Partitioned Cross-Validation for Divide-and-Conquer Density Estimation

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Abstract

We present an efficient method to estimate cross-validation bandwidth parameters for kernel density estimation in very large datasets where ordinary cross-validation is rendered highly inefficient, both statistically and computationally. Our approach relies on calculating multiple cross-validation bandwidths on partitions of the data, followed by suitable scaling and averaging to return a partitioned cross-validation bandwidth for the entire dataset. The partitioned cross-validation approach produces substantial computational gains over ordinary cross-validation. We additionally show that partitioned cross-validation can be statistically efficient compared to ordinary cross-validation. We derive analytic expressions for the asymptotically optimal number of partitions and study its finite sample accuracy through a detailed simulation study. We additionally propose a permuted version of partitioned cross-validation which attains even higher efficiency. Theoretical properties of the estimators are studied and the methodology is applied to the Higgs Boson dataset with 11 million observations.

Key words. Big data; Bandwidth; Cross-validation; Kernel density estimate; Permutation
1 Introduction

With dramatic advances in data acquisition and storage techniques, modern applications routinely necessitate the analysis of massive datasets. Accordingly, there has been a flurry of recent activity in the analysis of big data (Jordan, 2013), with emphasis on the divide-and-conquer strategy. Broadly speaking, the divide-and-conquer approach splits the data into disjoint subgroups, performs statistical analyses on all subgroups, and pools together one or more statistics calculated from each subgroup to obtain global estimates. Such an exercise is typically necessitated when the statistical approach under consideration is computationally expensive to implement on the full dataset. The data may also be too big to load onto the memory on a single machine, or may be split across different administrative units. Recent statistical applications of the divide-and-conquer approach include parametric models (Li et al., 2013), bag of little bootstraps (Kleiner et al., 2014), kernel ridge regression (Zhang et al., 2015), semi-parametric heterogeneous models (Zhao et al., 2016) and parallel MCMC for Bayesian methods (Scott et al., 2016; Johndrow et al., 2015), among others. It has been recently observed that divide-and-conquer procedures can achieve minimax optimality in non/semi-parametric models (Zhang et al., 2015; Zhao et al., 2016), provided the smoothing parameters are chosen appropriately. However, theoretical justifications for choosing smoothing parameters in a fully data dependent fashion are yet to be developed in this context.

In this article, we focus on kernel density estimation (Silverman, 1986) for massive datasets. Given the linearity of kernel density estimates, such methods are naturally amenable to divide-and-conquer as simple averaging over partitions of the data suffice to compute a global estimate, provided the bandwidth parameter is specified. The choice of the kernel bandwidth is an ubiquitous problem to which a large literature has been devoted (Sheather, 2004). We specifically focus on the cross-validation (CV) approach (Hall and Marron, 1987) in this article. For big datasets, the CV criterion becomes prohibitively expensive to compute. With this motivation, we consider a partitioned cross-validation (PCV) approach which partitions the data into subgroups, calculates an ordinary CV bandwidth for each subgroup
and scales and averages these bandwidths to return a bandwidth for the entire data. The idea of PCV was first put forward by Marron (1987), who minimized the average of CV curves computed over different partitions. Our approach instead separately minimizes each CV curve to obtain a group specific CV bandwidth before averaging them. Although the relative ordering of averaging and minimizing has a negligible impact asymptotically, the proposed approach requires less communication between the different partitions and is therefore more amenable to parallelization. Moreover, since we only calculate CV bandwidths on partitions of the data, we obtain computational gains in orders of magnitude over ordinary CV. However, more interestingly, we exhibit that PCV can be statistically more efficient than ordinary CV. It is well known that the CV bandwidth converges to the (MISE) optimal bandwidth at the notoriously slow rate of $n^{-1/10}$. We argue that PCV can substantially improve this rate to $n^{-1/6}$. This behavior indicates that divide-and-conquer has a fundamentally broader statistical appeal than computational tractability alone.

We provide a default choice for the number of subgroups under normality which works well in practice for a wide range of densities. While not explored empirically, we additionally describe a model-averaging approach instead of using a fixed number of subgroups. The finite sample efficacy of PCV over ordinary CV is demonstrated through a number of replicated simulation studies. As a further improvement over PCV, we present a permuted PCV (PCVP) approach that calculates multiple PCV bandwidths on random permutations of the data. We theoretically and empirically demonstrate that permuted PCV can achieve substantial variance reduction compared to PCV. In fact, it can improve the PCV rate of convergence from $n^{-1/6}$ to $n^{-2/11}$. The PCV and permuted PCV approaches are applied to the Higgs Boson data, publicly available at the UCI machine learning repository, with eleven million samples.
2 Methodology

2.1 Partitioned cross-validation

Suppose one observes a random sample \( X_1, \ldots, X_n \) from a density \( f \). The usual kernel density estimator of \( f(x) \) is

\[
\hat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^{n} K \left( \frac{x - X_i}{h} \right),
\]

where \( K \) is an appropriate kernel function, usually a unimodal density that is symmetric about 0 and having finite variance, and \( h \) is a positive number called the bandwidth. We are interested in cases where \( n \) is so large that \( \hat{f} \) cannot be computed directly. The divide and conquer solution to this problem begins by randomly dividing the original data set up into \( p \) mutually exclusive and exhaustive subsamples of equal size. A kernel estimate, call it \( \hat{f}_h(\cdot \mid i) \), is computed from the \( i \)th subsample, \( i = 1, \ldots, p \), and an overall estimate of \( f \) is the average of these \( p \) kernel estimates.

Due to the linearity of the kernel estimate, note that

\[
\hat{f}_h \equiv \frac{1}{p} \sum_{i=1}^{p} \hat{f}_h(\cdot \mid i).
\]

An omnipresent problem associated with kernel estimators is that of choosing the bandwidth \( h \). A natural method of so-doing in our divide and conquer situation is that of partitioned cross-validation (PCV), as proposed by Marron (1987). Before going into detail about PCV, we note at this point just two things about the method: (i) it involves partitioning the data, as is done in divide and conquer, and (ii) it leads to a more efficient bandwidth selector than does ordinary, leave-one-out cross-validation. The second point is interesting as it shows that partitioning, rather than leading to a loss of efficiency in choosing a bandwidth, can actually lead to an increase in efficiency.

Before further discussion of PCV, it will be useful to review some aspects of optimal bandwidth choice and cross-validation. It will be assumed throughout this paper that \( f \) is square integrable and has two continuous derivatives everywhere.
As a loss function we employ integrated squared error (ISE):

\[ ISE(\hat{f}_h, f) = \int_{-\infty}^{\infty} (\hat{f}_h(x) - f(x))^2 \, dx. \]

The optimal bandwidth \( h_{n,0} \) is defined to be the minimizer of mean integrated squared error (MISE), i.e., \( MISE(\hat{f}_h, f) = E[ISE(\hat{f}_h, f)] \). It is well known (see, e.g., Silverman [1986]) that if \( n \) tends to \( \infty \),

\[ h_{n,0} \sim D n^{-1/5}, \quad D = \left[ \frac{R(K)}{R(f''(x)) \sigma_K^2} \right]^{1/5}, \]

(1)

where \( R(g) = \int g^2(x) \, dx \) for any square integrable function \( g \) and \( \sigma_K^2 \) is the variance of \( K \).

The leave-one-out cross-validation (CV) criterion is

\[ CV(h) = \int_{-\infty}^{\infty} \hat{f}_h^2(x) \, dx - \frac{2}{n} \sum_{i=1}^{n} \hat{f}_h(X_i), \quad h > 0, \]

where \( \hat{f}_h \) is a kernel estimate computed with the \( n - 1 \) observations other than \( X_i \). The CV bandwidth \( \hat{h} \) is the minimizer of \( CV(h) \). Hall and Marron (1987) show that

\[ n^{1/10} \left( \frac{\hat{h} - h_{n,0}}{h_{n,0}} \right) \xrightarrow{p} Z, \]

(2)

where \( Z \) is normally distributed with mean 0. This result shows that the CV bandwidth converges to the optimum bandwidth at the notoriously slow rate of \( n^{-1/10} \). Note that in our divide and conquer setting it is not possible to compute \( \hat{h} \) because of a prohibitively large value of \( n \).

Use of PCV, as proposed by Marron (1987), can improve upon the slow rate of convergence of the CV bandwidth. This result seems not to be very well known, but has important implications for the divide-and-conquer setting. Our version of PCV proceeds as follows:

- Given a random sample of size \( n \), randomly partition it into \( p \) groups of equal size.

- Compute the usual CV bandwidth for each group, and denote these bandwidths by \( \hat{b}_i, \ i = 1, \ldots, p \).
Each bandwidth \( \hat{b}_i \) estimates an optimal bandwidth for sample size \( n/p \), and so, as suggested by (1), bandwidths appropriate for a sample of size \( n \) are \( \hat{h}_i = p^{-1/5} \hat{b}_i, i = 1, \ldots, p \).

The PCV bandwidth is \( \hat{h}_{PCV} = \sum_{i=1}^p \hat{h}_i/p \).

PCV results in a bandwidth that is less variable, but more biased, than the CV bandwidth. However, it turns out that there are many choices of \( p \) such that the reduction in variance more than offsets the increase in squared bias, resulting in a bandwidth \( \hat{h}_{PCV} \) such that \( E \left[ \left( \hat{h}_{PCV} - h_{n,0} \right)/h_{n,0} \right]^2 \) converges to 0 at a faster rate than \( n^{-1/5} \), which is the corresponding rate for the CV bandwidth \( \hat{h} \).

The version of PCV proposed by Marron (1987) averages the CV criteria from the \( p \) groups, and then chooses a bandwidth to minimize the average criterion. We prefer our version since it requires no communication between groups. Results of Hall and Marron (1987) or Scott and Terrell (1987) entail that if \( n, p \) and \( n/p \) all tend to \( \infty \), then \( \text{Var}(\hat{h}_{PCV}) \sim A^* n^{-3/5} p^{-4/5} \) for a positive constant \( A^* \) defined in (11), and hence \( \text{Var}(\hat{h}_{PCV})/h_{n,0}^2 \) is asymptotic to \( Ap^{-4/5} n^{-1/5} \) for \( A = A^*/D^2 \). This asymptotic variance is identical to that obtained by Marron (1987) for his version of PCV.

Now consider

\[
E(\hat{h}_{PCV}) = h_{n,0} + B_{1,n,p} + B_{2,n,p},
\]

where

\[
B_{1,n,p} = p^{-1/5} h_{n/p,0} - h_{n,0} \quad \text{and} \quad B_{2,n,p} = E(\hat{h}_{PCV}) - p^{-1/5} h_{n/p,0}.
\]

Marron (1987) obtains an approximation to \( B_{1,n,p} \) that is of order \( n^{-3/5} p^{2/5} \), and implicitly assumes that \( B_{2,n,p} \) is of smaller order than \( B_{1,n,p} \). However, our Theorem 1 suggests that \( B_{2,n,p} \) is of larger order than \( B_{1,n,p} \). The rate of \( B_{2,n,p} \) is determined by the bias of the ordinary CV bandwidth as an estimator of \( h_{n,0} \). Because of the large variance of the CV bandwidth, this bias is small enough to ignore in the classic theory of the CV bandwidth (see (11)), but dictates the dominant bias term in PCV.
Scott and Terrell (1987) and Hall and Marron (1987) provide conditions under which

\[
\hat{h} - h_{n,0} = -\frac{CV'(h_{n,0})}{CV''(h_{n,0})} + o_p\left( \frac{CV'(h_{n,0})}{CV''(h_{n,0})} \right). \tag{4}
\]

Result (4) suggests that \( E(\hat{h} - h_{n,0}) \) may be approximated by applying the classic approximation of the expectation of a ratio of random variables to \( CV'(h_{n,0})/CV''(h_{n,0}) \).

Using the fact that \( E[CV'(h_0)] = 0 \), said classic approximation is

\[
E\left[ \frac{CV'(h_{n,0})}{CV''(h_{n,0})} \right] \approx \text{Cov}(CV'(h_{n,0}), CV''(h_{n,0}))/M''(h_{n,0})^2 = E[CV'(h_{n,0})CV''(h_{n,0})]/M''(h_{n,0})^2, \tag{5}
\]

where \( M(h) \equiv MISE(\hat{f}_h, f) \). Theorem 1 provides a first order approximation of (5).

**Theorem 1.** Suppose that \( K \) is a symmetric-about-0 density function satisfying the following:

1. The first two derivatives of \( K \) exist everywhere.
2. As \( u \) tends to infinity, both \( K(u) \) and \( K'(u) \) are \( o(\exp(-a_1u^{a_2})) \) for positive constants \( a_1 \) and \( a_2 \).

Assume also that the first three derivatives of \( f \) exist and are bounded and continuous. Letting \( \hat{h} \) and \( h_{n,0} \) be as defined earlier in this section,

\[
E[CV'(h_{n,0})CV''(h_{n,0})]/M''(h_{n,0})^2 = B^* n^{-2/5} + o(n^{-2/5})
\]

as \( n \to \infty \), where \( B^* \) is a positive constant defined by (28) in the Appendix.

Assuming that indeed \( E(\hat{h}) = h_{n,0} - B^* n^{-2/5} + o(n^{-2/5}) \), we have

\[
B_{2,n,p} = -B^* n^{-2/5} p^{1/5} + o(n^{-2/5} p^{1/5})
\]

as \( n, p \) and \( n/p \) tend to \( \infty \). This entails that

\[
E\left[ \frac{\hat{h}_{PCV} - h_{n,0}}{h_{n,0}} \right]^2 \sim An^{-1/5} p^{-4/5} + Bn^{-2/5} p^{2/5}, \tag{6}
\]
with \( B = (B^*/D)^2 \). The asymptotically optimal \( p \) minimizes (6) and equals \((2A/B)^{5/6}n^{1/6}\).

The optimal rate of convergence of \( \hat{h}_{PCV} \) is \( n^{-1/6} \), a substantial improvement over the rate of \( n^{-1/10} \) for the CV bandwidth.

The asymptotically optimal \( p \) has the form \( Cn^{1/6} \), where \( C \) depends on \( A \) and \( B \). These constants depend on the kernel \( K \) and the unknown density \( f \). The dependence on \( K \) is not problematic, but dependence on \( f \) potentially is. However, our experience is that the latter dependence is not a big problem. The range of choices for \( p \) that lead to an improvement over ordinary CV is so large that it is not difficult to find a value of \( p \) that works reasonably well. We have had success using a “normal reference” choice for \( C \). In other words, we use the value of \( C \) for the case where \( f \) is normal. This value, call it \( C_N \), is 5.51. Interestingly, \( C \) is invariant to the location and scale of \( f \), so \( C \) is parameter-free for any specified location-scale family. Although \( C_N \) is not generally optimal, we have found that it is usually close enough to optimal to deliver a substantial improvement over ordinary CV. Furthermore, since \( C_N n^{1/6} \) has the correct rate, it will deliver an asymptotic improvement over CV.

It is conceivable that \( n \) is so large that a kernel estimate cannot be computed from a sample size of \( C_N n^{1/6} \). In such a case one could simply take \( p \) so that \( n/p \) is the largest sample size that still allows computation of the kernel estimate.

### 2.2 Using more partitions

It seems unsatisfactory that the PCV bandwidth should be determined by a particular ordering of the data. In principle one could determine all possible partitions (for given \( p \)), compute a PCV bandwidth for each partition, and then average the resulting bandwidths. This idea was put forward in the article of Marron [1987]. Of course, there are far too many partitions for this to be feasible in practice. Instead one may choose some manageable number of random partitions. Choosing a precise number of partitions is not so important since any number of partitions greater than 1 will result in a bandwidth with smaller asymptotic variance than that of a PCV bandwidth based on a single partition. As stated in Theorem 2 below, if one uses a
number of partitions equal to $N$ at every sample size $n$, then the asymptotic variance of the average of the $N$ PCV bandwidths is $AV_1/N$, where $AV_1$ is the asymptotic variance of $\hat{h}_{PCV}$. However, there is a limit to the rate at which the variance can tend to 0, and the limit is $AV_1/p$. This asymptotic variance is attained when $N$ tends to infinity and is of larger order than $p$. If $N$ is taken to be $rp$ for a constant $r$, then the asymptotic variance is $(1 + r^{-1})AV_1/p$.

**Theorem 2.** Suppose that the first four derivatives of $f$ exist and are bounded and continuous. Assume also that $K$ satisfies the conditions of Theorem 1. Define $\bar{h}_N$ to be the average of PCV bandwidths computed from $N$ random permutations of the data $X_1, \ldots, X_n$. Then if $p$ tends to $\infty$ with $p = o(n^{4/9})$,

$$\lim_{n \to \infty} \frac{\text{Var}(\bar{h}_N)}{\text{Var}(\hat{h}_{PCV})} \cdot \left[ \frac{1}{N} + \frac{(N - 1)}{Np} \right]^{-1} = 1.$$  

We may use Theorem 2 to determine the optimal rate at which $\bar{h}_N$ converges to the optimal bandwidth $h_{n,0}$. If $N$ tends to $\infty$ at a faster rate than $p$, then

$$E \left[ \frac{(\bar{h}_N - h_{n,0})}{h_{n,0}} \right]^2 \sim An^{-1/5}p^{-9/5} + Bn^{-2/5}p^{2/5}. \tag{7}$$

This implies that the asymptotically optimal choice of $p$ is

$$p = \left( \frac{9A}{2B} \right)^{5/11} n^{1/11},$$

and the optimal rate of convergence for $\bar{h}_N$ is $n^{-2/11}$. Recall that the optimal rates for ordinary cross-validation and PCV are $n^{-1/10}$ and $n^{-1/6}$, respectively.

### 2.3 Unequal group sizes

When PCV is used to deal with a single massive data set that makes ordinary computation infeasible, it seems natural to partition the data set into groups of equal size. However, in some cases (an example of which is seen in Section 5) it may be impossible or impractical to use equal group sizes, and hence it is of interest to determine what effect this has on PCV. Suppose that $p$ different kernel
estimates and $p$ different cross-validation scores are computed, and that the results are combined to obtain a single density estimate. Let the $p$ data sets have sample sizes $n_1 < \cdots < n_p$ with $n = \sum_{i=1}^{p} n_i$. Applying CV to group $i$ yields a bandwidth $\hat{b}_i$, which is adjusted for sample size yielding $\hat{h}_i = (n/n_i)^{-1/5} \hat{b}_i$, $i = 1, \ldots, p$. The asymptotic variance of $\hat{h}_i$ is proportional to $n_i^{-1/5} n^{-2/5}$ as $n_i$ and $n$ tend to $\infty$, $i = 1, \ldots, p$. The weighted average of $\hat{h}_1, \ldots, \hat{h}_p$ that minimizes asymptotic variance has weights that are inversely proportional to variances, and hence we propose using the bandwidth

$$\hat{h} = \frac{\sum_{i=1}^{p} n_i^{1/5} \hat{h}_i}{\sum_{i=1}^{p} n_i^{1/5}}.$$  

(8)

To determine the asymptotic mean squared error of $\hat{h}$ we need to make an assumption about how the sample sizes behave for large $n$. We will assume that the sizes are balanced in a certain sense. Let $Q$ be the quantile function of $Y$, a positive, absolutely continuous random variable with finite mean $\mu$. We assume that

$$n_i = \frac{n Q(i/p)}{\sum_{j=1}^{p} Q(j/p)}, \quad i = 1, \ldots, p.$$

It is straightforward to argue that both the variance and bias of $\hat{h}$ depend on $n_1, \ldots, n_p$ only through $\sum_{i=1}^{p} n_i^{1/5}$. Defining $\mu_{1/5} = E(Y^{1/5})$, we have

$$\sum_{i=1}^{p} n_i^{1/5} \sim p^{1/5} n^{1/5} \frac{\mu_{1/5}}{\mu^{1/5}}$$

as $p$ and $n$ tend to $\infty$ with $p = o(n)$.

Finally, applying previous results, we have

$$E \left[ \frac{(\hat{h} - h_{MISE})}{h_{MISE}} \right]^2 \sim An^{-1/5} p^{-4/5} \left( \frac{\mu_{1/5}}{\mu_{1/5}} \right) + Bn^{-2/5} p^{2/5} \left( \frac{\mu_{1/5}}{\mu_{1/5}} \right)^2,$$

where $A$ and $B$ are the same constants as in [6].

### 2.4 Model averaging as an alternative to choosing group size $p$

In Section 2.1 we suggested choosing $p$ to be the value, $C_N n^{1/6}$, that is asymptotically optimal when the underlying density is normal. This is analogous to using a normal
reference bandwidth, although the choice of $p$ is arguably not so crucial since it has only a second order effect on the bandwidth. Nonetheless, to protect against the possibility that $Cn^{1/6}$ is far from an optimal choice for $p$, one may use a form of model averaging wherein bandwidths arising from different choices of $p$ are averaged.

The asymptotically optimal choice of $p$ has the form $Cn^{1/6}$. To gain insight about what sort of model averaging would be appropriate, we study how the optimal constant $C$ varies with density $f$. As a functional of $f$, $C$ is proportional to

$$\frac{\left[\int (f''(x))^2 \, dx\right]^{1/6}}{\left[\int f^2(x) \, dx\right]^{5/6}}. \quad (9)$$

We study the distribution of $C$ by randomly generating normal mixtures, each of which has the form

$$f(x) = \sum_{i=1}^{M} w_i \frac{1}{\sigma_i} \phi \left( \frac{x - \mu_i}{\sigma_i} \right).$$

The densities were generated as follows:

- A value of $M$ between 2 and 20 is selected from a distribution such that the probability of $m$ is proportional to $m^{-1}$, $m = 2, \ldots, 20$.

- Given $m$, values $w_1, \ldots, w_m$ are selected from the Dirichlet distribution with all parameters equal to $1/2$.

- Given $m$ and $w_1, \ldots, w_m$, $1/\sigma_1^2, \ldots, 1/\sigma_m^2$ are independent and identically distributed as gamma with shape and rate each $1/2$, and conditional on $\sigma_1, \ldots, \sigma_m$, $\mu_1, \ldots, \mu_m$ are independent with $\mu_j$ distributed $N(0, \sigma_j^2)$, $j = 1, \ldots, m$.

One hundred thousand values of $C$ were obtained by generating densities in the manner just described. The range of the 100,000 values of $C$ was $(5.4, 1397.21)$. Since $C_N = 5.51$, this suggests that $C_N$ is close to being a lower bound on the optimal constant. In Figure 1 we provide a kernel density estimate computed over the interval $(4,16.27)$, the upper endpoint of which is the 95th percentile of the 100,000 values generated. To see how the optimal constant correlates with the values of $I_0 = \int f^2(x) \, dx$ and $I_2 = \int (f''(x))^2 \, dx$, we provide Figure 2. The red points in the scatterplot correspond to the values of $C$ that were larger than 16.27.
Figure 1: *Kernel density estimate of constant in asymptotically optimal choice of p. The vertical line indicates the constant of 5.51 when the underlying density is normal.*

To the extent that our generated densities represent the distribution of densities in practice, values of $C$ larger than 16 are rare, and extremely rare when $I_0$ is not small.

How can the information just discussed be used to compute an average of PCV bandwidths? Let $\hat{h}(p)$ be a PCV bandwidth when the number of partitions is $p$, and let $1 < p_1 < p_2 < \cdots < p_J < n$ be some appropriate set of choices for $p$. Now, let $\pi$ be a prior density for the optimal constant $C$. One possibility for $\pi$ would be the kernel density estimate in Figure 1. Then we may define

$$\hat{h}_{\text{MA}} = \frac{\sum_{j=1}^{J} \pi(n^{-1/6}p_j)\hat{h}(p_j)}{\sum_{j=1}^{J} \pi(n^{-1/6}p_j)},$$

where MA stands for “model average.” This bandwidth is a weighted average of PCV bandwidths, where the weight on $\hat{h}(p_j)$ is the prior probability that $\hat{h}(p_j)$ is the (asymptotically) optimal PCV bandwidth. Although we do not further explore this idea in the current paper, we refer the reader to Hoeting et al. (1999) for a discussion of the merits of model averaging in a larger context.
Figure 2: Scatterplot of $I_2^{1/6}$ versus $I_0^{5/6}$. The red points correspond to cases where the optimal constant is larger than 16.27.

3 Simulation study

We study various aspects of the proposed methodology through a number of replicated simulation studies. Throughout the simulations, we use three densities from Marron & Wand (1992) as ground truth. Each of these densities is a mixture of normals which facilitates comparison as various population quantities can be calculated analytically. We refer to these densities as MW1, MW2 and MW8 being consistent with the numbering of Marron & Wand (1992). The exact forms are

(i) $MW1 \equiv N(0, 1)$.
(ii) $MW2 \equiv 0.2 N(0, 1) + 0.2 N(1/2, (2/3)^2) + 0.6 N(13/12, (5/9)^2)$.
(iii) $MW8 \equiv 0.75 N(0, 1) + 0.25 N(3/2, (1/3)^2)$.

MW 2 and 8 respectively have a skewed unimodal and asymmetric bimodal shape.

Throughout the study we use a standard normal kernel.

We first study the finite sample accuracy of Theorem 1 in characterizing the bias of ordinary CV bandwidths. Letting $\hat{h}_n = h_{n,0} - B^* n^{-2/5}$, Theorem 1 suggests that $E\hat{h} = \hat{h}_n + o(n^{-2/5})$. We let the sample size vary from 100 to 20000, and
analytically calculate $h_{n,0}$ and $\tilde{h}_n$ for each sample size. We then generate $T = 2000$ independent datasets for each sample size and numerically minimize the CV criterion to calculate $T$ CV bandwidths $\hat{h}^{(1)}, \ldots, \hat{h}^{(T)}$. The Monte Carlo estimate $\hat{h}_{MC} = (T)^{-1} \sum_{i=1}^{T} \hat{h}^{(i)}$ of the CV bandwidth along with $h_{n,0}$ and $\tilde{h}_n$ are reported in Table 1. We also calculate a $t$-statistic for testing $E\hat{h} = \tilde{h}_n$ based on the 2000 CV samples for each sample size. It is evident from Table 1 that with increasing sample size, the magnitude of the $t$-statistic monotonically decreases for each of the three MW curves, taking on reasonably moderate values for $n \geq 1000$ and being practically insignificant for $n \geq 10000$.

|   | MW1 |        |        | t     | MW2 |        |        | t     | MW8 |        |        | t     |
|---|-----|--------|--------|-------|-----|--------|--------|-------|-----|--------|--------|-------|
|   | Opt | Exp    | MC     |       | Opt | Exp    | MC     |       | Opt | Exp    | MC     |       |
| 100| 44.55 | 41.66  | 44.06  | 8.99  | 30.53 | 28.20  | 30.69  | 9.98  | 31.79 | 30.87  | 35.15  | 14.94 |
| 250| 36.51 | 34.51  | 35.74  | 6.27  | 24.85 | 23.65  | 24.50  | 6.43  | 24.15 | 23.52  | 25.31  | 11.23 |
| 500| 31.50 | 29.99  | 30.58  | 3.86  | 21.36 | 20.45  | 20.80  | 3.33  | 20.12 | 19.64  | 20.42  | 7.22  |
| 1000| 27.24 | 26.09  | 26.52  | 3.50  | 18.42 | 17.72  | 17.95  | 2.70  | 16.97 | 16.61  | 16.90  | 3.62  |
| 5000| 19.53 | 18.92  | 19.01  | 1.14  | 13.15 | 12.79  | 12.88  | 1.79  | 11.78 | 11.58  | 11.66  | 2.06  |
| 10000| 16.95 | 16.49  | 16.47  | -0.42 | 11.40 | 11.13  | 11.14  | 0.25  | 10.13 | 9.99   | 10.01  | 0.70  |
| 20000| 14.78 | 14.38  | 14.33  | -0.92 | 9.90  | 9.69   | 9.70   | 0.29  | 8.75  | 8.64   | 8.63   | -0.62 |

Table 1: Bias of CV bandwidths for various choices of $n$ and the three MW curves. Opt and Exp respectively denote $(100\times)$ the MISE optimal bandwidth $h_{n,0}$ and $\tilde{h}_n$, the approximation to $E\hat{h}$. MC denotes $(100\times)$ the Monte Carlo estimate of the CV bandwidth based on 2000 independent replicates and $t$ denotes a $t$-statistic based on the 2000 CV samples for testing $E\hat{h} = \tilde{h}_n$.

Our next set of simulations investigates aspects of the proposed PCV approach. At the outset, we comment on the computational superiority of PCV over ordinary CV. Figure 3 shows a plot of the ratio of computational times between ordinary CV and PCV with increasing sample size. The PCV was implemented with the asymptotically optimal number of subgroups at normality for each sample size. To avoid numerical instabilities, the computational times for each approach were calculated by averaging over 10 datasets at each sample size. A cross-validation function written by the authors was used in each case to have a fair comparison.
As evident from Figure 3, PCV is close to 25 times more efficient than ordinary CV when $n = 5000$, and about 45 times more efficient when $n = 25000$. The computational gains would be even more pronounced for larger values of $n$. However, for $n > 25000$, our cross-validation function cannot be implemented due to memory and storage issues. We should also mention that we did not take advantage of the embarrassingly parallel nature of PCV, which would have resulted in further time gains in the order of the number of partitions.

We now comment on the statistical efficiency of PCV over ordinary CV. We calculated the ordinary CV and PCV bandwidths for each of the three MW curves over 1000 datasets at sample size $n = 25000$; box plots of the bandwidths over the simulation replicates are provided in Figure 4. As before, the optimal group size at normality was used for PCV. The variance reduction achieved by PCV over ordinary CV is strikingly evident in Figure 4. To quantify this variance reduction, we compare the empirical variances with their asymptotic counterparts. As noted in Section 2,

$$\text{Var}(\hat{h}_{PCV}) \sim A^* n^{-3/5} p^{-4/5}, \quad \text{Var}(\hat{h}_{CV}) = p^{4/5} \text{Var}(\hat{h}_{PCV}),$$

(10)
Figure 4: CV and PCV bandwidths over 1000 simulation replicates for \( n = 25000 \). The MISE optimal bandwidths are 0.140, 0.094 and 0.084 for MW1, 2 and 8.

where

\[
A^* = \frac{8}{25} \cdot \left( \frac{\int V^2}{(\int \phi^2)^{7/5}} \right) \cdot \left( \frac{\int f^2}{(\int (f'')^2)^{3/5}} \right).
\]  

(11)

In the above display, \( \phi \) is the standard normal density and \( V \), defined in (19) in the Appendix, is determined by the kernel, with \( \int V^2 = 0.0954 \) for the Gaussian kernel. When the true density \( f \) is a mixture of normals as in our case, the quantities \( \int f^2 \) and \( \int (f'')^2 \) can be analytically calculated. We report the asymptotic and empirical variances along with the variance reduction factor \( \text{Var}(\hat{h}_{CV})/\text{Var}(\hat{h}_{PCV}) \) in Table 2. The empirical variance reduction factor is closest to the asymptotic approximation for the standard normal curve MW1, with more than 15-fold variance reduction for PCV. Even for the MW8 curve, where the asymptotic approximations seem to require a larger sample size, PCV achieves a 9-fold variance reduction. We also calculated the empirical sum of squared errors \( \sum_{i=1}^{1000} (\hat{h}_n^{(i)} - h_{n,0})^2 \) for ordinary CV and PCV. PCV had the smaller value for all three curves compared to CV, with the ratio of CV to PCV sums of squares being 14.91, 13.09 and 1.98 for the three curves respectively. The relatively smaller gain for MW8 compared to the other two curves.
stems mainly from the larger bias incurred by the PCV in this case. Specifically, for MW8 we have $h_{n,0} = 0.0835$, with $E\hat{h}_{CV} = 0.0820$, $\text{Var}(\hat{h}_{CV}) = 1.01 \times 10^{-4}$, while $E\hat{h}_{PCV} = 0.0899$, $\text{Var}(\hat{h}_{PCV}) = 1.13 \times 10^{-5}$. Thus, the bias somewhat offsets the variance reduction for PCV in this case.

|         | MW1     | MW2     | MW8     |
|---------|---------|---------|---------|
| Asymptotic | CV: 29.54, PCV: 1.95, VRF: 15.11 | CV: 11.89, PCV: 0.78, VRF: 15.11 | CV: 54.81, PCV: 3.62, VRF: 15.11 |
| Empirical    | CV: 46.60, PCV: 2.94, VRF: 15.86 | CV: 17.29, PCV: 1.34, VRF: 12.81 | CV: 10.15, PCV: 1.13, VRF: 8.97 |

Table 2: Variances ($\times 10^5$) of CV and PCV bandwidths for the three MW curves with $n = 25000$. The asymptotic approximations in (10) and empirical estimates from 1000 replicates are reported along with the variance reduction factor (VRF).

Next, we investigate the performance of PCV for larger sample sizes $n = 5 \times 10^4, 10^5$. Due to the aforementioned difficulty with implementing ordinary CV for large sample sizes, we use $\hat{h}_n$ as a proxy for the CV bandwidth. Along with the asymptotically optimal $p$ at normality, we also report the PCV bandwidth for a range of values for $p$ in Table 3; the reported bandwidths are averages over 1000 simulation replicates. The last row of the table reports the PCV bandwidth obtained by averaging over the different choices of $p$. We picked $p = 50$ as the largest subgroup size to ensure at least 1000 samples per subgroup. Table 3 clearly suggests the PCV bandwidths are fairly robust with respect to choice of the subgroup size.

In Table 4 we report the asymptotic and empirical estimates for the variances of the PCV bandwidths. For the MW1 and MW2 curves, the scenario is fairly consistent with the $n = 25000$ case in Table 2; the empirical variance consistently overshot the asymptotic approximation, typically by a factor of around 1.5. However, for the MW8 curve, the reverse phenomenon was observed when $n = 25000$, suggesting the necessity of larger sample sizes for the asymptotic approximation to be accurate.

Our final set of simulations study the amount of variance reduction achieved by permuted PCV. In the setting of Table 3 we also calculated the permuted PCV
Table 3: PCV bandwidths for sample sizes $n = 5 \times 10^4, 10^5$. 1000 simulation replicates were considered. Opt and CV respectively denote (100$x$) the MISE optimal bandwidth $h_{n,0}$ and $\tilde{h}_n$, the approximation to $E\hat{h}$. PCV$_{opt}$ denotes (100$x$) PCV bandwidth using $p = C_N n^{1/6}$, the optimal number of subgroups at normality, while PCV$_p$ used to $p$ subgroups. The value of $C_N n^{1/6}$ is 33 at $n = 5 \times 10^4$ and 38 at $n = 10^5$.

|         | MW1   | MW2   | MW8   |
|---------|-------|-------|-------|
|         | $5 \times 10^4$ | $10^5$ | $5 \times 10^4$ | $10^5$ | $5 \times 10^4$ | $10^5$ |
| Opt     | 12.23 | 10.63 | 8.21  | 7.14  | 7.22  | 6.27  |
| CV      | 11.99 | 10.45 | 8.07  | 7.03  | 7.15  | 6.21  |
| PCV$_{opt}$ | 12.05 | 10.45 | 8.18  | 7.10  | 7.59  | 6.49  |
| PCV$_{30}$ | 12.05 | 10.45 | 8.18  | 7.08  | 7.56  | 6.45  |
| PCV$_{35}$ | 12.06 | 10.45 | 8.20  | 7.09  | 7.62  | 6.48  |
| PCV$_{40}$ | 12.07 | 10.46 | 8.21  | 7.10  | 7.66  | 6.49  |
| PCV$_{45}$ | 12.08 | 10.46 | 8.21  | 7.10  | 7.71  | 6.52  |
| PCV$_{50}$ | 12.10 | 10.49 | 8.24  | 7.12  | 7.75  | 6.54  |
| PCV$_{avg}$ | 12.07 | 10.46 | 8.20  | 7.10  | 7.65  | 6.50  |

Table 4: Variances ($\times 10^5$) of PCV bandwidths with $n = 5 \times 10^4$ and $10^5$. The asymptotic approximations in (10) and empirical estimates from 1000 replicates are reported.

|         | MW1   | MW2   | MW8   |
|---------|-------|-------|-------|
|         | $5 \times 10^4$ | $10^5$ | $5 \times 10^4$ | $10^5$ | $5 \times 10^4$ | $10^5$ |
| Asymptotic | 1.17  | 0.70  | 0.47  | 0.28  | 0.22  | 0.13  |
| Empirical  | 1.74  | 1.02  | 0.67  | 0.44  | 0.62  | 0.32  |

bandwidths with 2 and 5 permutations respectively. The number of subgroups was fixed at the optimal $p$ at normality for PCV. In the following table, we report Monte Carlo estimates of the ratio of variances between the permuted PCV and PCV bandwidths based on 1000 datasets. The numerical results overall agree with the conclusions of Theorem 2; one obtains a variance reduction of approximately 1/2.
with two permutations and 1/5 with five. An exception is the MW8 curve for which the variance reduction with five permutations was about 1/3, again suggesting that the asymptotics kick in slower for this curve.

| method | MW1  | MW2  | MW8  |
|--------|------|------|------|
| PCVP₂  | 0.51 | 0.50 | 0.55 |
| PCVP₅  | 0.24 | 0.23 | 0.33 |

Table 5: *Ratio of variances between permuted PCV (PCVP) and PCV bandwidths based on 1000 datasets. The subscript for PCVP denotes the number of permutations.*

Theorem 2 also suggests a phenomenon of diminishing returns in the reduction of variance as the number of permutations increases. More precisely, Theorem 2 entails that further reductions in variance are minimal when the number of permutations exceeds $p$. To study this, we continued with $n = 5 \times 10^4, 10^5$, and took $p$ to be its optimal value at normality, 33 and 38 in this case. The number of permutations considered ranged from 1 to 40. A plot of the Monte–Carlo estimates of the ratio of variance versus the number of permutations is shown in Figure 5.

Figure 5: *Ratio of variances between the permuted PCV and PCV bandwidths based on 1000 datasets versus the number of permutations. The solid/dashed/dashed-dotted curves indicate MW1/2/8. Sample sizes are $5 \times 10^4$ and $10^5$ in the left and right panels respectively.*
variances between the permuted PCV and PCV bandwidths based on 1000 datasets against the number of permutations is provided in Figure 5, which clearly shows the efficacy of permuted PCV in reducing variance. In Figure 5, we observe rapid reductions in variance initially but then a stabilizing variance ratio beyond 15-20 permutations. For $n = 5 \times 10^4$, the variance reduction for the MW8 curve plateaus quickly compared to the other two curves, consistent with the observation in Table 5. With 40 permutations, MW8 achieves a variance reduction of about 0.20, while the reductions for MW1 and MW2 are 0.05 and 0.10 respectively. The reductions are more comparable for $n = 10^5$, with a reduction factor of 0.13 for MW8 compared to 0.05 and 0.07 for MW1 and MW2.

4 Analysis of Higgs boson data

Verifying the existence of Higgs boson is a central problem in particle physics. Experiments are conducted in which particles collide at very high speeds, producing exotic particles, such as the Higgs boson. Simulated collision data have been used to study statistical properties of various classification schemes that are applied to collider data. An example of such data are the 11 million simulated collision events studied by Baldi et al. (2014). These data may be found at the UCI Machine Learning Repository, archive.ics.uci.edu/ml/datasets/HIGGS. Roughly half of the 11 million simulated collisions are signal, meaning that they produced Higgs bosons, and the rest are background, which produced other types of particles. Each of the 11 million observations has 28 variables, or features. Here we consider just two of the 28 features, referred to as jet 4 $\eta$ and $m_{jjj}$. (These two variables are columns 20 and 24 of the dataset at the UCI data repository.) Our goal is to produce a total of 4 density estimates, a signal and background estimate for each of jet 4 $\eta$ and $m_{jjj}$.

The size of the Higgs data set presented challenges in our analysis. It was not possible to read the entire data set into an R session in a Linux environment. Instead, we divided the data into 110 data sets of size 100,000 each. We then analyzed these 110 sets separately, with not more than one data set occupying memory at the same time. Even still there were computational issues with data sets of size 50,000
(the typical size of a signal or background data set.) Not enough memory could be allocated to run the cross-validation function written by the authors, and the R function `bw.ucv` always produced a bandwidth at the upper endpoint of the interval over which the CV curve was minimized. It was thus necessary to partition each data set of size 50,000 into at least two subgroups in order to avoid these computational issues.

![Boxplots of data-driven bandwidths for jet 4 η background data. The left hand plot is for 110 PCV bandwidths and the right hand plot for 110 permuted PCV bandwidths based on 10 random permutations.](image)

Previously we suggested that the asymptotically optimal choice of \( p \) at normality would be a reasonable choice of \( p \) in general. For partitioned cross-validation, with \( n = 11,000,000 \) and using a Gaussian kernel, this value of \( p \) is 82. In the same setting, the optimal value of \( p \) for permuted PCV is 16. So, clearly we are in a situation where the sheer size of the data set requires more partitioning than is optimal. We will apply PCV using the smallest feasible number of partitions, two, for each of the 110 data sets, yielding a \( p \) of 220. While this seems far from the PCV-optimal value of 82, using 220 instead of 82 actually leads to a fairly small increase in the mean squared error of the optimal bandwidth. When \( p \) is equal to \( k \)
times the optimal value of $p$, it is straightforward to show that (6) takes the form
\[ 2^{-2/3}A^{1/3}B^{2/3}n^{-1/3}(k^{-4/5} + 2k^{2/5}). \]
If we use $p = 220 = 2.68(82)$, the approximate ratio of the PCV bandwidth MSE to the optimum MSE is thus $[2.68^{-4/5} + 2(2.68)^{2/5}] / 3 = 1.14$. This is a fairly small increase and suggests that the PCV bandwidth using $p = 220$ will still be much more efficient than the ordinary CV bandwidth.

Figure 7: Boxplots of data-driven bandwidths for $m_{jjj}$ background data. The left hand plot is for 110 PCV bandwidths and the right hand plot for 110 permuted PCV bandwidths based on 10 random permutations.

Let $n$ be the total sample size of 11 million, and let $n_{i0}$ and $n_{i1}$ be the number of background and signal observations, respectively, in data set $i$, $i = 1, \ldots, 110$. For a given set of jet 4 $\eta$ background observations, let $\hat{b}_{ij}$ be the ordinary CV bandwidth for the $j$th partition of the $i$th data set, $i = 1, \ldots, 110$, $j = 1, 2$. Sample size adjusted bandwidths are $\hat{h}_{ij} = n^{-1/5}(n_{i0}/2)^{1/5}\hat{b}_{ij}$, $i = 1, \ldots, 110$, $j = 1, 2$. Finally, the overall PCV bandwidth is defined as in (8), namely
\[ \hat{h} = \sum_{i=1}^{110} \sum_{j=1}^{2} n_{i0}^{1/5} \hat{h}_{ij} \left( 2 \sum_{i=1}^{110} n_{i0}^{1/5} \right)^{-1}. \]
Table 6: PCV bandwidths for the Higgs boson data. The left hand number in each cell is a PCV bandwidth, and the right hand number uses permuted PCV based on ten random permutations.

| Feature | Background | Signal |
|---------|------------|--------|
| jet 4 $\eta$ | 0.02588, 0.02593 | 0.02653, 0.02648 |
| $m_{jjj}$ | 0.00398, 0.00400 | 0.00667, 0.00666 |

Applying the same procedure to each combination of feature and background/signal led to the bandwidths shown in Table 6.

Because of the computational issues discussed previously, we do not permute the entire data set of 11 million observations. Instead, we apply the permutation idea separately to the 110 smaller data sets, and then average results. The algorithm for a single data set is described as follows:

- Compute a PCV bandwidth based on two partitions.
- Repeat the previous step a total of ten times for ten random permutations of the data.
- Average the ten PCV bandwidths and adjust the average in the usual way to produce a bandwidth for a sample of size $n$.

Having produced 110 bandwidths as described above, we then average them to obtain the final bandwidth. The four bandwidths so determined are given in Table 6. Obviously the bandwidths chosen by the two methods are quite similar. An impression of the relative variability of the methods is obtained from the boxplots in Figures 6 and 7. We also applied a modified version of permuted PCV to the data.

Our theory indicates that were we able to consider ten random permutations of the entire data set, then the variance of the PCV bandwidth could be reduced by a factor of $1/10 + (9/10)/220 = 0.104$, since we use $p = 220$ partitions. However, applying permuted PCV separately to the 110 data sets leads to a reduction of just $1/10 + (9/10)/2 = 0.55$. Note that the width of the boxplots for the permuted PCV
Figure 8: Density estimates for jet 4 $\eta$ data. The solid and dashed lines are for the signal and background data, respectively.

Figure 9: Density estimates for $m_{jjj}$ data. The solid and dashed lines are for the signal and background data, respectively.
bandwidths is about $3/4$ of that for the PCV bandwidths, which agrees with the factor of $\sqrt{0.55} = 0.742$.

Finally, we wish to produce density estimates using bandwidths from Table 6. For a given feature, it is of interest to compare the density estimates for signal and background. A basic principle of comparing density estimates is to use a common bandwidth for the estimates being compared, especially when the estimates are similar in shape (see Bowman and Young 1996). We therefore use the average of permuted PCV bandwidths across rows of Table 6 as the common bandwidth for signal and background. This yields bandwidths of 0.02621 and 0.00533 for jet 4 $\eta$ and $m_{jjj}$, respectively. Separate density estimates were computed for the 110 data sets, and then a weighted average of these estimates was computed, where the weights were proportional to sample size. In Figures 8 and 9 we see that the signal and background estimates are quite similar for both features. This gives one an inkling of the complexity of the Higgs classification problem since one must try to distinguish between background and signal in a case where the marginal distributions of these two populations are very similar for all 28 features.

5 Concluding remarks

Use of partitioned cross-validation to choose the bandwidth of a kernel density estimator has been studied in the context of big data and the divide-and-conquer scenario. It was argued that PCV provides substantial improvements in both statistical and computational efficiency over ordinary CV. PCV involves randomly partitioning the data into $p$ subsets. Asymptotics show that the PCV bandwidth based on a single partitioning can converge to the optimal bandwidth at a faster rate than does the ordinary CV bandwidth. Intuition suggests that it is desirable to average the bandwidths resulting from multiple random partitionings of the data. Rather remarkably, it turns out that when the number of random partitionings is of a larger order than $p$, the variance of such an average converges to 0 at a faster rate than does the variance of the PCV bandwidth.

Obviously partitioned cross-validation can be applied in other contexts as well. A
particularly important setting is that of nonparametric regression, where estimation could be based on kernel-type estimators or splines. In either approach it is necessary to choose smoothing parameters, and cross-validation is a commonly used method for doing so. It seems fair to conjecture that partitioned cross-validation will lead to improvements in statistical efficiency in the regression context as well.

6 Appendix A

Proof of Theorem 1. We shall use $M(h)$ to succinctly denote $MISE(\hat{f}_h, f)$ as a function of $h$. Recall that $E\{CV(h)\} = M(h) - \int f^2$, and $\hat{h}$ and $h_{n,0}$ are the respective minimizers of $CV(h)$ and $M(h)$. Define the functions $L$ and $H$ by

$$L(u) = -uK'(u), \quad H(u) = -uL'(u).$$ \hspace{1cm} (12)

Using integration by parts and the assumptions on $K$, $L$ and $H$ are both kernel functions in that

$$\int L(u) du = \int H(u) du = 1$$

and

$$\int uL(u) du = \int uH(u) du = 0.$$ \hspace{1cm} (13)

The kernel $H$ satisfies the further moment condition

$$\int u^2H(u) du = 0.$$ \hspace{1cm} (14)

Let $\tilde{f}_h$ and $f^*_h$ denote the kernel density estimates corresponding to $L$ and $H$, i.e.,

$$\tilde{f}_h(x) = \frac{1}{nh} \sum_{i=1}^{n} L\left(\frac{x-X_i}{h}\right), \quad f^*_h(x) = \frac{1}{nh} \sum_{i=1}^{n} H\left(\frac{x-X_i}{h}\right).$$ \hspace{1cm} (15)

Invoking (14),

$$CV'(h) = 2 \int \hat{f}_h(x) \frac{d}{dh} \hat{f}_h(x) dx - 2 \frac{n}{h} \sum_{i=1}^{n} \frac{d}{dh} \tilde{f}_h^i(x)$$

$$= -\frac{2}{h} \int \hat{f}_h(x)[\hat{f}_h(x) - \tilde{f}_h(x)] dx + \frac{2}{nh} \sum_{i=1}^{n} [\hat{f}_h^i(X_i) - \tilde{f}_h^i(X_i)]$$

$$= -\frac{2}{h} \int \tilde{f}_h^2(x) dx + \frac{2}{h} \int \hat{f}_h(x)\tilde{f}_h(x) dx + \frac{2}{nh} \sum_{i=1}^{n} \hat{f}_h^i(X_i) - \frac{2}{nh} \sum_{i=1}^{n} \tilde{f}_h^i(X_i).$$ \hspace{1cm} (16)
Differentiating (15) and invoking (14) on multiple occasions,
\[
CV''(h) = \frac{6}{h^2} \int \hat{f}_h^2(x)dx + \frac{2}{h^2} \int \check{f}_h^2(x)dx - \frac{10}{h^2} \int \hat{f}_h(x)\check{f}_h(x)dx + 2 \frac{h^2}{n} \sum_{i=1}^{n} \hat{f}_h^i(X_i) + 6 \frac{h^2}{n} \sum_{i=1}^{n} \check{f}_h^i(X_i)
\]
- \frac{2}{nh^2} \sum_{i=1}^{n} f_{\ast}^i(X_i).
\]
(16)

We now introduce some further notation to express \(CV'(h)\) in (15) and \(CV''(h)\) in (16) in a compact fashion. Define the convolutions
\[
A(x) = \int K(x-u)K(u)du, \quad B(x) = \int K(x-u)L(u)du
\]
(17)
\[
C(x) = \int L(x-u)L(u)du, \quad D(x) = \int K(x-u)H(u)du.
\]
(18)

We now record a result which expresses the individual terms appearing in (15) and (16) as U-statistics; the proof is deferred to Appendix B.

**Lemma 6.1** We have
\[
\int \hat{f}_h^2(x)dx = \frac{1}{n^2h} \sum_{i=1}^{n} \sum_{j=1}^{n} A \left( \frac{X_i - X_j}{h} \right), \quad \int \check{f}_h^2(x)dx = \frac{1}{n^2h} \sum_{i=1}^{n} \sum_{j=1}^{n} C \left( \frac{X_i - X_j}{h} \right),
\]
\[
\int \hat{f}_h(x)\check{f}_h(x)dx = \frac{1}{n^2h} \sum_{i=1}^{n} \sum_{j=1}^{n} B \left( \frac{X_i - X_j}{h} \right)
\]
and
\[
\int \hat{f}_h(x)f_{\ast}^i(x)dx = \frac{1}{n^2h} \sum_{i=1}^{n} \sum_{j=1}^{n} D \left( \frac{X_i - X_j}{h} \right).
\]

Using Lemma 6.1 in (15) and recalling the definition of \(\hat{f}_h^i, \check{f}_h^i\), we have
\[
CV'(h) = -\frac{2}{n^2h^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left[ A \left( \frac{X_i - X_j}{h} \right) - B \left( \frac{X_i - X_j}{h} \right) \right]
\]
\[
+ \frac{2}{n(n-1)h^2} \sum_{i \neq j} \left[ K \left( \frac{X_i - X_j}{h} \right) - L \left( \frac{X_i - X_j}{h} \right) \right].
\]

Defining
\[
V(u) = A(u) - B(u) - K(u) + L(u),
\]
(19)
it can be verified that
\[ \int V(u)du = 0, \int uV(u)du = 0, \int u^2V(u)du = 0. \]

Noting that \(-2/(n^2h^2) = -2/(n(n-1)h^2) + 2/(n^2(n-1)h^2)\), we can write
\[
CV'(h) = -\frac{2}{hn(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{h} V \left( \frac{X_i - X_j}{h} \right)
+ \frac{2}{hn^2(n-1)} \sum_{i\neq j} \sum_{j=1}^{n} \frac{1}{h} \left[ A \left( \frac{X_i - X_j}{h} \right) - B \left( \frac{X_i - X_j}{h} \right) \right].
\]

Therefore, \(CV'(h) - E\{CV'(h)\}\) may be expressed as
\[
-\frac{2}{hn(n-1)} \sum_{i\neq j} \sum_{j=1}^{n} \left[ \frac{1}{h} V \left( \frac{X_i - X_j}{h} \right) - E_h \right]
+ \frac{2}{hn^2(n-1)} \sum_{i\neq j} \sum_{j=1}^{n} \left\{ \frac{1}{h} \left[ A \left( \frac{X_i - X_j}{h} \right) - B \left( \frac{X_i - X_j}{h} \right) \right] - E_{h1} \right\},
\]
where
\[
E_h = E \left[ \frac{1}{h} V \left( \frac{X_1 - X_2}{h} \right) \right], \quad E_{h1} = E \left\{ \frac{1}{h} \left[ A \left( \frac{X_1 - X_2}{h} \right) - B \left( \frac{X_1 - X_2}{h} \right) \right] \right\}.
\]

We used the fact that the terms corresponding to \(i = j\) in the first sum are canceled since they are constants. In the expression for \(CV'(h) - E\{CV'(h)\}\) in (20), the second term in the right hand side has exactly the same form as the first with the exception that it has an extra \(n^{-1}\), so that it is negligible compared to the first. We therefore conclude,
\[
CV'(h) - E\{CV'(h)\} = -\frac{2}{hn(n-1)} \sum_{i\neq j} \sum_{j=1}^{n} \left[ \frac{1}{h} V \left( \frac{X_i - X_j}{h} \right) - E_h \right] + R'_n, \quad (22)
\]
where \(R'_n\) is negligible.

Using the same argument, we can express \(CV''(h)\) in (16) in a more concise fashion as
\[
CV''(h) - E\{CV''(h)\} = \frac{2}{h^2 n(n-1)} \sum_{i\neq j} \sum_{j=1}^{n} \left[ \frac{1}{h} W \left( \frac{X_i - X_j}{h} \right) - E_{h2} \right] + R''_n,
\]
\[
(23)
\]
where

\[ W(u) = 3A(u) + C(u) - 5B(u) + D(u) - 2K(u) + 3L(u) - H(u), \]  

(24)

with

\[ \int W(u)du = 0, \int uW(u)du = 0, \int u^2W(u)du = 0, \int u^3W(u)du = 0, \]

and \( R''_n \) is negligible as before.

Ignoring terms that are negligible, we therefore have from (23) and (22) that

\[
\begin{align*}
- \frac{h^3 n^2 (n - 1)^2}{4} & \text{Cov}\{CV'(h), CV''(h)\} \\
& = E \left\{ \sum_{i \neq j} \sum_{k \neq l} \left[ \frac{1}{h} V\left( \frac{X_i - X_j}{h} \right) - E_h \right] \times \left[ \frac{1}{h} W\left( \frac{X_k - X_l}{h} \right) - E_{h^2} \right] \right\} \\
& = 2n(n - 1)T_1 + 4n(n - 1)(n - 2)T_2 + n(n - 1)(n - 2)(n - 3)T_3,
\end{align*}
\]

where

\[
\begin{align*}
T_1 &= E \left\{ \left[ \frac{1}{h} V\left( \frac{X_1 - X_2}{h} \right) - E_h \right] \times \left[ \frac{1}{h} W\left( \frac{X_1 - X_2}{h} \right) - E_{h^2} \right] \right\}, \\
T_2 &= E \left\{ \left[ \frac{1}{h} V\left( \frac{X_1 - X_2}{h} \right) - E_h \right] \times \left[ \frac{1}{h} W\left( \frac{X_1 - X_3}{h} \right) - E_{h^2} \right] \right\}, \\
T_3 &= E \left\{ \left[ \frac{1}{h} V\left( \frac{X_1 - X_2}{h} \right) - E_h \right] \times \left[ \frac{1}{h} W\left( \frac{X_3 - X_4}{h} \right) - E_{h^2} \right] \right\}.
\end{align*}
\]

Note that \( T_3 = 0 \), and

\[
T_1 = \int \int \frac{1}{h^2} V\left( \frac{x - y}{h} \right) W\left( \frac{x - y}{h} \right) f(x)f(y)dxdy - E_hE_{h^2}
\]

\[
= \frac{1}{h} \int V(u)W(u)du \int f^2(x)dx + o(1).
\]

Using a Taylor series expansion of \( f \), the fact that \( f \) has three bounded and continuous derivatives, and \( \int u^jV(u)du = 0, j = 0, 1, 2 \), it is easy to check that \( T_2 = O(h^5) \).

Taking \( h = h_{n,0} \) and combining results we have thus obtained the key approximation

\[
ECV'(h_{n,0})CV''(h_{n,0}) \sim - \frac{8}{h_{n,0}^4 n^2} \int V(u)W(u)du \int f^2(x)dx. \tag{25}
\]
Expression [25] needs to be divided by $M''(h_{n,0})^2$ in order to determine $B^*$. It suffices to replace $M(h)$ by its well-known asymptotic expression, which we shall continue to denote by $M$, so that

$$M(h) = \frac{\int K^2(u)du}{nh} + \frac{\sigma_k^2 h^4 \int (f''(x))^2 dx}{4} = \frac{C_1}{nh} + C_2 h^4.$$ (26)

Solving $M'(h) = 0$, we get $h_{n,0} \sim \{C_1/(4C_2)\}^{1/5} n^{-1/5}$. Differentiating $M'(h)$ and using this identity, we obtain

$$M''(h_{n,0}) \sim 5 \frac{4^{3/5} C_1^{2/5} C_2^{3/5}}{n^{2/5}} n^{-2/5}.$$ (27)

Using (27) and simplifying,

$$\frac{E[CV'(h_{n,0})CV''(h_{n,0})]}{M''(h_{n,0})^2} = - \frac{8}{25} n^{-2/5} \frac{\int V(u)W(u)du \int f^2(x)dx}{\left[ \int K^2(u)du \right]^{8/5} \left[ \int \sigma_k^4 \int (f''(x))^2 dx \right]^{2/5} + o(n^{-2/5}),}$$

which defines $B^*$ and concludes the proof of Theorem 1.

**Proof of Theorem 2.** Let $\hat{h}_1, \ldots, \hat{h}_N$ be PCV bandwidths corresponding to $N$ random permutations of the data. The PCVP bandwidth is $\bar{h} = \sum_{i=1}^{N} \hat{h}_i$. We have

$$\hat{h}_i = \frac{1}{p} \sum_{j=1}^{p} \hat{h}_{ij},$$

where $\hat{h}_{i1}, \ldots, \hat{h}_{ip}$ are the bandwidths computed on the $p$ groups of the $i$th partitioning, $i = 1, \ldots, N$. Furthermore,

$$\hat{h}_{ij} = p^{-1/5} \hat{b}_{ij},$$

where $\hat{b}_{ij}$ is the usual CV bandwidth for the data in the $j$th group of the $i$th partitioning.

Because the data are independent and identically distributed,

$$\text{Var}(\bar{h}) = \frac{1}{N} \text{Var}(\hat{h}_1) + \left( \frac{N-1}{N} \right) \text{Cov}(\hat{h}_1, \hat{h}_2)$$

$$= \frac{1}{N} \text{Var}(\hat{h}_1) + \left( \frac{N-1}{N} \right) \text{Cov}(\hat{h}_{11}, \hat{h}_{21}).$$ (29)
Let $m = n/p$ and without loss of generality let the data from which $\hat{h}_{11}$ is calculated be $X_1, \ldots, X_m$. The data from which $\hat{h}_{21}$ is calculated are $X_{i_1}, \ldots, X_{i_m}$, where $i_1, \ldots, i_m$ are a random sample (without replacement) from $1, \ldots, n$. We may write

$$\text{Cov}(\hat{h}_{11}, \hat{h}_{21}) = \sum_{r=1}^{m} \text{Cov}(\hat{h}_{11}, \hat{h}_{21}|A_r)p_r,$$

where $A_r$ is the event that exactly $r$ of $i_1, \ldots, i_m$ are in $\{1, \ldots, m\}$ and

$$p_r = P(A_r) = \frac{\binom{m}{r} \binom{n-m}{m-r}}{\binom{n}{m}}.$$ 

Because the data are independent of the chosen permutation,

$$\text{Cov}(\hat{h}_{11}, \hat{h}_{21}|A_r) = p_r^{-2/5}\text{Cov}(\hat{b}_{11}, \hat{b}^{(r)}),$$

where $\hat{b}_{11}$ and $\hat{b}^{(r)}$ are the usual CV bandwidths computed from $X_1, \ldots, X_m$ and $Y = (X_1, \ldots, X_r, X_{m+1}, \ldots, X_{2m-r})$, respectively.

Let $CV_{11}(b)$ and $CV_r(b)$ be the cross-validation curves for $X_1, \ldots, X_m$ and $Y$, respectively. Arguing as in the proof of Scott and Terrell (1987), as $m \to \infty$

$$\text{Cov}(\hat{b}_{11}, \hat{b}^{(r)}) \sim \text{Cov}(CV'_{11}(b_0), CV'_r(b_0)) [M''(b_0)]^{-2},$$

where $b_0$ is the MISE optimal bandwidth for a sample of size $m$ and $M''(b)$ is the usual first order approximation of the second derivative of MISE. Arguing as in the proof of Theorem 1

$$4b_0^{-2}m^{-2}(m-1)^{-2}\text{Cov}\left(\sum_{i=1}^{m} \sum_{j=1}^{m} \frac{1}{b_0} V\left(\frac{X_i - X_j}{b_0}\right), \sum_{j=1}^{m} \sum_{k=1}^{m} \frac{1}{b_0} V\left(\frac{X_{ij} - X_{ik}}{b_0}\right)\right),$$

where $V$ is defined by (19).

We may write

$$\sum_{i=1}^{m} \sum_{j=1}^{m} \frac{1}{b_0} V\left(\frac{X_i - X_j}{b_0}\right) = S_r + \delta_{r1}$$

and

$$\sum_{j=1}^{m} \sum_{k=1}^{m} \frac{1}{b_0} V\left(\frac{X_{ij} - X_{ik}}{b_0}\right) = S_r + \delta_{r2},$$

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where
\[ S_r = \sum_{i=1}^{r} \sum_{j=1}^{r} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right), \]

\[
\delta_{r1} = \sum_{i=1}^{r} \sum_{j=r+1}^{m} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) + \sum_{i=r+1}^{m} \sum_{j=1}^{r} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) + \sum_{i=r+1}^{m} \sum_{j=r+1}^{m} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right)
\]

and
\[
\delta_{r2} = \sum_{i=1}^{r} \sum_{j=m+i}^{2m-r} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) + \sum_{i=m+1}^{2m-r} \sum_{j=1}^{r} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) + \sum_{i=m+1}^{2m-r} \sum_{j=m+1}^{2m-r} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right).
\]

It follows that
\[
\text{Cov}(CV'_{11}(b_0), CV'_r(b_0)) \sim
\]
\[
4b_0^{-2}[m(m-1)]^{-2} \left[ \text{Var}(S_r) + 2\text{Cov}\left( S_r, \sum_{i=1}^{r} \sum_{j=m+1}^{r} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) \right) \right. \\
+ 2\text{Cov}\left( S_r, \sum_{i=1}^{r} \sum_{j=r+1}^{m} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) \right) + \text{Cov}(\delta_{r1}, \delta_{r2}) \left].
\]

(30)

Again using Scott and Terrell (1987),

\[
\text{Var}(S_r) = 2r(r-1)b_0^{-1} \left[ \int V^2(u) \, du \int f^2(x) \, dx + o(1) \right] + 4r(r-1)(r-2)o(b_0^6),
\]

where both o terms immediately above are independent of r. By inspection

\[
\text{Cov}\left( S_r, \sum_{i=1}^{r} \sum_{j=m+1}^{r} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) \right) = \text{Cov}\left( S_r, \sum_{i=1}^{r} \sum_{j=r+1}^{m} \frac{1}{b_0} V \left( \frac{X_i - X_j}{b_0} \right) \right).
\]

The latter covariance is
\[
b_0^{-2} \sum_{i=1}^{r} \sum_{j=1}^{r} \sum_{k=1}^{r} \sum_{\ell=r+1}^{m} \text{Cov}\left( V \left( \frac{X_i - X_j}{b_0} \right), V \left( \frac{X_k - X_\ell}{b_0} \right) \right) =
\]

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\[ 2b_0^{-2} \sum_{i=1}^{r} \sum_{j=1}^{r} \sum_{\ell=r+1}^{m} \text{Cov} \left( V \left( \frac{X_i - X_j}{b_0} \right), V \left( \frac{X_i - X_\ell}{b_0} \right) \right) = \]
\[ 2b_0^{-2} r(r-1)(m-r) \text{Cov} \left( V \left( \frac{X_1 - X_2}{b_0} \right), V \left( \frac{X_1 - X_3}{b_0} \right) \right). \]

Now,
\[
\text{Cov}(\delta_{r1}, \delta_{r2}) = 4b_0^{-2} \text{Cov} \left( \sum_{i=1}^{r} \sum_{j=r+1}^{m} V \left( \frac{X_i - X_j}{b_0} \right), \sum_{i=1}^{r} \sum_{j=m+1}^{2m-r} V \left( \frac{X_i - X_j}{b_0} \right) \right)
\]
\[= 4b_0^{-2} r(m-r)^2 \text{Cov} \left( V \left( \frac{X_1 - X_2}{b_0} \right), V \left( \frac{X_1 - X_3}{b_0} \right) \right). \]

We see then that \(
\text{Cov}(\delta_{r1}, \delta_{r2}) \) and the sum of the other two covariance terms in (30) are identical except for the factors \( r(m-r)^2 \) and \( r(r-1)(m-r) \). For later reference note that
\[
\sum_{r=1}^{m} r(m-r)^2 p_r = \frac{m^4}{n} (1 + o(1))
\]
and
\[
\sum_{r=1}^{m} r(r-1)(m-r)p_r \sim \frac{m^5}{n^2}.
\]

The sum of the first and second covariance terms in (30) contributes the following to \( \text{Cov}(\hat{h}_{11}, \hat{h}_{21}) \):
\[
\frac{32}{p^{2/5} m^4 b_0^4 M''(b_0)^2} \text{Cov} \left( V \left( \frac{X_1 - X_2}{b_0} \right), V \left( \frac{X_1 - X_3}{b_0} \right) \right) \sum_{r=1}^{m} r(r-1)(m-r)p_r \sim
\]
\[
C_1 m^{8/5} p^{-2/5} m^{-4} \frac{m^5}{n^2} \text{Cov} \left( V \left( \frac{X_1 - X_2}{b_0} \right), V \left( \frac{X_1 - X_3}{b_0} \right) \right),
\]
where \( C_1 \) is a positive constant. We have
\[
E \left[ V \left( \frac{X_1 - X_2}{b_0} \right) \right] = \int \int V \left( \frac{x-y}{b_0} \right) f(x) f(y) \, dx \, dy
\]
\[= b_0 \int f(x) \int V(u) f(x-b_0u) \, du \, dx.
\]
Since \( \int u^j V(u) \, du = 0, j = 0, 1, 2, 3, \) and \( f \) has first four derivatives that are bounded and continuous,
\[
E \left[ V \left( \frac{X_1 - X_2}{b_0} \right) \right] = O(b_0^5).
\]
Similarly,
\[ E \left[ V \left( \frac{X_1 - X_2}{b_0} \right) V \left( \frac{X_1 - X_3}{b_0} \right) \right] = O(b_0^0), \]
and hence \( \text{Cov} \left( V \left( \frac{X_1 - X_2}{b_0} \right), V \left( \frac{X_1 - X_3}{b_0} \right) \right) = O(b_0^0). \) Therefore, the covariance term in question contributes a term of the following order to \( \text{Cov}(\hat{h}_{11}, \hat{h}_{21}) \):
\[
m^{8/5} p^{-2/5} m m^{-2} = p^{-2/5} m^{3/5}.
\]
(31)

The term in (30) involving \( \text{Var}(S_r) \) contributes the following to \( \text{Cov}(\hat{h}_{11}, \hat{h}_{21}) \):
\[
\frac{4}{p^{2/5} m^4 b_0^2 M''(b_0)^2} \left[ \frac{2m^4}{b_0 n^2} \int V^2(u) du \int f^2(x) dx \sum_{r=1}^{m} r(r-1)p_r \right]
+ o(b_0^6) \sum_{r=1}^{m} r(r-1)(r-2)p_r,
\]
which is
\[
\frac{4}{p^{2/5} m^4 b_0^2 M''(b_0)^2} \left[ \frac{2m^4}{b_0 n^2} \int V^2(u) du \int f^2(x) dx + o(m^4 b_0^{-1} n^{-2}) + o(b_0^6 m^6 n^{-3}) \right].
\]
(32)

We have
\[
o(b_0^6) m^6 n^{-3} \left[ \frac{m^4}{b_0 n^2} \right]^{-1} = o(b_0^6) \frac{m^2}{n} = o(m/n),
\]
which tends to 0 as \( m, n \to \infty \) since \( m = o(n) \). So, the the term involving (32) is asymptotic to
\[
\frac{8}{p^{2/5} m^4 b_0^3 M''(b_0)^2 n^2} \int V^2(u) du \int f^2(x) dx = \frac{1}{p} \text{AV}(\hat{h}_1),
\]
(33)
where \( \text{AV}(\hat{h}_1) \) is the asymptotic variance of \( \hat{h}_1 \). The order of (33) is \( m^{7/5} p^{-2/5} n^{-2} \), and hence larger than (31).

The term in (30) involving \( \text{Cov}(\delta_{r1}, \delta_{r2}) \) contributes the following to \( \text{Cov}(\hat{h}_{11}, \hat{h}_{21}) \):
\[
\frac{16}{p^{2/5} m^4 b_0^4 M''(b_0)^2} \text{Cov} \left( V \left( \frac{X_1 - X_2}{b_0} \right), V \left( \frac{X_1 - X_3}{b_0} \right) \right) \sum_{r=1}^{m} r(m-r)^2 p_r,
\]
which is of order \( m^{8/5} m^{-4} p^{-2/5} m^{-2} m^4 n^{-1} = (pm)^{-2/5} n^{-1} = n^{-7/5} \).

Collecting previous results, we have
\[
\text{Cov}(\hat{h}_{11}, \hat{h}_{21}) = \frac{1}{p} \text{AV}(\hat{h}_1) + O(n^{-7/5}) + o \left( \frac{1}{p} \text{AV}(\hat{h}_1) \right).
\]
(34)
Since $p^{-1}AV(\hat{h}_1)$ is asymptotic to $C_4p^{-9/5}n^{-3/5}$, it follows that $n^{-7/5}$ is of smaller order than $p^{-1}AV(\hat{h}_1)$ when $p = o(n^{4/9})$. Combining (34) with (29), and assuming that $N \sim p^a$ for $a > 1$, we have

$$\text{Var}(\bar{h}) \sim \frac{1}{p}AV(\hat{h}_1).$$

On the other hand, if $N$ is fixed, then $\text{Var}(\bar{h})$ is asymptotic to $\text{Var}(\hat{h}_1)/N$ as $n$ and $p$ tend to $\infty$.

7 Appendix B

Proof of Lemma 6.1. We prove the first equality; the rest follow similarly. We have

$$\int \hat{f}_h^2(x)dx = \frac{1}{n^2h^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \int K\left(\frac{x-X_i}{h}\right)K\left(\frac{x-X_j}{h}\right)dx$$

$$= \frac{1}{n^2h} \sum_{i=1}^{n} \sum_{j=1}^{n} \int K\left(\frac{X_i-X_j}{h} - u\right)K(u)du$$

$$= \frac{1}{n^2h} \sum_{i=1}^{n} \sum_{j=1}^{n} A\left(\frac{X_i-X_j}{h}\right).$$

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