistic.
The rather large amount of smoothing chosen by these methods is beneficial w.r.t. $L_1$ risk for the Cauchy density (number 6), which is mainly due to the fact that the $L_1$ loss penalizes errors in the tails quite heavily.

The method L2NR chooses bandwidths that are much smaller than those chosen by the other methods. Although it is guaranteed to asymptotically choose the $L_2$ optimal bandwidth for the normal density, the results for both $L_1$ and $L_2$ risk are poor even when the true density is the normal (number 11). The small bandwidths seem to be helpful for capturing the fine structure of multimodal densities 23, 27 and (less pronounced) 24.

Except for 8, 15 and 19 all densities are bounded and hence fulfill the assumptions of Theorem 2.2, such that the estimate based on a bandwidth chosen using E-LR will be almost surely consistent w.r.t. the $L_1$-distance.

Density 8 is the density of $U^2$, where $U$ is a uniform random variable on $[0, 1]$. This corresponds to the density in Example 2.1 for $\varepsilon = 1/2$, such that using E-LR to select the bandwidth will result in a consistent estimate w.r.t. $L_1$-loss. The density is not in $L_2$. With respect to $L_1$-risk, at least for larger sample sizes all versions of the discrepancy principle except L2NR perform better than L2CV. The distribution function corresponding to density 15 is in $C^{0, \alpha}$ for any $\alpha < 1$, and hence using E-LR to select the bandwidth will also lead to $L_1$-consistent estimates by Theorem 2.2 and Corollary 2.1. This density is in $L_2$. Again, L2CV performs worse than all variants of the discrepancy principle except L2NR. Density number 19 is the density of $N^3$, where $N$ is a standard normal random variable. It is not in $L_2$ and it can be shown that

$$|F(h) - F * K_h(h)| = \frac{1}{\sqrt{2\pi}} h^{\frac{3}{2}} (1 + o(1)),$$

where $F$ is the distribution function and $K_h$ the Epanechnikov-kernel with bandwidth $h$. Hence, for $h$ small enough, the conditions of Theorem 2.3 are fulfilled with $\varepsilon = 1/3$ and any $0 < c < (\sqrt{2\pi})^{-1}$. From this it follows that every version of the discrepancy principle considered in the simulation study will lead to inconsistent estimates w.r.t. $L_1$-loss almost surely. The main Theorem in
Table 1: Results of the simulation study: Estimated $L_1$ risk for kernel estimators

Table 1 shows that $L2CV$ performs even worse than most versions of the discrepancy principle in our simulations (with the versions choosing larger bandwidths doing relatively better).

Overall, if the discrepancy principle is to be used for choosing a bandwidths, from the simulations it seems that $V$ and $E-LR$ would be the versions of choice. Although they perform similarly in the simulation study, there are good theoretical reasons for preferring $E-LR$ as consistency can be guaranteed can be guaranteed for a large class of densities. Generally, the simulations show that the asymptotic results are of limited use for the sample sizes considered here (even for $n = 2500$!). This is not so much of a surprise since the asymptotic analysis is largely based on the law of the iterated logarithm.

5 Conclusions

The discrepancy principle is a fast and simple method of parameter choice that is also easy to implement. Although it is very popular in other branches of applied mathematics (namely in ill-posed problems theory), it has only rarely been used in density estimation. While there are many shortcomings – it is not optimal in any sense and it can even lead to inconsistent estimates for some densities with infinite peaks –, some variants do work surprisingly well for a large set of different

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[Devroye (1989)] which states that selecting the bandwidth using $L2CV$ will lead to $L_1$-inconsistent estimators for any sufficiently sharply peaked density is not applicable to density 19. However, Table 1 shows that $L2CV$ performs even worse than most versions of the discrepancy principle in our simulations (with the versions choosing larger bandwidths doing relatively better).
Table 2: Results of the simulation study: Estimated squared $L_2$ risk for kernel estimators

| Density | n  | L2CV | E-LR | V  | KS .5 | KS .95 | Kuip .5 | Kuip .95 | L2NR |
|---------|----|------|------|----|-------|--------|--------|---------|------|
| 1       | 100| 0.0774| 0.0726| 0.0755| 0.0939 | 0.152 | 0.0889 | 0.117 | 0.251 |
|         | 1000| 0.0205| 0.0248| 0.022 | 0.0295 | 0.0526 | 0.0245 | 0.0349 | 0.0215 |
|         | 2500| 0.012 | 0.0156| 0.013 | 0.0169 | 0.0299 | 0.0138 | 0.019 | 0.0122 |
| 6       | 100| 0.008 | 0.008 | 0.0082| 0.0129 | 0.0336 | 0.0111 | 0.0203 | 0.0529 |
|         | 1000| 0.0014| 0.0016| 0.0014| 0.0021 | 0.0055 | 0.0016 | 0.0027 | 0.0028 |
|         | 2500| 8e-04| 8e-04| 8e-04| 9e-04 | 0.0024 | 7e-04 | 0.0012 | 0.001 |
| 11      | 100| 0.0072| 0.007 | 0.0069| 0.0104 | 0.0342 | 0.0088 | 0.0177 | 0.037 |
|         | 1000| 0.0011| 0.0011| 0.0011| 0.0014 | 0.004 | 0.0011 | 0.0018 | 0.0036 |
|         | 2500| 6e-04| 6e-04| 6e-04| 7e-04 | 0.0017 | 6e-04 | 0.0012 | 0.0012 |
| 12      | 100| 0.0235| 0.0213| 0.0221| 0.0309 | 0.0639 | 0.0325 | 0.0541 | 0.1137 |
|         | 1000| 0.0043| 0.0049| 0.0044 | 0.0059 | 0.0118 | 0.006 | 0.0103 | 0.0063 |
|         | 2500| 0.0022| 0.0027| 0.0022| 0.0029 | 0.0058 | 0.003 | 0.0052 | 0.0025 |
| 13      | 100| 0.0039| 0.0039 | 0.0039| 0.0051 | 0.1017 | 0.0048 | 0.0086 | 0.1124 |
|         | 1000| 0.0124| 0.013 | 0.0137 | 0.017 | 0.0264 | 0.0148 | 0.0192 | 0.0126 |
|         | 2500| 0.0077| 0.0103| 0.0088 | 0.011 | 0.0169 | 0.0094 | 0.0122 | 0.0076 |
| 15      | 100| 0.3402| 0.2946| 0.3034 | 0.3663 | 0.5308 | 0.397 | 0.5167 | 0.7157 |
|         | 1000| 0.1059| 0.1104| 0.1043| 0.122 | 0.181 | 0.1338 | 0.1836 | 0.1262 |
|         | 2500| 0.0688| 0.075 | 0.0682 | 0.0784 | 0.1128 | 0.0862 | 0.1168 | 0.0788 |
| 22      | 100| 0.0124| 0.0119| 0.0125 | 0.0181 | 0.0337 | 0.0176 | 0.0263 | 0.0725 |
|         | 1000| 0.0021| 0.0028| 0.0023 | 0.0036 | 0.0081 | 0.0032 | 0.006 | 0.0034 |
|         | 2500| 0.0013| 0.0015| 0.0011 | 0.0017 | 0.0039 | 0.0014 | 0.0027 | 0.0013 |
| 23      | 100| 0.0536| 0.0546 | 0.0544 | 0.0572 | 0.0768 | 0.0561 | 0.0639 | 0.1051 |
|         | 1000| 0.0485| 0.034 | 0.0238 | 0.0457 | 0.0472 | 0.0319 | 0.0501 | 0.0074 |
|         | 2500| 0.0236| 0.0202 | 0.011 | 0.0244 | 0.05 | 0.014 | 0.0317 | 0.0033 |
| 24      | 100| 0.0444| 0.0547 | 0.0597 | 0.0856 | 0.127 | 0.0777 | 0.1073 | 0.0813 |
|         | 1000| 0.0116| 0.028 | 0.0239 | 0.034 | 0.0578 | 0.0269 | 0.0392 | 0.0117 |
|         | 2500| 0.0091| 0.0292 | 0.0153 | 0.022 | 0.0378 | 0.017 | 0.0248 | 0.0075 |
| 27      | 100| 0.0205| 0.0198 | 0.02 | 0.0211 | 0.0239 | 0.0208 | 0.0222 | 0.0185 |
|         | 1000| 0.0192| 0.0188 | 0.0146 | 0.0191 | 0.0192 | 0.0178 | 0.0176 | 0.0023 |
|         | 2500| 0.0171| 0.0123 | 0.007 | 0.0146 | 0.0181 | 0.0085 | 0.0174 | 0.0014 |

densities in simulations and consistency can – at least for some versions – be guaranteed for a large class of densities including all square-integrable ones. The simulations also show that the behavior of methods based on the discrepancy principle may be quite different from the asymptotic behavior even for sample sizes as large as $n = 2500$. Generally, asymptotic results do not help much in choosing the threshold function $s(n)$ – the most striking example being the $L_2$ normal reference version $L2NR$ which is guaranteed to asymptotically choose the $L_2$ optimal bandwidth for the normal distribution but performs very poorly even when the true density is the normal. Also taking into account the inconsistency for some densities (a problem that is actually shared by many popular bandwidth selectors), the method cannot be recommended in general.

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References

Aidu, F., and Vapnik, V. (1989), “Estimation of Probability Density on the Basis of the Method of Stochastic Regularization,” Automation and Remote Control, 50, 499–509.
Table 3: Results of the simulation study: Chosen Bandwidth

| Density | n  | L2CV | E-LR | V  | KS .5 | KS .95 | Kuip .5 | Kuip .95 | L2NR |
|---------|----|------|------|----|-------|--------|---------|---------|------|
| 1       | 100| 0.2267| 0.2206| 0.2443| 0.3609| 0.6297| 0.3342| 0.4784| 0.0292|
| 6       | 100| 1.1911| 1.1651| 1.2968| 1.9599| 3.0053| 1.7881| 2.6064| 1.438 |
| 8       | 100| 0.0862| 0.0439| 0.0946| 0.2425| 0.5993| 0.3342| 0.4784| 0.0292|
| 11      | 100| 0.9621| 0.9097| 1.0118| 1.4927| 2.4632| 1.7347| 1.9009| 0.977 |
| 12      | 100| 0.4389| 0.4123| 0.4865| 0.6981| 1.2262| 0.7236| 0.7321| 0.6845|
| 13      | 100| 0.4289| 0.4148| 0.4889| 0.7277| 1.3762| 0.6792| 0.9784| 0.0684|
| 15      | 100| 0.0903| 0.0631| 0.0703| 0.1044| 0.2223| 0.1286| 0.2116| 0.0113|
| 22      | 100| 0.8416| 0.8513| 0.9462| 1.3895| 2.3862| 1.3423| 1.937 | 0.1067|
| 23      | 100| 0.7869| 0.7691| 0.7671| 1.1304| 1.9354| 1.0402| 1.4971| 0.0718|
| 24      | 100| 0.7473| 0.7096| 0.8144| 1.2902| 2.7506| 1.1366| 1.815 | 0.097 |
| 27      | 100| 5.7691| 3.8767| 4.3972| 6.8032| 12.1572| 6.2664| 9.1095| 0.4075|

Table 3: Results of the simulation study: Chosen Bandwidth

Berlinet, A., and Devroye, L. (1994), “A Comparison of Kernel Density Estimates,” *Publications de l’Institute de Statistique de L’Universite de Paris*, 38, 3–59.

Bogachev, V. (2007), *Measure Theory. Volume 2.*, New York: Springer.

Cao, R., Cuevas, A., and González Manteiga, W. (1994), “A Comparative Study of Several Smoothing Methods in Density Estimation,” *Computational Statistics and Data Analysis*, 17, 153–176.

Celisse, A., and Robin, S. (2008), “Nonparametric Density Estimation by Exact Leave-p-Out Cross-Validation,” *Computational Statistics and Data Analysis*, 52, 2350–2368.

Davies, P.L. (1995), “Data Features,” *Statistica Neerlandica*, 49, 185–245.

Davies, P.L. (2008), “Approximating Data (with discussion),” *Journal of the Korean Statistical Society*, 37, 191–240.

Davies, P.L., Gather, U., Nordman, D.J., and Weinert, H. (2009), “A Comparison of Automatic Histogram Constructions,” *ESAIM: Probability and Statistics*, 13, 181–196.

Davies, P.L., and Kovac, A. (2004), “Densities, Spectral Densities and Modality,” *The Annals of Statistics*, 32, 1093–1136.
Devroye, L. (1989), “On the Non-Consistency of the $L_2$-Cross-Validated Kernel Density Estimate,” *Statistics and Probability Letters*, 8, 425–433.

Devroye, L. (1997), “Universal Smoothing Factor Selection in Density Estimation: Theory and Practice (with discussion),” *Test*, 6, 223–320.

Devroye, L., and Györfi, L. (1985), *Nonparametric Density Estimation. The $L_1$ View*, New York: Wiley.

Eggermont, P., and LaRiccia, V. (1996), “A simple and Effective Bandwidth Selector for Kernel Density Estimation,” *Scandinavian Journal of Statistics*, 23, 285–301.

Eggermont, P., and LaRiccia, V. (1997), “Nonlinearly Smoothed EM Density Estimation With Automated Smoothing Parameter Selection for Nonparametric Deconvolution Problems,” *Journal of the American Statistical Association*, 92, 1451–1458.

Eggermont, P., and LaRiccia, V. (2001), *Maximum Penalized Likelihood Estimation. Volume I: Density Estimation*, New York: Springer.

Hjort, N., and Walker, S. (2001), “A Note on Kernel Density Estimators with Optimal Bandwidths,” *Statistics and Probability Letters*, 54, 153–159.

Katznelson, Y. (2004), *An Introduction to Harmonic Analysis. Third Edition*, Cambridge: Cambridge University Press.

Markovich, N. (1989), “Experimental Analysis of Nonparametric Density Estimates and of Methods for Smoothing Them,” *Automation and Remote Control*, 50, 941–948.

Mildenberger, T. (2011), “Das Diskrepanzprinzip in der Nichtparametrischen Kurvenschätzung,” Ph.D. dissertation (in German), TU Dortmund University, Faculty of Statistics.

Mildenberger, T., and Weinert, H. (2012), “The benchden Package: Benchmark Densities for Nonparametric Density Estimation,” *Journal of Statistical Software*, 46, 1–14.

Mildenberger, T., Weinert, H., and Tiemeyer, S. (2012), *benchden: 28 Benchmark Densities from Berlinet/Devroye (1994)*, R package version 1.0.5.

Morozov, V.A. (1966), “On the Solution of Functional Equations by the Method of Regularization,” *Soviet Mathematics*, 7, 414–417.

Shapiro, H. (1969), *Smoothing and Approximation of Functions*, New York: Van Nostrand Reinhold.

Vapnik, V. (1998), *Statistical Learning Theory*, New York: Wiley.

Vapnik, V. (2000), *The Nature of Statistical Learning Theory. Second Edition*, New York: Springer.

Vapnik, V., and Stefanyuk, A. (1978), “Nonparametric Methods of Reconstructing the Probability Density,” *Automation and Remote Control*, 39, 1127–1140.

Wand, M., and Jones, M. (1995), *Kernel Smoothing*, Boca Raton: Chapman and Hall.

Yamamoto, H. (1973), “Uniform Convergence of an Estimator of a Distribution Function,” *Bulletin of Mathematical Statistics*, 15, 69–78.