BANDWIDTH SELECTION FOR A CLASS OF DIFFERENCE - BASED VARIANCE ESTIMATORS IN THE NONPARAMETRIC REGRESSION: A POSSIBLE APPROACH

by

Michael Livine
Purdue University

Technical Report #05-05

Department of Statistics
Purdue University

April 2005

Bandwidth selection for a class of difference-based variance estimators in the nonparametric regression: a possible approach

M. Levine
Department of Statistics
Purdue University
West Lafayette, IN 47907
Tel.765-496-7571
Fax 765-494-0558

Abstract

A possible approach to bandwidth selection for difference-based variance estimators in the nonparametric regression is proposed. The approach is based on the crossvalidation-type idea modified for the case of correlated data. The method is compared to an alternative plug-in style method. Difficulties in implementing the latter are highlighted and it is argued that the proposed method represents a better alternative. Simulations for several models are given that illustrate good practical performance of the proposed method.

KEYWORDS: Bandwidth selection, crossvalidation, correlated data

1. INTRODUCTION

The model we consider in this article is the non-parametric regression model

$$y_i = g(x_i) + \sqrt{f(x_i)}\epsilon_i, i = 1, \ldots, n \tag{1}$$

where $g(x)$ and $f(x)$ are unknown mean and variance functions, respectively. It is assumed that $f(x) \in C^p$ belong to some functional smoothness classes. The errors ϵ_i, $i = 1, \ldots, n$ are independent standard normal random variables $N(0, 1)$. For convenience purposes, we further assume that $x \in [0, 1]$ and the (fixed) design is equispaced, t.i. $x_i = \frac{i}{n}$. Our problem of interest is estimating the variance function $f(x)$ in the presence of the (infinite dimensional) nuisance parameter $g(x)$.

It was pointed out in the late 1980's in [1] that variance (and not only the mean) estimation is also an important problem. As a practical example, we may need to construct confidence(prediction) intervals for the mean function or to analyze immunoassay(building prediction and calibration intervals) - either task will require an estimate of the variance. At first, only the mean was assumed to be functionally dependent on the predictor variable and the error variance was assumed to be constant. A few of the articles that dealt with estimating the constant variance are [18], [7], and [8]. The heteroscedastic case is a fairly recent research topic. Some notable publications dedicated to it are [15], [10], [6] and [3]. The functional nature of the variance means that different local estimation techniques,uch as local polynomial estimation, are needed. The author in his dissertation (see [14]) proposed a class of Nadaraya-Watson type local kernel estimators of the variance function.

It is well-known that for any kernel estimator to become a workable procedure it has to be accompanied by a bandwidth selection procedure. The traditional application field for the kernel estimation - estimation of the mean function in nonparametric regression - contains many different bandwidth selection procedures.

Two most common classes of those procedures are

- plug-in type procedures
- data-driven procedures that minimize some estimator of the mean squared error (MSE)

However, the same problem with respect to the kernel variance estimators has received scant attention so far.

In this article, we work with the variance estimation method described in [14]. First, we briefly describe the method. Next, we introduce a suitable crossvalidation-type method for use with this procedure. The next step is investigating its properties in Monte-Carlo settings. We will also show why an alternative approach via a plug-in type procedure does not seem to be a good option for our variance estimation approach although it is very attractive conceptually. As a sidenote, there are other possible nonconstant variance estimation procedures that have been suggested in recent years. We can mention, among others, the approach in [6] that is based on smoothing squared residuals from the local linear fit of the mean function. [16] uses a similar idea, only in place of local linear regression the Gasser-Müller kernel estimation is used. As for the bandwidth selection procedures, [6] uses the bandwidth selection method from [5]; as possible alternatives, the crossvalidation bandwidth rule or the plug-in approach of [20] are also mentioned. [16] (1994) uses a simple "leave-one-out" crossvalidation. Note that those are not methods designed specifically for the bandwidth selection in the variance estimation context: since the problem of variance estimation in both of the abovementioned articles is being reduced to the local linear regression, the methods used are the classical ones designed in the local polynomial regression setting.

2. METHOD DESCRIPTION

Once again, we consider a model (1). What follows is a brief review of the method to be used to estimate the variance. For a more detailed treatment of this subject please see [14].

Definition 2..1. A difference sequence of order r is a sequence of real numbers $d_i, i = 0, \ldots, r$ such that its elements sum up to zero:

$$\sum_{i=0}^{r} d_i = 0 \tag{2}$$

while the sum of squares is 1

$$\sum_{i=0}^{r} d_i^2 = 1 \tag{3}$$

The first step is to construct the building blocks for the variance estimator. We call them pseudoresiduals of order r and use the following definition.

Definition 2..2. A pseudoresidual of order r is

$$\Delta_i = \sum_{j=0}^{r-1} d_j y_{j+i} \tag{4}$$

where $\{d_i\}_{i=1}^{r}$ is a difference sequence as defined in (2) and (3).

Example The (unique) difference sequence of order 2 is $\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\}$. The corresponding pseudoresidual is $\Delta_i = \frac{y_i - y_{i-1}}{\sqrt{2}}$.

Remark 2..3. It is also possible to define the pseudoresidual Δ_i as being symmetric around y_i:

$$\Delta_i = \sum_{j=0}^{r-1} d_j y_{i-\left[\frac{r+1}{2}\right]+j+1} \tag{5}$$

Note that this choice does not influence any asymptotic results.

Next, we define the variance estimator as the weighted local average of the squared pseudoresiduals of order r. Each pseudoresidual is a normalized difference of $r+1$ observations; it can be viewed as the rough first-step estimate of the variance function $f(x)$. If this view is adopted, the next step of taking a weighted local average is nothing else but smoothing of several rough estimates to produce a more precise one. The following definition should provide a clear insight into the nature of this estimator.

Definition 2..4. Let us assume that the kernel function $K(\cdot)$ is a proper density on $[-1, 1]$. Then, the variance estimator of order r is defined as

$$\hat{f}_h(x) = \frac{\sum_{i=1}^{n-r} \Delta_{r,i}^2 K\left(\frac{x-x_i}{h}\right)}{\sum_{i=1}^{n-r} K\left(\frac{x-x_i}{h}\right)} \tag{6}$$

Remark 2..5. By definition, any kernel function $K(\cdot)$ must satisfy $\int K(u)\, du = 1$ but it need not be the proper density. (see, e.g. [11]). We can also define (6) with this more general kernel in mind. In such a case, the "best " bandwidth has to be defined in the minimax sense over a certain class of variance functions $\mathcal{F}$ and the rates of convergence are then different from those we obtain. The functional class $\mathcal{F}$ has to be wide enough to contain the set of twice continuously differentiable functions we use in this article. For example, we can assume that $\mathcal{F} = W_2^2$ - an L_2-based Sobolev space.

Remark 2..6. This estimator is conceptually equivalent to a NW kernel estimator though of course $\Delta_{r,i}^2$ are not independent.

Various properties of this estimator were derived in [14] including closed form expressions of the asymptotically optimal bandwidth and integrated mean squared error (MISE). Ignoring the higher-order bias terms that depend on r, [14] showed that for fixed r, $h \to 0$, $n \to \infty$ and $nh \to \infty$ the asymptotically optimal (in the sense of [17] and [19]) bandwidth $h \sim O(n^{-1/5})$ while $MISE \sim O(n^{-4/5})$. Unfortunately, these results do not provide us with a bandwidth selection algorithm which is an obvious priority before the method can be used in practice.

3. PLUG-IN APPROACH TO BANDWIDTH SELECTION

From [14], we know that the exact optimal bandwidth is

$$h = n^{-1/5} \left[\frac{C R_K \int f^2(x)\, dx}{2\sigma_K^4 \int [f''(x)]^2\, dx} \right]^{1/5} \tag{7}$$

where

$$C = 2 \left(2 \sum_{k=1}^{r} \left(\sum_{j=0}^{r-k} d_j d_{j+k} \right)^2 + 1 \right)$$

is the constant that depends on the chosen difference sequence $\{d_i\}$. (see [14]). The expression (7) contains quadratic functionals of the unknown variance function, namely $\int f^2(x)\, dx$ and $\int [f''(x)]^2\, dx$. A common notation for them is

$$R(f) \doteq \int f^2(x)\, dx \tag{8}$$

and

$$R(f'') \doteq \int [f''(x)]^2\, dx \tag{9}$$

(see,for example, [21]). Then, if some estimates of these functionals $\hat{R}(f)$ and $\hat{R}(f'')$ are available, the plug-in estimator of the optimal bandwidth h is

$$\hat{h} = n^{-1/5} \left[\frac{C R_K \hat{R}(f)}{2\sigma_K^4 \hat{R}(f'')} \right]^{1/5} \tag{10}$$

This suggests using (10) to derive a possible bandwidth selection method. However, we have not found this method to be practicable.

Remark 3..1. To help the reader to understand why this method cannot be applied easily note that already at this stage in order to estimate one unknown quantity (bandwidth h) we have to estimate two (functionals (8) and (9)).

It seems that estimating bandwidth by a plug-in method is a more complicated problem than the original problem of variance estimation itself. That makes the alternative approach that we consider in the next chapter all the more attractive.

4. CROSSVALIDATION APPROACH

The basic idea of any crossvalidation-type method is to estimate the true MISE (mean integrated squared error). By definition, MISE depends on the unknown function $f(x)$; thus, we want to have a data-driven estimator that mimics its behavior

In order to make it easier to follow we will use the notation $\hat{f}_h(x)$ to stress the fact that the variance function estimate depends on the bandwidth h. Remember that the integrated squared error is a global measure of risk defined as

$$MISE = \int E\,(\hat{f}_h(x) - f(x))^2\,dx \tag{11}$$

We will also introduce its discrete counterpart that we are going to call discrete mean squared error (DMSE)

$$DMSE = n^{-1}\sum_{i=1}^{n} E\,(\hat{f}_h(x_i) - f(x_i))^2 \tag{12}$$

Both (11) and (12) depend on the unknown variance function $f(x)$ and so we need to estimate them.

One possible way of estimating (11) can be briefly described as follows. Partition the data $\{x_i, y_i\}$ at random into K approximately equal and disjoint subsets. Each of these subsets consists of about k_j pairs where $\sum k_j = n$. Let the $\{\tilde{x}_i^j, \tilde{y}_i^j\}$, $i = 1, \ldots, k_j$ denote the pairs in the j_{th} subset with the values of $\tilde{x}_i^j$ arranged in ascending order; that is, $\tilde{x}_i^j \leq \tilde{x}_i^{j+1}$, $i = 1, \ldots, k_j - 1$. Similarly, let $\{x_i^j, y_i^j\}$, $i = 1, \ldots, n - k_j$ denote the pairs in the complement of the jth subset, again with the x_i^j arranged in ascending order. Using the terminology that originates in machine learning we call the

set $\{x_i^j\}$ the training dataset and the set $\{\tilde{x}_i^j\}$ a validation dataset. Now, let Δ_i^j, $\tilde{\Delta}_i^j$ denote the pseudoresiduals formed from $\{x_i^j, y_i^j\}$ and $\{\tilde{x}_i^j, \tilde{y}_i^j\}$, respectively. Then, let $\hat{f}_h^j$ denote the estimator derived from the jth subset $\{(x_i^j, y_i^j\}$ when using bandwidth h and squared pseudoresiduals $(\Delta_i^j)^2$. Unless stated otherwise, the superscript j will be omitted for the values of the argument x to simplify the notation.

We estimate the MISE as follows. First, define

$$CV^j(h) = \sum_{l=1}^{k_j} \left((\tilde{\Delta}_l^j)^2 - \hat{f}_h^j(\tilde{x}_l) \right)^2 \tag{13}$$

Then, the crossvalidation criterion is

$$CV(h) = \frac{1}{n} \sum_{j=1}^{K} CV^j(h) \tag{14}$$

As a final step of the algorithm, we choose as optimal bandwidth

$$h_{CV} = argmin_{h \in H} CV(h) \tag{15}$$

where $H \in [0, 1]$ is the finite grid that we use for simulation purposes.

The question about what happens to crossvalidation when the data is correlated has been partly investigated before. In particular, C.-K. Chu and J.S. Marron found (see [2]) that, in the case of "leave-one-out" crossvalidation (which corresponds to $K = n$) and positively correlated data, the crossvalidation will produce very small bandwidths resulting in undersmoothed estimates; on the other hand, if the observations are negatively correlated, then crossvalidation will produce very large bandwidths that result in oversmoothed estimates. It is unclear in general if the same happens for K-fold crossvalidation when $K < n$. Thus, our method may have properties that are somewhat different from the standard K-fold crossvalidation. It was established in [14] that for many potential applications only small values of r, such as $r = 2$ or $r = 3$ are needed. We conjecture that for small values of r the performance of this method will not be very different from that of the usual K-fold crossvalidation for fairly large data sets.

The following heuristics should help to understand why the algorithm described by (13)-(14) works. Note that the CV criterion as defined in (14)

gives

$$\begin{aligned}\frac{1}{n}\sum_{j=1}^{K}\sum_{l=1}^{k_j}[(\tilde{\Delta}_l^j)^2 - \hat{f}_h^j(\tilde{x}_l)]^2 &= \frac{1}{n}\sum_{j=1}^{K}\sum_{l=1}^{k_j}[(\tilde{\Delta}_l^j)^2 - f(\tilde{x}_l)]^2 + \\ \frac{1}{n}\sum_{j=1}^{K}\sum_{l=1}^{k_j}[f(\tilde{x}_l) - \hat{f}_h^j(\tilde{x}_l)]^2 &+ \frac{2}{n}\sum_{j=1}^{K}\sum_{l=1}^{k_j}[(\tilde{\Delta}_l^j)^2 - f(\tilde{x}_l)][f(\tilde{x}_l) - \hat{f}_h^j(\tilde{x}_l)]\end{aligned} \tag{16}$$

Looking at the terms one by one, we note that the first term in (16) does not depend on the bandwidth h. More precisely, it is easy to check that the first term on the right side of (16) behaves asymptotically as

$$2\int f^2(u)\,du + O(n^{-2}) \tag{17}$$

when $n \to \infty$. Thus, the first term is approximately a constant for large n

To check this, note that since $(\tilde{\Delta}_l^j)^2$ can be viewed as an estimator of the variance function $f(x)$ at the point $\tilde{x}_l$ the expected value of the first term in (16)

$$E\,[(\tilde{\Delta}_l^j)^2 - \hat{f}_h^j(\tilde{x}_l)]^2 \tag{18}$$

is the mean squared error of $\tilde{\Delta}_l^2$ as an estimator of $\hat{f}_h^j(\tilde{x}_l)$. Let us approximate $[(\tilde{\Delta}_l^j)^2 - f(\tilde{x}_l)]^2$ by its expectation

$$[(\tilde{\Delta}_l^j)^2 - f(\tilde{x}_l)]^2 \approx Bias^2(\tilde{\Delta}_l^j)^2 + Var\,(\tilde{\Delta}_l^j)^2 \tag{19}$$

The notation $\bar{y}_i \doteq y_i - g(x_i)$ (where i is the generic index)will be used for centered observations. Next, using the first-order Taylor formulas for both $f(x)$ and $g(x)$ we find

$$\begin{aligned}E\,(\tilde{\Delta}_l^j)^2 &= E\left[\sum_{j=0}^{r-1} d_j g(\tilde{x}_{j+l}) + \sum_{j=0}^{r-1} d_j \bar{y}_{j+l}\right]^2 \\ &= \left[\sum_{j=0}^{r-1} d_j \left(g(\tilde{x}_l) + g'(\tilde{x}_l + \delta_1)\frac{j}{n}\right)\right]^2 + f(\tilde{x}_l) + n^{-1}\sum_{j=0}^{r-1} j d_j^2 f'(\tilde{x}_l + \delta_2) \\ &\le f(\tilde{x}_l) + \frac{C_1}{n^2}\left(\sum_{j=1}^{r-1} j d_j^2\right)^2 + n^{-1}C_2\sum_{j=1}^{r-1} j d_j^2\end{aligned} \tag{20}$$

where $0 < \delta_i < 1$, $i = 1, 2$, $C_1 > 0$ and $C_2 > 0$ are constants that depends on the choice of $g(x)$ and $f(x)$ only. Thus, the squared bias of $(\tilde{\Delta}_l^j)^2$ is of the order $O(n^{-2})$ as $n \to \infty$.

Next, note that $(\tilde{\Delta}_l^j)^2$ is a scaled $\chi_1^2(0)$ where the scaling factor is equal to $f(\tilde{x}_l)$ plus the terms of the order $o(1)$. As a result, it is easy to check that the variance of the squared pseudoresidual $(\tilde{\Delta}_l^j)^2$ is

$$Var\,(\tilde{\Delta}_l^j)^2 = 2f^2(\tilde{x}_l) + O(n^{-2}). \tag{21}$$

(21) and the asymptotic behavior of the bias of $(\tilde{\Delta}_l^j)^2$ mean that (17) is true.

The second term is an approximation for the average integrated mean squared error (MISE) of the estimator $\hat{f}_h(x)$. If we can argue that the expected value of the third term goes to zero at the rate faster than the second, the minimizer of the left-hand side in (16) (the crossvalidation criterion as we defined it) can be expected to mimick the behavior of the minimizer of the mean squared error of $\hat{f}_h(x)$.

To analyze the third term, note that the estimator $\hat{f}_h^j(x)$ is the same as the generic variance estimator $\hat{f}_h(x)$ except that it is defined using not the entire data set of size n but only $n - k_j$ points $\{x_i^j\}$, $i = 1, \ldots, n - k_j$.

Thus, at any point $\tilde{x}_l$ from the validation data set we have

$$\hat{f}_h^j(\tilde{x}_l) = \frac{\sum_{m=1}^{n-k_j} (\Delta_m^j)^2 K\left(\frac{\tilde{x}_l - x_m}{h}\right)}{\sum_{m=1}^{n-k_j} K\left(\frac{\tilde{x}_l - x_m}{h}\right)} \tag{22}$$

Using the notation first introduced in [11], we denote

$$W(\tilde{x}_l - x_m) = \frac{K\left(\frac{\tilde{x}_l - x_m}{h}\right)}{\sum_{m=1}^{n-k_j} K\left(\frac{\tilde{x}_l - x_m}{h}\right)} \tag{23}$$

thus enabling us to write the estimator (22) in the form

$$\hat{f}_h^j(\tilde{x}_l) = \sum_{m=1}^{n-k_j} (\Delta_m^j)^2 W(\tilde{x}_l - x_m) \tag{24}$$

Remember that the pseudoresiduals Δ_m^j form an r-dependent sequence; this means that the number of those Δ_m^j that are correlated with $\tilde{\Delta}_l^j$ is $O(r)$. Let us represent (24) as

$$\hat{f}_h^j(\tilde{x}_l) = \hat{f}_{h,r}^j(\tilde{x}_l) + \hat{f}_{h,-r}^j(\tilde{x}_l) \tag{25}$$

where

$$\hat{f}_{h,r}^j(\tilde{x}_l) = \sum_{m \in J_1} (\Delta_m^j)^2 W(\tilde{x}_l - x_m) \tag{26}$$

and

$$\hat{f}^j_{h,-r}(\tilde{x}_l) = \sum_{m \in J_2} (\Delta^j_m)^2 W(\tilde{x}_l - x_m) \tag{27}$$

Here the index set J_1 includes those pseudoresiduals Δ^j_m that are correlated with $\tilde{\Delta}^j_l$. Clearly, the cardinality of this set is at most $O(r)$. The index set J_2 is its complement. Of course, $|J_1| + |J_2| = n - k_j$. The crossproduct term

$$C_{2n} = \frac{2}{n} \sum_{j=1}^{K} \sum_{l=1}^{k_j} [(\tilde{\Delta}^j_l)^2 - f(\tilde{x}_l)][f(\tilde{x}_l) - \hat{f}^j_h(\tilde{x}_l)] \tag{28}$$

can be now split into two terms:

$$\begin{aligned} C_{2n} &= \frac{2}{n} \sum_{j=1}^{K} \sum_{l=1}^{k_j} [((\tilde{\Delta}^j_l)^2 - f(\tilde{x}_l))(f(\tilde{x}_l) - \hat{f}^j_{h,-r}(\tilde{x}_l))] \\ &- \frac{2}{n} \sum_{j=1}^{K} \sum_{l=1}^{k_j} [((\tilde{\Delta}^j_l)^2 - f(\tilde{x}_l))\hat{f}^j_{h,r}(\tilde{x}_l)] \end{aligned} \tag{29}$$

It is easy to analyze the first term. The factors that comprise it are independent; also, as was pointed out before in (20), the bias of $(\tilde{\Delta}^j_l)^2$ as an estimator of $f(\tilde{x}_l)$ is of the order $O(n^{-1})$. At the same time, note that the second factor can be viewed as the bias of $\hat{f}^j_{h,-r}$ used as an estimator of $f(\tilde{x}_l)$. Since the cardinality of the set J_1 is $O(r)$, we can easily conclude that $|J_2| = O(n)$. Hence, this bias is asymptotically the same as the order of the bias of the regular estimator $\hat{f}_h(\tilde{x}_l)$: $E[f(\tilde{x}_l) - \hat{f}^j_{h,-r}(\tilde{x}_l)] = O(h^2)$. Consequently, choosing the usual optimal bandwidth $h = O(n^{-1/5})$ we find that

$$\begin{aligned} &E[(\tilde{\Delta}^j_l)^2 - f(\tilde{x}_l)][f(\tilde{x}_l) - \hat{f}_{h,-r}(\tilde{x}_l)] \\ &= E[(\tilde{\Delta}^j_l)^2 - f(\tilde{x}_l)]E[f(\tilde{x}_l) - \hat{f}_{h,-r}(\tilde{x}_l)] \\ &= O\left(\frac{1}{n}\right) O(h^2) = O\left(\frac{h^2}{n}\right) = O(n^{-7/5}) \end{aligned}$$

Thus, the first term in (29) goes to zero much faster than $O(n^{-4/5})$.

Analyzing the second term in (29), it is important to remember that $\hat{f}^j_{h,r}(\tilde{x}_l)$ is based on the finite number of terms only. Without loss of generality, it is possible to assume that the mean $g(x) \equiv 0$ for the purpose of this

analysis. Then, using the representation (26) for $\hat{f}_{h,r}(\tilde{x}_l)$, we find that

$$\begin{aligned}
&\sum_{l=1}^{k_j}(\tilde{\Delta}_l^j)^2 \hat{f}_{h,r}^j(\tilde{x}_l) \\
&= \sum_{l=1}^{k_j}(\tilde{\Delta}_l^j)^2 \sum_{k\in J_1}(\Delta_k^j)^2 W(\tilde{x}_l - x_k) \\
&= \sum_{l=1}^{k_j}\sum_{k\in J_1}\left(\sum_{p,q=0}^{r-1} d_p d_q \tilde{y}_{p+l} y_{q+k}\right)^2 W(\tilde{x}_l - x_k)
\end{aligned}$$

In order to estimate the expected value of the above, we will use the upper bound for the absolute sth moment of quadratic forms in independent random variables due to [22]. It allows us to conclude that

$$\begin{aligned}
&E\left(\sum_{p,q=0}^{r-1} d_p d_q \tilde{y}_{p+l} y_{q+k}\right)^2 \qquad (30)\\
&\leq C\sum_{p,q=0}^{r-1} d_p^2 d_q^2 (E\,\tilde{y}_{p+l}^4)^{1/4}(E\,y_{q+k}^4)^{1/4} \\
&= C\sum_{p,q=0}^{r-1} d_p^2 d_q^2 \sqrt{f(x_{p+l})f(x_{q+k})}
\end{aligned}$$

where the constant C depends on r and the choice of the difference sequence $\{d_i\}$. As the function $f(x)$ is bounded the expression (30) is bounded as well. This allows us to conclude that

$$\sum_{l=1}^{k_j}(\tilde{\Delta}_l^j)^2 \hat{f}_{h,r}^j(\tilde{x}_l) \leq C\sum_{l=1}^{k_j}\sum_{k\in J_1} W(\tilde{x}_l - x_k) \qquad (31)$$

for some constant C. By definition, the coefficients $W(\tilde{x}_l - x_k)$ are normalized and add up to one:

$$\sum_{k=1}^{n-k_j} W(\tilde{x}_l - x_k) = 1$$

Since the kernel function $K(\cdot)$ is assumed bounded, it is easy to see that asymptotically, as $n \to \infty$, each coefficient $W(\tilde{x}_l - x_k)$ behaves as $O(\frac{1}{n})$.

The number of observations in J_1 is finite (at most $O(r)$), and thus

$$\frac{1}{n}E\sum_{j=1}^{K}\sum_{l=1}^{k_j}(\tilde{\Delta}_l^j)^2\hat{f}_{h,r}^j(\tilde{x}_l) = O(1) \tag{32}$$

It was shown in [14] that the estimator $\hat{f}_{h,r}^j(x_l)$ is asymptotically consistent and, in particular,

$$\hat{f}_{h,r}^j(x) = f(x) + \frac{1}{\sqrt{n}}O_p(1) \tag{33}$$

As the variance function $f(x)$ is bounded, (33) means that the expected value of the product $f(x_l)\hat{f}_{h,r}^j(x_l)$ is bounded as well. This fact and (32) mean that the expectation of the second term in (29) is of the order $O\left(\frac{1}{n}\right)$. As the first term goes to zero much faster, the expectation of the entire crossproduct (16) is also of the order $O\left(\frac{1}{n}\right)$.

We know that the first term in (16) behaves as a constant asymptotically, the second term imitates MISE of the variance estimator $\hat{f}_h(x)$ and the third one tends to zero at the rate of $O(\frac{1}{n})$. Thus, minimizing the crossvalidation criterion CV(h) mimics equivalent to minimizing the MISE of the variance estimator $\hat{f}_h(x)$ and the minimizer of the crossvalidation criterion (14) mimics the behavior of the minimizer of the MISE of the variance estimator $\hat{f}_h(x)$.

5. THE FINITE SAMPLE PERFORMANCE OF THE METHOD AND THE CHOICE OF K: THE FIRST CASE STUDY

It is known from [14] (and earlier literature cited there) that the shape of the mean function is not important asymptotically as long as the minimal smoothness condition (the existence and continuity of the first derivative $g'(x)$) is satisfied. However, the mean function can become rather important in finite samples. The mean-function related bias term can be easily estimated for any sample size n. It was shown in [14] that asymptotically this term becomes approximately equal to

$$\frac{C(\{d_i\},r)[g'(x)]^2}{n^2} \tag{34}$$

where $C(\{d_i\},r)$ is the constant that depends on the choice of the difference sequence $\{d_i\}$ and its order r. It is possible to show that, given the order

r, the difference sequence can be uniquely selected in a way that minimizes the variance of the estimator (6) under the constraints (2) and (3). Such a sequence cannot be written down in the closed form but it is possible to calculate its elements for any order r; for details, see [14] and [8]. If this optimal difference sequence is chosen, the constant $C(\{d_i\}, r)$ becomes $\frac{(2r+1)(r+1)}{12}$ (see, for example [4]).

Example Suppose our variance function is constant: $f(x) \equiv 1$ while the mean function is such that it has large (in absolute value) first derivative; for example, let us define

$$g(x) = \begin{cases} 100x & \text{if } 0 \leq x < 1 \\ 0 & \text{otherwise} \end{cases} \tag{35}$$

Then, it is easy to check that for $n \approx 112$ the term (34) is of the same magnitude as the variance function (parameter to be estimated) itself; its absolute value is approximately equal to 1. Clearly, in this example the bias-related mean term is anything but negligible. □

Thus, it is important to investigate how our method will perform for finite samples. Another important issue is a choice of parameter K. The opinion prevailing in the literature (see, for example [12]) is that $K = 5$ or $K = 10$ should be used; however, it is better to run a test to see what the experience may suggest in our case.

In order to do this, we run a fixed model with different choices of K. We use a simple choice of smooth quadratic variance function $f(x) = (x-0.5)^2 + 0.5$ and a constant mean function $g(x) = \frac{3}{4}$. The design is equispaced and fixed; in other words, $x_i = \frac{i}{n}$, $i = 1, 2, \ldots, n$. We use three different sample sizes: first, $n = 500$, then $n = 1000$ and $n = 2000$ data points on $[0, 1]$. For each of the choices of n we try three different choices of K: $K = 5$, 10 and 15 successively. Results are shown in figures (1),(2) and (3). All of them employ the following convention.

On the X-axis are the values of the discreet oracle loss which is denoted

$$ODMSE = \min_{h \in H} n^{-1} \sum_{i=1}^{n} \left[\hat{f}_h(x_i) - f(x_i) \right]^2 \tag{36}$$

Here, ODMSE stands for Oracle Discreet Mean Squared Error. Of course, we can calculate ODMSE only because we work with the simulated data where $f(x)$ is known beforehand. The Y-coordinate is a crossvalidation DMSE (CDMSE) that is defined as

$$CDMSE = n^{-1} \sum_{i=1}^{n} \left[\hat{f}_{h_{CV}}(x_i) - f(x_i) \right]^2 \tag{37}$$

with h_{CV} defined by (15). Clearly, ODMSE $\leq$ CDMSE. The closer CDMSE is to the ODMSE, the better choice of the bandwidth has been made.

First, note that for the fairly low sample size of $n = 500$, increasing K seem to decrease slightly the variability of CDMSE values. At the same time, the method performance is also getting better (in case of $K = 15$, all values of CDMSE except for three outliers are less then 0.025 while for $K = 5$ the largest non-outlier value is above 0.03). This is not true for larger sample sizes, though. When $n = 1000$, we have values of CDMSE that are highly spread out. Increasing K does little to reduce the variability of CDMSE; only the choice of $K = 15$ seems to offer some improvement over $K = 5$, but the reduction isn't great. At the same time, the method performance as measured by the difference between ODMSE and CDMSE gets worse as K increases; when $K = 15$, the largest values of CDMSE are over 0.015 while for $K = 5$ they are (except for a very few outliers) staying close to 0.010. The same trends hold when sample size is $n = 2000$. In other words, increasing K does very little, if anything, to decrease the variability while making the method performance worse.

One of the few literary sources on the subject, [12] suggests $K = 5$ or $K = 10$ as an optimal choice. The argument goes that the choice of K is, probably, the matter of bias-variance tradeoff for the K-fold crossvalidation criterion as an estimator of the global mean squared error. Our empirical analysis suggests that, unless the sample size is quite small, $K = 10$ is, probably, the better option.

6. SECOND CASE STUDY

To test how well the method performs for different possible mean functions, the following study design was followed. We chose a smooth quadratic variance function

$$f(x) = \left(x - \frac{1}{2}\right)^2 + \frac{1}{2} \tag{38}$$

that remained fixed throughout this study. The mean function choices ranged from ones with the small mean-related bias term (34) to less smooth ones. Since this term, if measured globally over $[0, 1]$, is asymptotically proportional to the

$$R(g') = \int [g'(x)]^2 \, dx \tag{39}$$

we will use the quadratic functional (39) as a measure of the mean function influence on the variance estimation. Clearly, the larger (39) is, the more distortion the mean function would be expected to bring to the process.

Next we define a sequence of mean functions we use for our simulation study. Let us define first the indicator function

$$I(A) = \begin{cases} 1 & \text{if x} \in \text{A} \\ 0 & \text{otherwise} \end{cases} \tag{40}$$

for any set A. Then, the following choices are considered:

1. $g(x) = \frac{3}{4}$
2. $g(x) = (x + \frac{\sqrt{3}}{2})^2 * I(x < 0.5) + (\frac{2+\sqrt{3}}{2} - x)^2 * I(x > 0.5)$
3. $g(x) = \frac{3}{4} * \sin(16\pi\, x) + \frac{3}{4}$

The setup (1)-(3) is fairly logical. Function choices range from constant to the sinusoid (thus increasing the value of (39)). The mean function (1) is constant, thus all its derivatives and the functional (39) are equal to zero. Consequently, the mean-related bias term is also zero and the difference between the small sample and large sample performance of the method is, probably, not very large. This is clearly not the case for (2) and (3); it is easy to calculate the value of $R(g^{'})$ for each of them and find out that (39) is greater for (3) than it is for (2). Consequently, the finite sample performance is likely to be the best for (1) and the worst for (3)

As before, we consider an equidistant design with $x_i = \frac{i}{n}$, $i = 1, \ldots, n$ where the number of observations n is first assumed to be 500, then 1000 and, finally, 2000. We perform 100 simulations for each choice of n and use $K = 10$.

Definition 6..1. We define the oracle bandwidth as

$$h_o = \text{argmin}_{h \in H} DMSE(h) \tag{41}$$

and the crossvalidation bandwidth as before in (15)

Remark 6..2. The ODMSE, previously defined in (36), can be also described as $R_o = DMSE(h_o)$ while CDMSE is $R_{CV} = DMSE(h_{CV})$. As before, $R_{CV} \geq R_o$. The smaller (and closer to the oracle loss, respectively) the crossvalidation loss is, the better the performance of our method.

In the graphs (4)-(6), the oracle risk is shown using a straight line (and not 100 separate points for each simulation) to serve as a benchmark against which values of the crossvalidation risk are plotted. We show three graphs corresponding to the three possible mean function choices for each of the sample sizes $n = 500$, $n = 1000$ and $n = 2000$. In each panel, we move clockwise from (1) to (3).

Tables (1)-(2) summarize values of $R(g^{'})$ for each of the choices (1)-(3). It also gives the respective median oracle loss and median crossvalidation loss for every combination of the mean function (1)-(3) and the sample size. We report both ODMSE and CDMSE in the form of approximate 95% binomial confidence interval (Np_1, Np_2) where the percentiles $p_1 = 0.5 - \frac{1.96}{\sqrt{2n}}$, $p_2 = 0.5 + \frac{1.96}{\sqrt{2n}}$, and N is the number of simulations performed (which in our case is equal to 100).

Note that for different choices of the mean function the differences in ODMSE do not look statistically significant as the confidence intervals overlap strongly. This seems to be true for each of the three sample sizes considered. In other words, the oracle loss changes very little, if at all, with the introduction of a more complicated mean function.

It is not entirely clear at this stage what is the influence of the particular choice of the mean on the performance of the bandwidth selection method. There seems to be a tendency towards increased crossvalidation loss as the mean function curvature increases; however, the effect is not very pronounced. Tables (1)-(2) show that overlap between confidence intervals for CDMSE and ODMSE is still present for all choices of the mean function at any given sample size, although it becomes very small for quadratic and sinusoid mean functions for large $n = 1000$ and $n = 2000$. More extensive simulations with wider choice of the mean function are necessary to clarify this issue better.

7. THIRD CASE STUDY

Of course, the most important issue is whether the method performs well for variance functions of different smoothness. As a smoothness measure of the variance function the following quadratic functional is used:

$$R(f^{''}) = \int [f^{''}(x)]^2 \, dx \tag{42}$$

The reason for this choice is that the asymptotically optimal bandwidth for the estimator (6) is inversely proportional to (42). The larger (42) is, the

smaller the optimal bandwidth has to be chosen to pick up ever smaller details of the original function $f(x)$.

We use the following study design:

1. We assume that the mean function is constant; for example, $g(x) = \frac{1}{2}$ for $x \in [0, 1]$. Our main purpose here is to keep the asymptotic mean-related bias term equal to zero so that only the variance function $f(x)$ contributes to the mean squared error asymptotic expansion of the estimator (6)

2. We will consider several choices of the variance function $f(x)$. They are arranged in a "ladder" of possible candidates from the ones having small (42) to those with a larger value of this functional. The choices are:

   (a) $f(x) = (x - 0.5)^2 + 0.5$
   (b) $f(x) = 2(x - 0.5)^2 + 0.5$
   (c) $f(x) = 4(x - 0.5)^2 + 0.5$

As we move from (2a) to (2c), the value of (42) increases; as a consequence, we expect the bandwidth selection to become increasingly more difficult.

As in the first study, we specify the crossvalidation parameter as $K = 10$. The sample size is first $n = 500$, then $n = 1000$ and eventually $n = 2000$. The number of Monte-Carlo simulations for each possible combination of the sample size and variance function is 100. Tables (3)-(4) give some indication of the performance of the method, together with plots (7)-(9).

The first conclusion we can make is that, indeed, the median oracle loss (ODMSE) seems to grow as the variance function becomes more difficult to handle. For each of the three sample sizes, ODMSE grows as we move from (2a) to the (2c) options for the variance functions. Note also that the median crossvalidation loss (CDMSE) exhibits the same tendency, in effect mimicking the oracle loss.

It is fairly clear just from the visual inspection of the graphs (7)-(9) that the distance between ODMSE and CDMSE is larger for more complicated choices of the variance function. For example, for $n = 1000$ and the simplest choice of the variance function (2a) the ODMSE and CDMSE confidence intervals still have a small overlap of 0.00027. However, for (2b) they do not overlap at all and the same is true for (2c). The situation is exactly the same for $n = 2000$. These results suggest that CDMSE becomes an increasingly poor estimator of ODMSE as the degree of the variance function curvature increases.

Visually, the performance of the method seems to improve for larger sample sizes. This improvement looks to be rather slow for the fixed choice of the variance function $f(x)$ which seems to indicate similarity between our method and the classical "leave-one-out" crossvalidation. It is known that the relative rate of convergence of the crossvalidation-selected bandwidth estimator to the oracle bandwidth is $O(n^{-1/10})$ (for details, see [9]). We may conjecture that the similar phenomenon is at work here as well. More extensive simulations with the wider choice of possible variance functions $f(x)$ are probably needed here.

8. CONCLUSIONS

At this point, we have a workable method that allows us to select the bandwidth for the general variance function estimator (6). The method can be easily implemented using any statistical software and is intuitively appealing. The method is reasonably insensitive to fluctuations in the mean function $g(x)$; however, it does tend to break down for highly variable variance functions, as shown in Fig. (7), (8) and (9).

There are a lot of questions that remain unanswered for now and that need a careful investigation. A number of theoretical questions are raised by this research. To begin with, it is unclear what is the rate at which the bandwidth estimated by our method converges to the minimizer of the (11). There is very little research done so far on the K-fold crossvalidation (except when $K = N$ - the standard "leave-one-out" crossvalidation) even under the ordinary assumption of independent data, let alone in a case like ours that deals with correlated data. We know that in the case of "leave-one-out "crossvalidation" having positively correlated data results in choosing a bandwidth that is smaller than the minimizer of MISE while the opposite is true for the negatively correlated data (see [2]). It is sensible to assume that having correlated data also influences K-fold crossvalidation to a degree; however, a precise theoretical investigation is very much in order here. Another interesting question that merits further discussion is whether there possibly exists an optimal value of K such that it minimizes the MISE. In much of our development here we have used $K = 10$ on the basis of simulations shown in graphs (1), (2) and (3).

9. ACKNOWLEDGEMENTS

The author would like to thank his advisor, Prof. Lawrence D. Brown for his invaluable help while preparing this article.

References

[1] Carroll, R., and Ruppert, D. (1988) *Transformation and Weighting in Regression*, Chapman& Hall

[2] Chu, C.-K., and Marron, J. S. (1991) "Comparison of two bandwidth selectors with dependent errors," *The Annals of Statistics*, 19 , pp. 1906-1918

[3] Dette, H. (2002) "A consistent test for heteroscedasticity in nonparametric regression based on the kernel method", *Journal of Statistical Planning and Inference*, 103 (1-2), pp.311-329

[4] Dette, H., Munk, A., and Wagner, T. (1998) "Estimating the variance in nonparametric regression-what is a reasonable choice?" *Journal of the Royal Statistical Society*, Ser. B, 60, Part 4, pp. 751-764

[5] Fan, J., and Gijbels, I. (1995) "Data-driven bandwidth selection in local polynomial fitting: variable bandwidth and spatial adaptation," *Journal of the Royal Statistical Society*, Ser. B, 57, pp. 371-394

[6] Fan. J., and Yao, Q. (1998) "Efficient estimation of conditional variance functions in stochastic regression", *Biometrika*, 85, pp.645-660

[7] Gasser, U., Sroka, L., and Jennen-Steinmetz, C. (1986) "Residual variances and residual pattern in the nonlinear regression," *Biometrika*, 73, pp. 625-33

[8] Hall, P., Kay. J.W., and Titterington, D.M. (1990) "Asymptotically optimal difference-based estimation of variance in nonparametric regression," *Biometrika* , 77, pp.521-528

[9] Härdle, W., Hall, P., and Marron, J.S. (1988) "How far are automatically chosen regression smoothing parameters from their optimum? (with discussion)," *Journal of the American Statistical Association*, 83, pp. 86-101

[10] Härdle, W., and Tsybakov, A. (1997) "Local polynomial estimators of the volatility function in nonparametric autoregression", *Journal of Econometrics*, 81 , pp.223-242

[11] Härdle, W. (1990) *Applied Nonparametric Regression*, Cambridge University Press

[12] Hastie, T., Tibshirani, R., and Friedman, J. (2001) *The Elements of Statistical Learning*, Springer

[13] Jones, M.C., Marron, J.S., and Sheather, S.J. (1996) "A brief survey of bandwidth selection for density estimation," *Journal of the American Statistical Association*, 91, pp. 401-407

[14] Levine, M. (2003) "Variance estimation for nonparametric regression and its applications,", *PhD Dissertation*, University of Pennsylvania

[15] Müller, H.-G., and Stadtmüller, U. (1993) "On variance function estimation with quadratic forms", *Journal of Statistical Planning Inference*, 35, 213-231.

[16] Neumann, M. (1994) "Fully data-driven nonparametric variance estimators," *Statistics*, 25, pp. 189-212

[17] Parzen, E. (1962)"On estimation of a probability density function and mode," *Annals of Mathematical Statistics*, 33, pp.1065-1076

[18] Rice, J. (1984) "Bandwidth choice for nonparametric kernel regression," *Annals of Statistics*, 12, pp. 1215-30

[19] Rosenblatt, M. (1956)"Remarks on some nonparametric estimates of a density function, "Annals of Mathematical Statistics", 27, pp. 832-837

[20] Ruppert, D., Sheather, S.J.& Wand, M.P.(1995) "An effective bandwidth selector for local least squares regression," *Journal of the American Statistical Association*, 90, pp. 1257-70

[21] Wand, M.P., and Jones, M.C. (1995) *Kernel Smoothing*, Chapman&Hall

[22] Whittle, P. (1960) "Bounds for the Moments of Linear and Quadratic Forms in Independent Variables," *Theory of Probability and its Applications*, 5, pp. 302-305

Figure 1. Sample size $n = 500$
Figure 2. Sample size $n = 1000$
Figure 3. Sample size $n = 2000$
Figure 4. Sample size $n = 100$
Figure 5. Sample size $n = 1000$
Figure 6. Sample size $n = 2000$
Figure 7. Sample size $n = 500$
Figure 8. Sample size $n = 1000$
Figure 9. Sample size $n = 2000$

Table 1: Performance under the changing curvature of the mean function

		Median ODMSE					
Mean function	$R(g^{'})$	$n = 500$		$n = 1000$		$n = 2000$	
Constant	0	0.00390	0.00609	0.00215	0.00375	0.00124	0.00206
Quadratic	5.07	0.00395	0.00663	0.00226	0.00329	0.00124	0.00216
Sinusoid	$72\pi^2 \approx 710.61$	0.00357	0.00503	0.00204	0.00314	0.00107	0.00177

Table 2: Performance under the changing curvature of the mean function

		Median CDMSE					
Mean function	$R(g^{'})$	$n = 500$		$n = 1000$		$n = 2000$	
Constant	0	0.00512	0.00780	0.00292	0.00464	0.00168	0.00284
Quadratic	5.07	0.00482	0.00814	0.00318	0.00442	0.00203	0.00263
Sinusoid	$72\pi^2 \approx 710.61$	0.00405	0.00568	0.00299	0.00441	0.00162	0.00235

Table 3: Performance under the changing curvature of the variance function

		Median ODMSE					
Variance function	$R(f'')$	$n = 500$		$n = 1000$		$n = 2000$	
(2a)	4	0.00423	0.00695	0.00223	0.00342	0.00113	0.00175
(2b)	16	0.00579	0.01073	0.00337	0.00496	0.00209	0.00321
(2c)	64	0.01330	0.02189	0.00765	0.01117	0.00438	0.00645

Table 4: Performance under the changing curvature of the variance function

		Median CDMSE					
Variance function	$R(f'')$	$n = 500$		$n = 1000$		$n = 2000$	
(2a)	4	0.00532	0.00818	0.00315	0.00430	0.00165	0.00235
(2b)	16	0.00775	0.01396	0.00505	0.00676	0.00344	0.00516
(2c)	64	0.02220	0.02967	0.01308	0.01750	0.00775	0.01014

Figure 1:

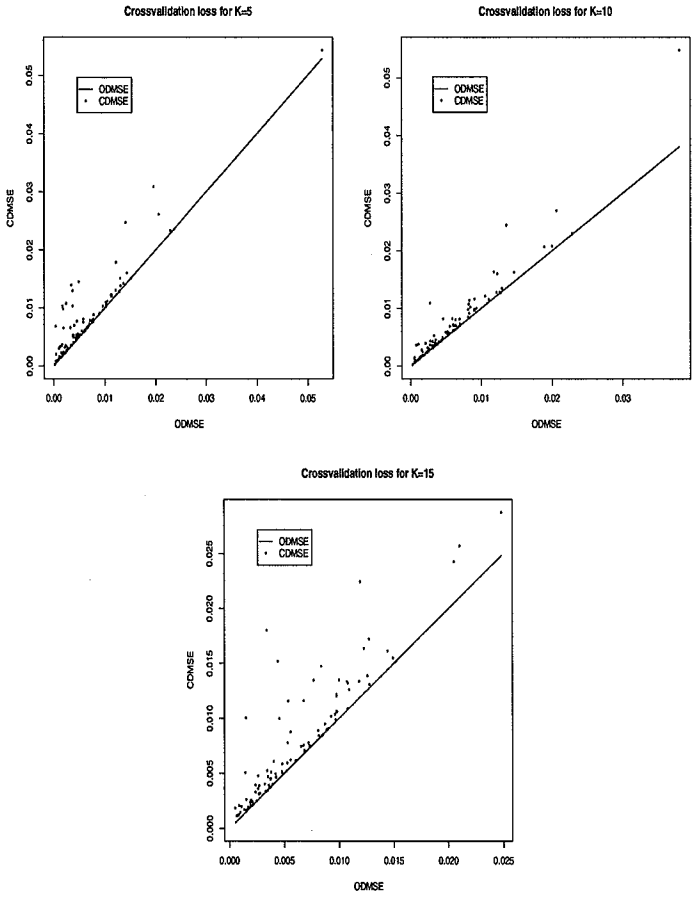

Crossvalidation loss for K=5
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation loss for K=10
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation loss for K=15
ODMSE
CDMSE
CDMSE
ODMSE

Figure 2:

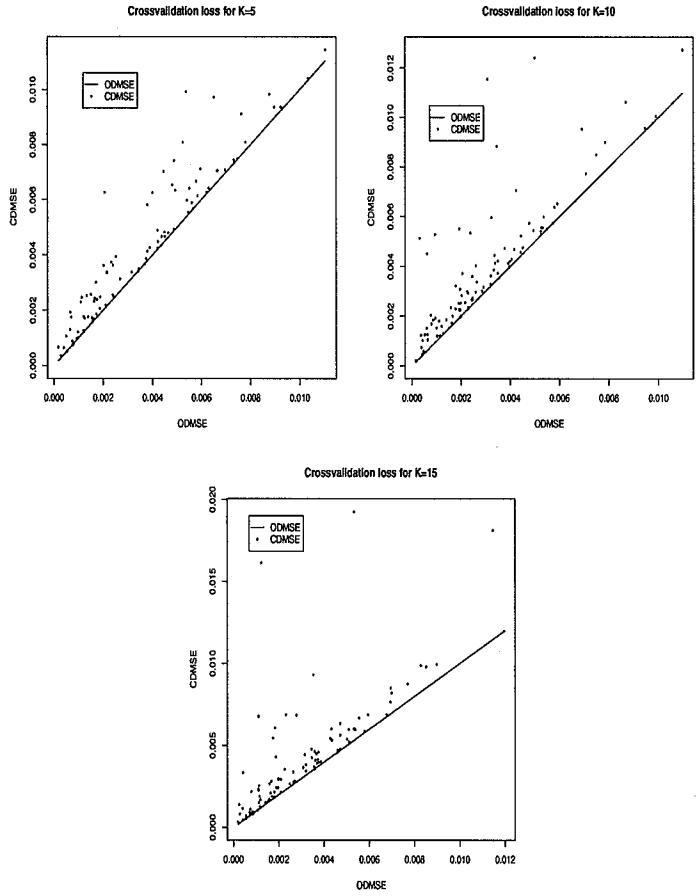

Crossvalidation loss for K=5
ODMSE
CDMSE
CDMSE
ODMSE
0.000
0.002
0.004
0.006
0.008
0.010
Crossvalidation loss for K=10
ODMSE
CDMSE
CDMSE
ODMSE
0.000
0.002
0.004
0.006
0.008
0.010
0.012
Crossvalidation loss for K=15
ODMSE
CDMSE
CDMSE
ODMSE
0.000
0.005
0.010
0.015
0.020
0.000
0.002
0.004
0.006
0.008
0.010
0.012

Figure 3:

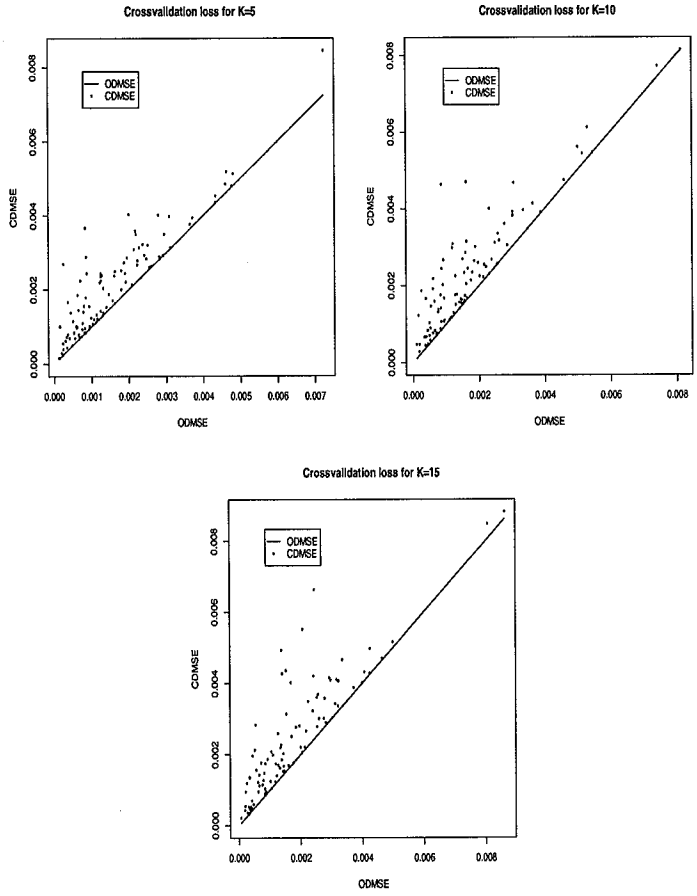

Crossvalidation loss for K=5
ODMSE
CDMSE
0.000
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
Crossvalidation loss for K=10
Crossvalidation loss for K=15

Figure 4:

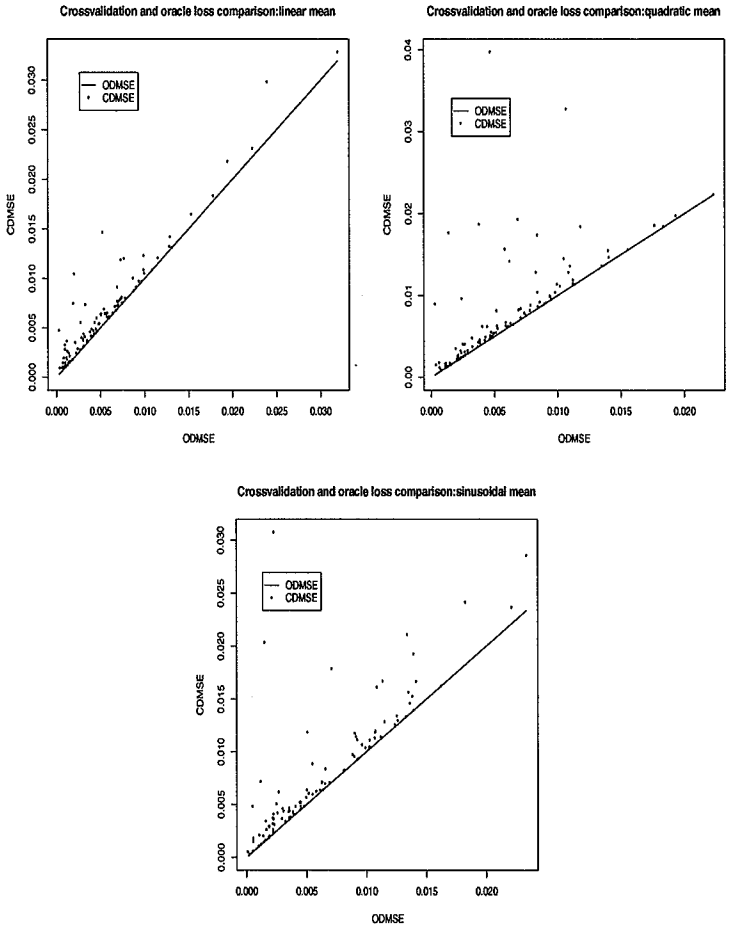

Crossvalidation and oracle loss comparison:linear mean
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation and oracle loss comparison:quadratic mean
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation and oracle loss comparison:sinusoidal mean
ODMSE
CDMSE
CDMSE
ODMSE

Figure 5:

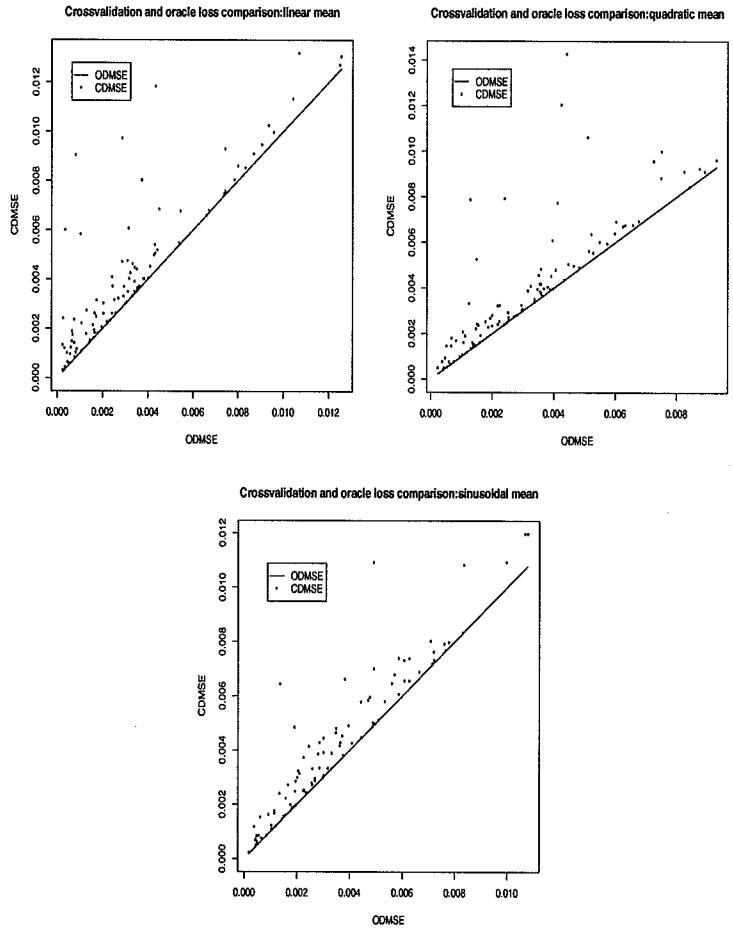

Crossvalidation and oracle loss comparison:linear mean
ODMSE
CDMSE
0.000
0.002
0.004
0.006
0.008
0.010
0.012
Crossvalidation and oracle loss comparison:quadratic mean
ODMSE
CDMSE
0.000
0.002
0.004
0.006
0.008
0.010
0.012
0.014
Crossvalidation and oracle loss comparison:sinusoidal mean
ODMSE
CDMSE
0.000
0.002
0.004
0.006
0.008
0.010
0.012

Figure 6:

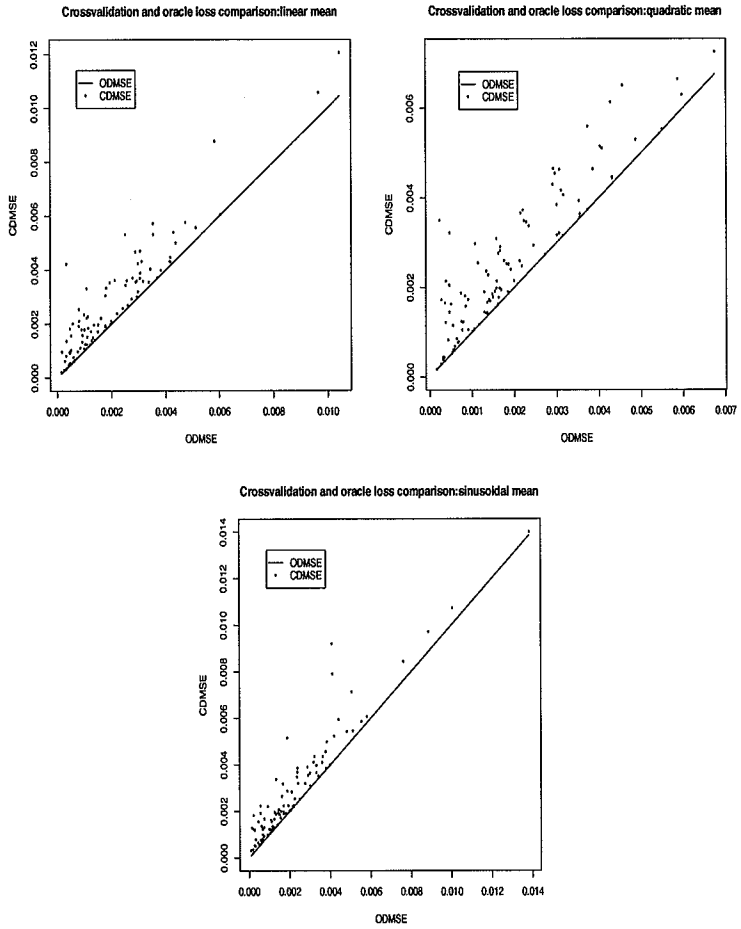

Crossvalidation and oracle loss comparison:linear mean
ODMSE
CDMSE
Crossvalidation and oracle loss comparison:quadratic mean
ODMSE
CDMSE
Crossvalidation and oracle loss comparison:sinusoidal mean
ODMSE
CDMSE

Figure 7:

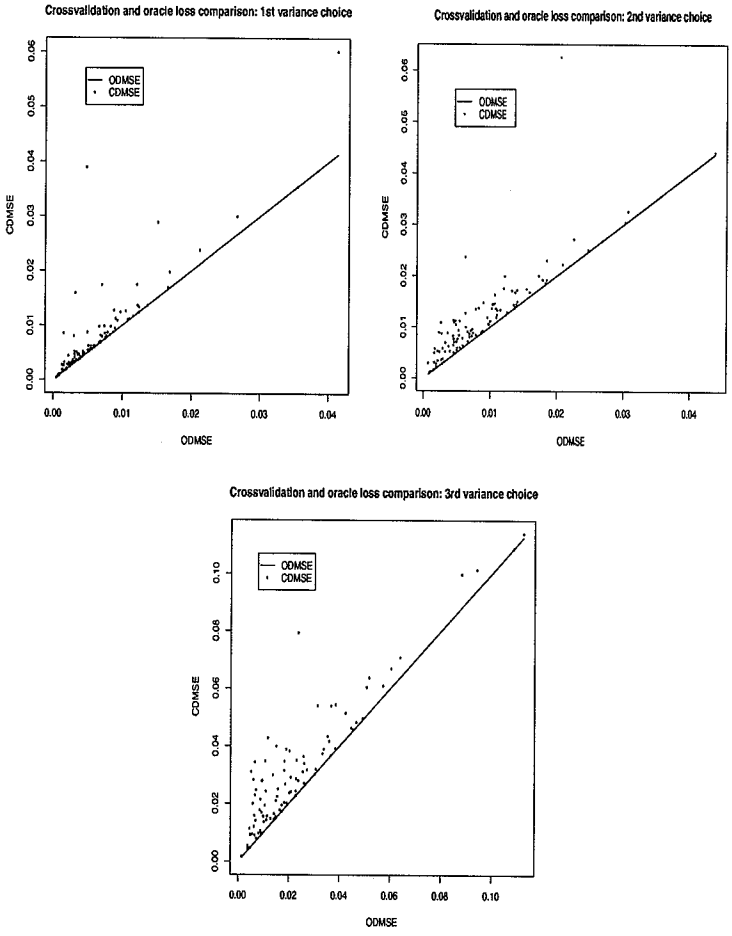

Crossvalidation and oracle loss comparison: 1st variance choice
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation and oracle loss comparison: 2nd variance choice
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation and oracle loss comparison: 3rd variance choice
ODMSE
CDMSE
CDMSE
ODMSE

Figure 8:

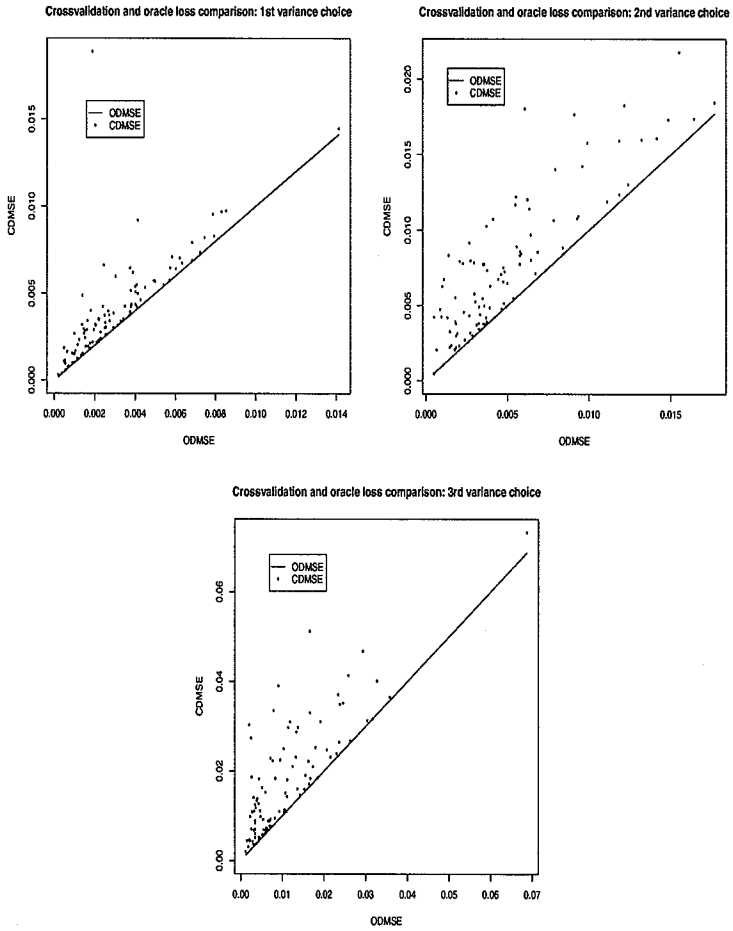
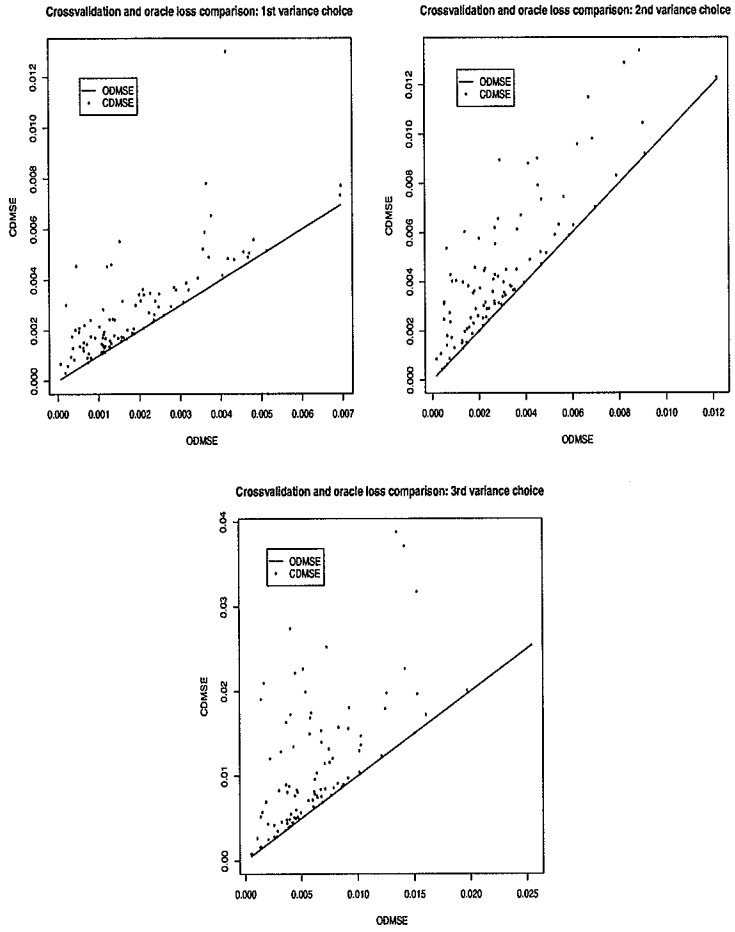

Crossvalidation and oracle loss comparison: 1st variance choice
ODMSE
CDMSE
0.000
0.005
0.010
0.015
0.000
0.002
0.004
0.006
0.008
0.010
0.012
0.014
CDMSE
ODMSE
Crossvalidation and oracle loss comparison: 2nd variance choice
ODMSE
CDMSE
0.000
0.005
0.010
0.015
0.020
0.000
0.005
0.010
0.015
CDMSE
ODMSE
Crossvalidation and oracle loss comparison: 3rd variance choice
ODMSE
CDMSE
0.00
0.02
0.04
0.06
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
CDMSE
ODMSE

Figure 9:


Crossvalidation and oracle loss comparison: 1st variance choice
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation and oracle loss comparison: 2nd variance choice
ODMSE
CDMSE
CDMSE
ODMSE
Crossvalidation and oracle loss comparison: 3rd variance choice
ODMSE
CDMSE
CDMSE
ODMSE