Bandwidth selection for local linear regression: A simulation study

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Summary

This paper provides a simulation study of several popular bandwidth selectors for local linear regression. The study also includes two new selectors which couple the non-asymptotic plug-in and the unbiased risk estimation techniques. These two new selectors are simple to describe, easy to implement and performed very well in our simulation study.

Keywords: Bandwidth selection, Least-square cross-validation, Local linear regression, Plug-in, PURE

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1 Introduction

In the past decade, local polynomial regression has emerged as an attractive procedure for nonparametric function estimation. Particularly in the case of random $X$'s, it has superior bias and variance properties (e.g., Fan & Gijbels 1996, Section 3.2.1) as well as avoiding boundary bias problems suffered by other methods such as various versions of kernel estimators (e.g., Fan & Gijbels 1996, Section 3.2.5).

The bandwidth of course has a crucial effect on the quality of the estimator, and a number of methods have been developed for the automatic choice of bandwidth. A natural bandwidth selector is least-squares cross-validation (LSCV); for example, see Fan & Gijbels (1996, Section 4.10.2). In addition, various methods based on the plug-in idea have also been proposed. Gasser, Kneip & Köhler (1991) and Ruppert, Sheather & Wand (1995) developed plug-in bandwidth selection methods which rely on some asymptotic expressions (the former was developed for a different nonparametric estimator, but applies also to local linear regression), while Fan & Gijbels (1995) developed some plug-in bandwidth selection methods which rely on non-asymptotic expressions.

The aim of this paper is twofold. First, we introduce a new method which can be applied to construct bandwidth selectors. This method is based on a coupling of the non-asymptotic Plug-in and the Unbiased Risk Estimation techniques. We call our method PURE and our work was inspired by the work of Chiu (1992), as we describe further below.

The second goal of the paper is to evaluate the practical performance of our new method as well as those above-mentioned existing bandwidth selection methods by means of a simulation study.

The rest of this paper is organized as follows. Section 2 provides some background of local linear regression. Section 3 surveys four existing bandwidth selectors while Section 4 presents our PURE methodology. Results of a simulation study are reported in Section 5. Section 6 discusses a special application of our PURE methodology, and Section 7 concludes this paper. In the sequel we write $X_1^n = \{X_1, \ldots, X_n\}$ and $Y = (Y_1, \ldots, Y_n)^T$.

2 Local Linear Regression

Suppose we observe $n$ pairs of measurements $(X_i, Y_i)$, $i = 1, \ldots, n$, relating to the model

$$Y_i = m(X_i) + \epsilon_i,$$
where \( \varepsilon \) is an iid \((0, \sigma^2)\) noise while \( m(X) \) is an unknown function of interest. We suppose \( X_i \) is drawn at random from an unknown sampling density \( p(x) \) with a known compact support \([a, b]\). The local linear regression estimator \( \hat{m}_h(x) \) is obtained by fitting local straight lines (e.g., see Wand & Jones 1995, Chapter 5 or Fan & Gijbels 1996, Chapter 1) and is given by

\[
\hat{m}_h(x) = w_{x,h}^T Y,
\]

where

\[
\begin{align*}
w_{x,h} &= (w_{x,h}(X_1), \ldots, w_{x,h}(X_n))^T, \\
w_{x,h}(X_i) &= \frac{\{s_2,x,h - s_1,x,h(X_i - x)\} K_h(X_i - x)}{n \{s_2,x,h s_0,x,h - (s_1,x,h)^2\}}, \\
s_{r,x,h} &= \sum_{i=1}^n (X_i - x)^r K_h(X_i - x).
\end{align*}
\]

Here \( h \) is the bandwidth and \( K(\cdot) \) is a nonnegative kernel obeying the standard conditions: \( \int K(u) du = 1, \int u K(u) du = 0 \) and \( 0 < \mu_2 = \int u^2 K(u) du < \infty \). The function \( K_h(u) \) is defined as \( K_h(u) = \frac{1}{h} K(\frac{u}{h}) \). The bandwidth \( h \) controls the size of "features" or "bumps" in the unknown function that maybe discerned from the available noisy data. It might better be called a characteristic length or resolution width rather than a bandwidth.

Amongst others, there are two legitimate measures of estimator quality, namely, the mean integrated squared error (MISE) and the weighted mean integrated squared error (WMISE). Note that the latter sometimes is called the predictive integrated squared error and that the mean in both MISE and WMISE is taken over the distribution of \( \varepsilon \). Also, there are both conditional and unconditional versions of these two measures. The conditional versions are

\[
\begin{align*}
\text{MISE}_c &= \mathbb{E} \left[ \int \{m(x) - \hat{m}_h(x)\}^2 dx | X_1^n \right], \\
\text{WMISE}_c &= \mathbb{E} \left[ \int \{m(x) - \hat{m}_h(x)\}^2 \ p(x) dx | X_1^n \right]
\end{align*}
\]

while the unconditional versions are

\[
\begin{align*}
\text{MISE}_u &= \mathbb{E}(\text{MISE}_c) \quad \text{and} \quad \text{WMISE}_u = \mathbb{E}(\text{WMISE}_c).
\end{align*}
\]

Notice that all these four measures are unknown quantities as \( m \) is unknown. Most existing methods aim at minimizing one of the two conditional measures (MISE\(_c\) or WMISE\(_c\)). The primary concern of this paper is also the conditional versions, but we also discuss how to apply our PURE idea to construct bandwidth selectors which aim to minimize either MISE\(_u\) or WMISE\(_u\).

A remark: there are conflicting views regarding the question of whether one should consider the unconditional versions at all (e.g., see Jones 1991 for such
a discussion in the density estimation context). In order to allow the readers to form their own views, we shall keep both the conditional and unconditional versions in our paper.

To aid with the description of some existing bandwidth selectors we note the asymptotic expression for \( \text{WMISE}_c \) (e.g., Ruppert et al., 1995)

\[
\text{AWMISE}_c = \frac{h^4 \mu_2}{4} \int \{m''(x)\}^2 p(x)dx + \frac{\sigma^2 R(K)(b-a)}{nh}
\]

(1)

where \( R(K) = \int K^2(u)du \). From this expression we find the asymptotically optimal bandwidth for minimizing \( \text{AWMISE}_c \) is

\[
h_{\text{AWMISE}} = \left\lfloor \frac{\sigma^2 R(K)(b-a)}{n\mu_2^2 \int \{m''(x)\}^2 p(x)dx} \right\rfloor^{\frac{1}{2}}
\]

\[
= C_1(K) \left\lfloor \frac{\sigma^2(b-a)}{n\theta_{22}} \right\rfloor^{\frac{1}{2}},
\]

(2)

where \( C_1(K) = \{R(K)/\mu_2^2\}^{\frac{1}{2}} \) and for later use we have introduced the array

\[
\theta_{rs} = \int m^{(r)}(x)m^{(s)}(x)p(x)dx, \quad r, s \geq 0, \quad r + s \text{ even}.
\]

Again for later use we write down the following estimator, with a bandwidth \( g \), for \( \sigma^2 \):

\[
\hat{\sigma}_g^2 = \frac{1}{\nu} \sum_{i=1}^{n} \{Y_i - \hat{m}_g(X_i)\}^2.
\]

(3)

This is simply a normalized residual sum of squares and the normalizing quantity \( \nu \), sometimes known as the degrees of freedom, is given by \( \nu = n - 2 \sum_i w_{X_i,h}(X_i) + \sum_{i,j} w_{X_i,h}^2(X_i) \). Its presence guarantees \( E(\hat{\sigma}_g^2|X_1, \ldots, X_n) = \sigma^2 \) whenever \( m(x) \) is either constant or linear.

### 3 Existing Bandwidth Selection Methods

In this section we briefly survey four existing bandwidth selection methods.

**Least–Squares Cross–Validation:** Perhaps the most well-known bandwidth selection method is least–squares cross–validation. It selects the bandwidth \( h \) that minimizes the cross–validation score

\[
\text{CV}(h) = \sum_{i=1}^{n} \{Y_i - \hat{m}_{h,-i}(X_i)\}^2,
\]

(4)
where \( \hat{m}_{n, -1}(X_i) \) is the usual "leave-one-out" estimate of \( m(X_i) \).

**Asymptotic Direct Plug-In:** Ruppert et al. (1995) developed a "direct plug-in" bandwidth selection procedure which relies on the asymptotically optimal bandwidth expression (2). The idea is to plug-in estimates of \( \sigma^2 \) and \( \theta_{22} \) into expression (2), and obtain an estimate of \( h_{\text{awmss}} \) as the chosen bandwidth.

**Asymptotic Iterative Plug-In:** An "iterative plug-in" bandwidth selection procedure for the Gasser–Müller kernel estimator (Gasser & Müller 1984) was developed by Gasser et al. (1991). This iterative plug-in scheme can also be applied to local linear regression. As for the direct plug-in approach, it relies on the asymptotic expression (2); i.e., it also aims to minimize \( \text{WMISE}_c \). However, the asymptotic optimal bandwidth \( h_{\text{awmss}} \) is estimated in an iterative manner.

**Non-Asymptotic Plug-In:** Fan & Gijbels (1995) developed some bandwidth selection procedures which also involve the plug-in notion. However, there is a major difference between their plug-in procedures and the two asymptotic procedures mentioned above: in their procedures the plug-in idea is only applied to *non-asymptotic* expressions. The particular procedure developed by Fan & Gijbels that we are interested here is the so-called global refined bandwidth selector. However, in this paper we shall call it non-asymptotic plug-in.

### 4 PURE Bandwidth Selectors

In this section we present two new PURE bandwidth selectors, one aims to minimize \( \text{MISE}_c \) while the other aims to minimize \( \text{WMISE}_c \). We begin with the \( \text{MISE}_c \). It is straightforward to show the bias–variance decomposition

\[
\text{MISE}_c = \int \left\{ m(x) - w_{z,h}^T \hat{m} \right\}^2 dx + \sigma^2 \int w_{z,h}^T w_{z,h} dx.
\]

One way to construct an estimator of \( \text{MISE}_c \) is to plug-in pilot local linear estimates \( \hat{m}_g(x) \) and \( \hat{\sigma}_g^2 \) (see (3)) into the above expression, and obtain

\[
\tilde{\text{MISE}}_c = \int \left\{ \hat{m}_g(x) - w_{z,h}^T \hat{m}_g \right\}^2 dx + \hat{\sigma}_g^2 \int w_{z,h}^T w_{z,h} dx,
\]

where \( \hat{m}_g = (\hat{m}_g(X_1), \ldots, \hat{m}_g(X_n))^T \). For simplicity we suggest choosing the pilot bandwidth \( g \) by LSCV, and we use simple quadrature to calculate the integrals. Our PURE bandwidth selector which aims to minimize \( \text{MISE}_c \) chooses the bandwidth as the minimizer of \( \text{MISE}_c \).
Similarly we can estimate \( \text{WMISE}_c \) by

\[
\int \left\{ \hat{m}_g(x) - w_{x,h}^T \hat{m}_g \right\}^2 p(x) dx + \sigma_g^2 \int w_{x,h}^T w_{x,h} p(x) dx.
\]

Now the first term is still a problem since we do not know \( p(x) \). A second use of the plug-in principle gives the estimator

\[
\text{WMISE}_c = \frac{1}{n} \sum_{j=1}^{n} \left\{ \hat{m}_g(X_j) - w_{X_j,h}^T \hat{m}_g \right\}^2 + \sigma_g^2 \int w_{X,h}^T w_{x,h} p(x) dx.
\]

Our PURE bandwidth selector which aims to minimize \( \text{WMISE}_c \) chooses the bandwidth as the minimizer of \( \text{WMISE}_c \).

Thus, the general idea of our PURE methodology is that, we first obtain an exact and suitable expression (see below) for \( \text{MISE}_c \) (or \( \text{WMISE}_c \)), and then apply the non-asymptotic plug-in principle to obtain an estimate of \( \text{MISE}_c \) (or \( \text{WMISE}_c \)). For simplicity we recommend using LSCV to obtain the relevant pilot bandwidth(s). Our numerical experience suggests that LSCV is very reasonable for pilot bandwidth selection.

In the above when we said an “exact and suitable expression” for \( \text{MISE}_c \), we meant the expression should be non-asymptotic and should not contain “higher order” quantities like \( m'' \). As a result, our two PURE bandwidth selectors, unlike other plug-in bandwidth selectors, do not require the existence of \( m'' \).

We have the following remarks.

1. The PURE methodology can be easily extended to higher-order local polynomials.

2. Our procedure was inspired by the “double CV” method of Chiu (1992) for kernel density estimation. Chiu (1992) also estimates terms in an exact MISE formula. He obtains a simple pilot density estimator in which the pilot bandwidth (actually a cutoff frequency) is chosen by CV. This pilot estimator is plugged into the exact MISE formula, and the bandwidth for the main density estimator is chosen by minimizing the resulting MISE expression. The procedure is also described by Hall, Marron & Park (1992) and called smoothed CV by them. We rather see it as a smoothed unbiased risk estimation procedure.

3. There are several features of Chiu’s method that we think are important. Firstly it is easy to describe and simple to implement — just two density estimators are used and two bandwidths are chosen (no asymptotic expressions are needed). Further the method has the potential to be applied in more complex bandwidth selection problems for inverse problems, such as nonlinear ones, where asymptotic expressions may
not be available. Our procedure then has the same simplicity and ease of implementation as Chiu’s method since no asymptotic expressions are needed.

4. Chiu (1991) also discusses nonparametric function estimation but only for regularly gridded data. Also he does not give an automatic method to choose the pilot bandwidth. Thus we see our work as a natural extension of his density estimation procedure.

5. A referee pointed out that our PURE methodology is closely related to the “double smoothing” methods described in H"ardle, Hall & Marron (1992) and Wand & Gutiérrez (1997). However we have pushed the simple idea of using LSCV to choose the pilot, and backed up our suggestion by numerical results to be reported in the next section. We would also like to mention that our work was done independently.

6. To facilitate the following discussion, we first distinguish pilot function estimate from final function estimate: for the current PURE context the pilot function estimate is the LSCV local linear regression estimate \( \hat{m}_2 \) (see expression for MISE or WMISE), while the final function estimate is the local linear regression estimate obtained using the minimizer of MISE or WMISE as bandwidth. Work of H"ardle et al. (1992) on kernel regression suggests that an optimal asymptotic MISE rate of \( 1/\sqrt{n} \) cannot be achieved if both the pilot and final function estimates are of the same structure. This issue can be dealt with by using higher order kernels in the pilot estimation stage (a point missed by H"ardle et al. 1992). The equivalent change in local polynomial regression is to use higher order polynomials for pilot estimation (e.g., see Fan & Gijbels 1996). We have repeated our simulation study using a pilot function estimate with local cubic, and obtained very similar results, and hence we do not report them here.

5 Simulation Study

5.1 Settings

A simulation study was conducted to evaluate the practical performance of the proposed bandwidth selectors, as well as the four existing bandwidth selectors discussed in Section 3. Four Test Functions were used:

1: \( \sin(10\pi x) \), \( x \in [0, 1] \),
2: \( 1 - 48x + 218x^2 - 315x^3 + 145x^4 \), \( x \in [0, 1] \),
3: \( \sin(2x) + 2\exp(-16x^2) \), \( x \in [-2, 2] \),
4: \( x + 2\exp(-16x^2) \), \( x \in [-2, 2] \).
Test Functions 1 and 2 were used by Ruppert et al. (1995) while Test Functions 3 and 4 were used by Fan & Gijbels (1995). Also, Test Functions 1 and 4 are of the same structural form as two of the test functions used by Gasser et al. (1991). These four functions, together with their Fourier representations, are plotted in Fig. 1.

Three signal–to–noise ratios (snrs) and two design densities were used. That is, each Test Function was tested with six combinations of snr and design density. Here snr is defined to be the variance of the function divided by the variance of the noise: \( \text{snr} = \frac{\text{var}(m)}{\sigma^2} \). The three snrs were: low = 2, medium = 4 and high = 8, and the two design densities were the uniform density and \( p_0(x) = 6x(1-x)I_{\{0 \leq x \leq 1\}} \) (for Test Functions 3 and 4 we used an adjusted version of \( p_0(x) \)).

The design density \( p_0(x) \) was used by Hastie & Loader (1993). Note that \( p_0(x) \) provides a sparse design near the boundaries, and that results for \( p_0(x) \) cannot be generalized to other non–uniform random designs such as one that is having positive limits at boundaries.

The kernel that we used was Gaussian, hence we did not have a lot of problems with data sparseness. But if sparseness did occur for a particular simulated data set, we replaced it with a new set (we only needed to replace less than 5% of data sets). One could also use the interpolation methods of Hall & Turlach (1997) to handle this data sparseness problem.

For each combination of Test Function, snr and design density, 200 sets of simulated data were generated, and the number of data points \( n \) for each data set was 50. We used one \( n \) because \( n \) and snr are interchangeable, as the (asymptotic) performance depends only on the ratio \( \sigma^2/n \). This simple observation does not seem to have been emphasized before.

For each of these generated data sets, we computed the following automatically selected bandwidths:

\[
\begin{align*}
  h_{\text{PURE}} & : \text{PURE bandwidth selector which aims to minimize} \ M\text{ISE}_c, \\
  h_{\text{PUREW}} & : \text{PURE bandwidth selector which aims to minimize} \ W\text{MISE}_c, \\
  h_{\text{LSCV}} & : \text{least–squares cross–validation} \text{ bandwidth selector}, \\
  h_{\text{DAPI}} & : \text{direct asymptotic plug–in} \text{ bandwidth selector}, \\
  h_{\text{IAP1}} & : \text{iterative asymptotic plug–in} \text{ bandwidth selector}, \\
  h_{\text{NAPI}} & : \text{non–asymptotic plug–in} \text{ bandwidth selector}.
\end{align*}
\]
Figure 1: Plots of Test Functions. Plots in the left column, from top to bottom, are Test Functions 1 to 4 respectively. Plots in the right column are the corresponding Fourier representations, plotted in a log scale. Notice that for Test Function 1, its Fourier representation is a delta function.
5.2 Results: Uniform Random Design

For the uniform design, in addition to the above six automatically computed bandwidths, we also computed the optimal but unknown bandwidth $h_{\text{ISE}}$, defined as the minimizer of a discretized version of

$$\text{ISE}(h) = \int \{m(x) - \tilde{m}_h(x)\}^2 \, dx$$

(note for uniform design ISE = WISE; see Section 5.3 for definition of WISE).

We only present results corresponding to median snr, as results for high and low snrs are similar.

Fig. 2 displays the boxplots of the bandwidth ratios

$$\frac{(h - h_{\text{ISE}})/h_{\text{ISE}}}{h_{\text{ISE}}}$$

where $h$ is any of the six automatically selected bandwidths. Also, boxplots of the ISE ratios

$$\log \left\{ \frac{\text{ISE}(h)}{\text{ISE}(h_{\text{ISE}})} \right\}$$

are given in Fig. 3.

For Test Function 1, both $h_{\text{DAPL}}$ and $h_{\text{API}}$ had a strong tendency to oversmooth. In fact, for some simulated data sets, both $h_{\text{DAPL}}$ and $h_{\text{API}}$ were far too large to the extent that the obvious sinusoidal structure of Test Function 1 was completely smoothed out!

For Test Function 2, $h_{\text{API}}$ performed slightly worse than the others. It seems that $h_{\text{API}}$ tended to undersmooth.

For Test Functions 3 and 4, all bandwidth selectors gave similar performance, with the slight exception that, $h_{\text{API}}$ sometimes produced a large ISE ratio.

Perhaps the most interesting observation is that, for most cases the performance of $h_{\text{SCV}}$ was actually better than $h_{\text{DAPL}}$ and $h_{\text{API}}$. We will return to this observation later.
Figure 2: Boxplots of \((h - h_{\text{ISE}})/h_{\text{ISE}}\) for various \(h\), uniform random design and medium snr. In each panel, the boxplots correspond to (from left to right) \(h_{\text{PUREM}}\), \(h_{\text{PUREW}}\), \(h_{\text{LSCV}}\), \(h_{\text{DAP1}}\), \(h_{\text{API}}\) and \(h_{\text{NAPI}}\).

Figure 3: Boxplots of \(\log \{\text{ISE}(h)/\text{ISE}(h_{\text{ISE}})\}\) for various \(h\), uniform random design and medium snr. In each panel, the boxplots correspond to (from left to right) \(h_{\text{PUREM}}\), \(h_{\text{PUREW}}\), \(h_{\text{LSCV}}\), \(h_{\text{DAP1}}\), \(h_{\text{API}}\) and \(h_{\text{NAPI}}\).
5.3 Results: Non–Uniform Random Design

Here we report our results when the design density was $p_0(x)$. Again, we only report results corresponding to medium snr.

For each of the 200 simulated data sets, we computed the six automatically selected bandwidths, the optimal but unknown bandwidth $h_{\text{ISE}}$, and the optimal but unknown bandwidth $h_{\text{WISE}}$ which minimizes a discretized version of

$$\text{WISE}(h) = \int \{m(x) - \hat{m}_h(x)\}^2 p(x)dx.$$

That is, eight bandwidths were computed.

Figs. 4 and 5 display the boxplots of

$$(h - h_{\text{ISE}})/h_{\text{ISE}} \quad \text{and} \quad \log \{\text{ISE}(h)/\text{ISE}(h_{\text{ISE}})\}$$

respectively, while Figs. 6 and 7 display the boxplots of

$$(h - h_{\text{WISE}})/h_{\text{WISE}} \quad \text{and} \quad \log \{\text{WISE}(h)/\text{WISE}(h_{\text{WISE}})\}$$

respectively. Here $h$ is any of the six automatically selected bandwidths.

In general, the relative ranking of the six bandwidth selectors is roughly the same in terms of both ISE($h$) and WISE($h$). However, it seems that $h_{\text{MAP}}$ was inferior to other selectors, while $h_{\text{QAP}}$ performed well if WISE($h$) is the criterion for measuring quality. For $h_{\text{MAP1}}$, it performed well for Test Function 4, but poorly for Test Function 1. For other cases, we feel that the performance of the bandwidth selectors was similar.
Figure 4: Boxplots of $(h - h_{ISE})/h_{ISE}$ for various $h$ with design density $p_0(x)$ and medium snr. In each panel, the boxplots correspond to (from left to right) $h_{PUREM}$, $h_{PUREW}$, $h_{LSCV}$, $h_{DAP1}$, $h_{API}$ and $h_{NAPI}$.

Figure 5: Boxplots of $\log \{\text{ISE}(h)/\text{ISE}(h_{ISE})\}$ for various $h$ with design density $p_0(x)$ and medium snr. In each panel, the boxplots correspond to (from left to right) $h_{PUREM}$, $h_{PUREW}$, $h_{LSCV}$, $h_{DAP1}$, $h_{API}$ and $h_{NAPI}$. 
Figure 6: Boxplots of \((h - h_{\text{wise}})/h_{\text{wise}}\) for various \(h\) with design density \(p_0(x)\) and medium snr. In each panel, the boxplots correspond to (from left to right) \(h_{\text{purem}}\), \(h_{\text{purew}}\), \(h_{\text{lsCV}}\), \(h_{\text{dapi}}\), \(h_{\text{iapi}}\) and \(h_{\text{napi}}\).

Figure 7: Boxplots of \(\log\{\text{WISE}(h)/\text{WISE}(h_{\text{wise}})\}\) for various \(h\) with design density \(p_0(x)\) and medium snr. In each panel, the boxplots correspond to (from left to right) \(h_{\text{purem}}\), \(h_{\text{purew}}\), \(h_{\text{lsCV}}\), \(h_{\text{dapi}}\), \(h_{\text{iapi}}\) and \(h_{\text{napi}}\).
5.4 Empirical Conclusion

No bandwidth selector performed uniformly the best in our simulation. However, there are a few important empirical conclusions:

1. the selectors \( h_{\text{DAPM}} \) and \( h_{\text{IAPM}} \) sometimes ridiculously oversmooth,
2. the selectors \( h_{\text{DAPM}} \), \( h_{\text{IAPM}} \), and \( h_{\text{NASM}} \), which have been shown to have faster rate of convergence than \( h_{\text{LSCV}} \), do not outperform \( h_{\text{LSCV}} \) in our study, and
3. the two new selectors \( h_{\text{PUREM}} \) and \( h_{\text{PUREW}} \), even though not always the best, compare favorably with other selectors in virtually all cases.

6 Unconditional Versions

In this section we briefly discuss how to adopt our PURE methodology to construct a bandwidth selector which aims to minimize the unconditional version of MISE, i.e., \( \text{MISE}_u \). The case of \( \text{WMISE} \) can be tackled in a similar manner, and hence is omitted.

We first express \( \text{MISE}_u \) in a form so that the PURE methodology can be directly applied. Recall that \( \text{MISE}_u = E(\text{MISE}_c) \) and let \( X_1^* = \{X_1^*, \ldots, X_n^*\} \) be \( n \) independent draws from \( p(x) \). Direct calculations give

\[
\text{MISE}_u = E^* \left[ \int (m(x) - w_{x,h}^* m^*)^2 \, dx \right] + \sigma^2 \int E^* (w_{x,h}^* w_{x,h}^*) \, dx,
\]

where \( m^* = (m(X_1^*), \ldots, m(X_n^*))^T \) and \( w_{x,h}^* = (w_{x,h}(X_1^*), \ldots, w_{x,h}(X_n^*))^T \).

Now we need to obtain an estimator of \( \text{MISE}_u \), and this can be achieved by using the bootstrap.

Let \( X_1^{bn} = \{X_1^{bn}, \ldots, X_n^{bn}\} \) be the \( b \)th bootstrap sample obtained from the original observed \( X_i \)'s. That is, each of the \( X_i^{bn} \)'s is drawn from \( \{X_1, \ldots, X_n\} \) with replacement. A natural estimator of \( \text{MISE}_u \) is:

\[
\widehat{\text{MISE}}_u = \frac{1}{B} \sum_{b=1}^{B} \int (m(x) - w_{x,h}^{b*} m^*)^2 \, dx + \frac{\sigma^2}{B} \sum_{b=1}^{B} \int w_{x,h}^{b*} w_{x,h}^{b*} \, dx,
\]

where \( m^b \) and \( w_{x,h}^{b*} \) are defined similarly to \( m^* \) and \( w_{x,h}^* \) (with \( X_1^{*bn} \) replaced by \( X_1^{bn} \)), and \( B \) is the number of bootstrap replicates. Thus, if the aim is to minimize \( \text{MISE}_u \), we can choose the bandwidth as the minimizer of \( \text{MISE}_u \).

However, this bootstrap or unconditional PURE approach has one major drawback: it is extremely computational intensive. It is \( B \) times slower than the non-bootstrap or conditional PURE.
Efron & Tibshirani (1993, Chapter 18) discuss another bootstrap procedure for estimating WMISE suited to this context. Their procedure is more elegant in that the pilot bandwidth estimation is not needed. However, their procedure also has the same drawback as the bootstrap PURE procedure: it is extremely computational intensive.

To study the performance of the bootstrap PURE procedure and the bootstrap procedure of Efron & Tibshirani, we performed a small experiment. We generated 50 data sets from Test Function 1 with sur=4 and a uniform design density. Again, the number of data points for each data set was 50, but we used a different error measure, PSE(h) instead of ISE(h):

\[ \text{PSE}(h) = \sum_{i=1}^{200} (y_i^* - \hat{m}_h(x_i^*))^2, \]

where \((x_i^*, y_i^*), i = 1, \ldots, 200\), are new simulated “future” data.

For each generated data set, we computed five bandwidths: 1. \(h_{\text{PSE}}\) (the optimal bandwidth which minimizes PSE); 2. \(h_{\text{PUREM}}\) (non-bootstrap PURE); 3. \(h_{\text{LSCV}}\) (least-square cross-validation); 4. \(h_{\text{BOOT}}\) (bootstrap PURE); and 5. \(h_{\text{BEST}}\) (Efron & Tibshirani’s selector).

The results are displayed in a similar fashion as before: Fig. 8 displays the boxplots of the bandwidth ratios \((h - h_{\text{PSE}})/h_{\text{PSE}}\), and the boxplots of the PSE ratios \(\log(\text{PSE}(h)/\text{PSE}(h_{\text{PSE}}))\). Here \(h\) is any of the four automatically selected bandwidths. The results seem to suggest that the extra effort of bootstrapping does not improve the performance. However, this statement is far from conclusive.

7 Discussion

In this paper we surveyed four existing bandwidth selectors and proposed two new bandwidth selectors for local linear regression. All six selectors were empirically assessed by means of a simulation study. Numerical results demonstrate that the two proposed selectors compare favorably with other selectors.

Numerical results also suggest that, some plug-in bandwidth selectors appearing in the literature are in fact inferior to the LSCV selector, even though these plug-in selectors have been shown to possess better theoretical properties than the LSCV selector. This observation agrees with the study reported in Chiu (1996) in the context of density estimation.
Figure 8: Results concerning the bootstrap-based procedures. Left: boxplots of \((h - h_{PSE})/h_{PSE}\) for various \(h\). Right: boxplots of \(\log \{PSE(h)/PSE(h_{PSE})\}\) for various \(h\). In each panel, the boxplots correspond to (from left to right) \(h_{LSCV}, h_{PUMEM}, h_{BOOT}\) and \(h_{ET}\).

The two new bandwidth selectors are based on the method of coupling the non-asymptotic plug-in and the unbiased risk estimation techniques. This method is very easy to use and requires little theory to explain. Also, this method can be applied to more complex problems whereas asymptotic plug-in rely on analytic expressions for bias, variance and optimal bandwidth which will not always be available. Theoretical properties of our method will be described elsewhere, but one can expect results similar to those of Chiu (1992).

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References


