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Bandwidth choice for density derivative

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ABSTRACT

The methods for choosing appropriate bandwidth (smoothing parameter) are important to approximate the regression function to the original function so that the error is as small as possible. It is always a good starting point, and that the smoothing accuracy depends only on the bandwidth, which in turn affects the degree of smoothing of the estimated curve and its proximity to the true curve. The equilibrium between bias and variance is called the smoothing parameter or the bandwidth parameter. Its value is greater than zero, which reduces the function and its value corresponds to the smallest standard, and that large values of (h) produce smoothed results, because it increases the bias and reduces the variance to estimate the original regression function. It is one of the methods to reduce the mean squares of error. This article explains the structured methods of bandwidth choice for estimating the r^{th} derivative of a univariate kernel employing techniques methods of cross-validation. We used kedd package proposed by Arsalane Chouaib Guidoum based on R programming with different kernel functions for computing bandwidth choice for density derivative. Simulation approaches are used to construct the method of bandwidth along with real-life data sets.

Keywords: Bandwidth, Kernel, derivatives, UCV, CCV, MCV.

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1. Introduction

In statistics and studies related field of wider applications, kernel density derivatives are highly adopted. The derivatives to probability density function with several statistical properties are important in estimation of distributions like extreme and point inflection that can be recognized. The kernel density derivative functions are applications used in time series analysis, clustering analysis, and estimation the location of a density estimate.

The research is structured as follows: Section 2 gives details about kernel density estimator and its derivatives. Section 3 summarizes the techniques methods for bandwidth kernel density estimator and its derivative. In section 4, Monte Carlo simulation is used to construct the method of bandwidth. Moreover, the results are applied based on real data. Finally, the research finishes with the "Conclusions".

2. Kernel estimation and derivatives

The univariate kernel estimate offers a brilliant base for showing characteristics in specified observations as a result of its straightforward application as compared with other complex estimators [1].

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

Accordingly,

K stands for kernel function.

$h > 0$ for bandwidth that is very important.

$X_i > 0$ for the observations.

n is the sample size.

The kernel function which satisfies the conditions is [2]:

$\int K(x)dx = 1, \int x\, K(x)dx = 0 \quad and \quad \int x^2 K(x)dx = k_2(K) > 0$ (2)

Let (X_1,X_2,……,X_n) with a probability density function and r times, then estimator of the r^{th} derivative to the kernel is [3] :

$$\hat{f}_h^{(r)}(x) = \frac{1}{nh^{r+1}} \sum_{i=1}^{n} K^{(r)}\left(\frac{x-X_i}{h}\right) \quad (3)$$

where $K^{(r)}$ is related to r^{th}. The choice method of h is an important problem since the effect of bandwidth is based on the estimator. If the value of bandwidth is big, we can obtain an over smooth estimator. On the other hand, if the value of bandwidth is small, the estimator can be obtained with under smooth estimator. Gaussian function with mean zero and variance one can be used since yield estimator is smooth density [4]. Gaussian function r^{th} density is estimated based on Gaussian kernel [5].

3. Method of bandwidth

The research is based on structured methods of bandwidth choice for estimating the r^{th} derivative to the kernel [2] , [6] as follows:

3.1. Unbiased cross-validation (UCV)

Method was proposed by Wolfgang et al.(1990) [7] to select rth derivative based on the kernel of density function , the minimization of ISE(h) defined [2]:

$$h_{ucv} = \underset{h>0}{argmax}\; UCV(h, r) \quad (4)$$

$$UCV(h, r) = \frac{R(K^{(r)})}{nh^{2r+1}} + \frac{(-1)^r}{n(n-1)/h^{2r+1}} \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} \left(K^{(r)} * K^{(r)} - 2K^{(2r)}\right) K\left(\frac{x_j - x_i}{h}\right) \quad (5)$$

The h. UCV for bandwidth is computing from Unbiased cross-validation (UCV) [2] ,[8].

3.2. Complete cross-validation (CCV)

Method was proposed by (Peter and Marron(1987)) [9] to obtain r^{th} for a kernel of density function given by:

$$CCV(h, r) = R\left(\hat{f}_h^{(r)}\right) - \bar{\theta}_{(r)}(h) + \tfrac{1}{2}\mu_2(K)h^2\, \bar{\theta}_{r+1}(h) + \tfrac{1}{24}\left(6\mu_2^2(K) - \delta(K)\right) h^4 \bar{\theta}_{r+2}(h) \quad (6)$$

where,

$$R\left(\hat{f}_h^{(r)}\right) = \frac{R(K^{(r)})}{nh^{2r+1}} + \frac{(-1)^r}{n(n-1)h^{2r+1}} \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} K^{(r)} * K^{(r)} K\left(\frac{x_j - x_i}{h}\right)$$

$$\bar{\theta}_{(r)}(h) = \frac{(-1)^r}{n(n-1)h^{2r+1}} \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} K^{(2r)} K\left(\frac{x_j - x_i}{h}\right) \quad (7)$$

and $\delta(K) = \int x^4\, K(x)dx$

The h. CCV for bandwidth is computed based on complete cross-validation (CCV) [2] ,[10].

3.3. Modified cross-validation (MCV)

This method was proposed on [2] , [11],to select the r^{th} derivative of a kernel of density function. The minimization of MCV(h) is defined:

$$MCV(h, r) = \frac{R(K^{(r)})}{nh^{2r+1}} + \frac{(-1)^r}{n(n-1)h^{2r+1}} \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} \varphi^{(r)}\left(\frac{x_j - x_i}{h}\right) \quad (8)$$

where,

$$\varphi^{(r)}(c) = \left(K^{(r)} * K^{(r)} - K^{(2r)} - \frac{\mu_2(K)}{2} K^{(2r+2)}\right)(c)$$

The h. MCV for bandwidth computed from modified cross-validation (MCV) [2] , [12]

4. Results and discussion

In this section, we consider the simulation as well as real life data sets to compare some methods techniques for bandwidth for the kernel estimation and its derivatives. Further, corresponding values for bandwidth are depicted and compared.

4.1. Monte Carlo simulation

In the Monte Carlo simulation study, data sets of size 45 have been generated with random variable $x\sim N(\mu = 0, \sigma^2 = 1)$ from R software. It is based on 10,000 replications to obtain the techniques of cross-validation methods (UCV,CCV,MCV) for bandwidth the kernel estimation and its derivatives [2] , [12] .

The following procedural code shows the method of unbiased cross-validation (UCV) for bandwidth the kernel estimation and its derivatives by using Data: x (45 obs.); Kernel: Gaussian

```
> iteration<-10000
> n<-45
> mu<-0
> sigmax<-1
> x<-rnorm(n,mu,sigmax)
> x
 [1] -0.54956389  1.04689009 -0.32569102  0.39324899  1.21368868  0.15185216
 [7]  0.01673154 -1.81966034  0.97438209 -0.32007329 -0.67662334  1.46333675
[13] -0.31761550 -0.79010354  0.69971357  1.50079303  1.42018723  0.44832012
[19]  0.87561001  0.87102969 -1.55306685  1.05567786 -0.22724150 -0.43851938
[25] -0.18134940 -1.15267252  1.25044104 -0.05823951 -0.07319079 -0.13568687
[31] -0.07421325  0.66530548 -1.21995170  2.13579256  0.47316818 -1.24977958
[37] -0.57386579 -0.21625646 -0.33441057 -0.81315883 -1.15983138  0.51516997
[43]  0.18838449  0.31007011 -0.03969973

> h2<-h.ucv(x = x, deriv.order = 0, kernel = "gaussian")
> h2
Call:        Unbiased Cross-Validation
Derivative order = 0
Data: x (45 obs.);     Kernel: gaussian
Min UCV = -0.2835591;   Bandwidth 'h' = 0.5944787

> h2<-h.ucv(x = x, deriv.order = 1, kernel = "gaussian")
> h2
Call:        Unbiased Cross-Validation
Derivative order = 1
Data: x (45 obs.);     Kernel: gaussian
Min UCV = -0.1199174;   Bandwidth 'h' = 0.7838137

> h2<-h.ucv(x = x, deriv.order = 2, kernel = "gaussian")
> h2
Call:        Unbiased Cross-Validation
Derivative order = 2
Data: x (45 obs.);     Kernel: gaussian
Min UCV = -0.1093683;   Bandwidth 'h' = 0.9782694

> h2<-h.ucv(x = x, deriv.order = 3, kernel = "gaussian")
> h2
Call:        Unbiased Cross-Validation
Derivative order = 3
Data: x (45 obs.);     Kernel: Gaussian
Min UCV = -0.1223378;   Bandwidth 'h' = 1.155548
```

We note from above that: Gaussian ; Derivative order = 0, 1,2,3; Bandwidth 'h' ≥ 0 corresponds to the lowest value for this criterion. Min UCV and large values of (h) produce smooth results because they increase bias and reduce variance,which affects the degree of smoothing of the estimated curve and its closeness to the true curve.

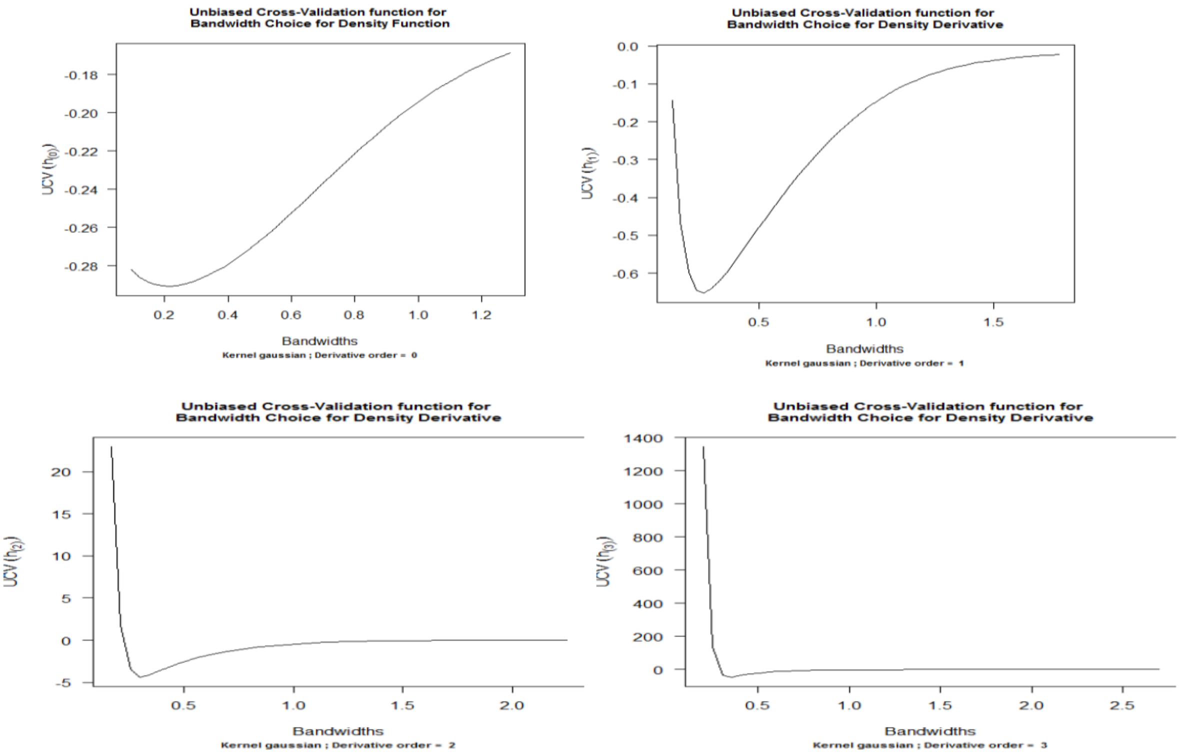

Figure 1. UCV for Bandwidth choice for density derivative

The following procedural code depicts the method of complete cross-validation (CCV) for bandwidth of kernel estimation and its derivatives based on Data: x (45 obs.); Kernel: Gaussian

```
> h4<-h.ccv(x = x, deriv.order = 0, kernel = "gaussian")
> h4
Call:      Complete Cross-Validation
Derivative order = 0
Data: x (45 obs.);    Kernel: gaussian
Min CCV = 0.01439067;   Bandwidth 'h' = 0.4746379

> h4<-h.ccv(x = x, deriv.order = 1, kernel = "gaussian")
> h4
Call:      Complete Cross-Validation
Derivative order = 1
Data: x (45 obs.);    Kernel: gaussian
Min CCV = -0.9627307;   Bandwidth 'h' = 0.149492
> h4<-h.ccv(x = x, deriv.order = 2, kernel = "gaussian")
> h4
Call:      Complete Cross-Validation
Derivative order = 2
Data: x (45 obs.);    Kernel: gaussian
Min CCV = -376.0201;    Bandwidth 'h' = 0.1502714
```

```
> h4<-h.ccv(x = x, deriv.order = 3, kernel = "gaussian")
> h4
Call:        Complete Cross-Validation
Derivative order = 3
Data: x (45 obs.);     Kernel: gaussian
Min CCV = -88037.8;    Bandwidth 'h' = 0.1596364
```

We note from above that the method of Complete cross-validation (CCV) for bandwidth of kernel estimation and its derivatives by using Data: x (45 obs.); Kernel: Gaussian ; Derivative order = 0, 1,2,3;; Bandwidth 'h' ≥ 0. It corresponds to the lowest value for this criterion Min CCV, large values of (h) produce smooth results because they increase bias and reduce variance,which affects the degree of smoothing of the estimated curve and its closeness to the true curve.

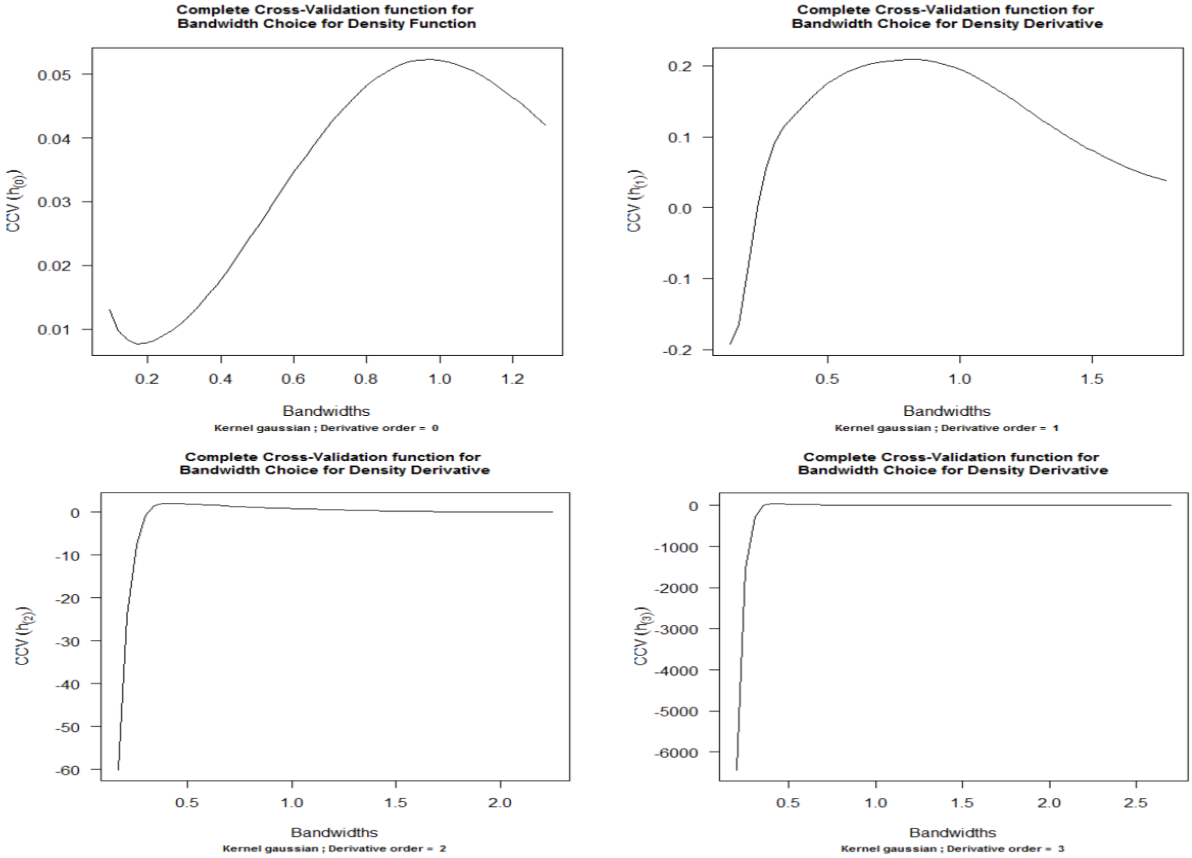

Figure 2. CCV for Bandwidth choice for density derivative

The following procedural code gives details about the procedure of modified cross-validation (MCV) for bandwidth the kernel estimation and its derivatives by using Data: x (45 obs.); Kernel: Gaussian

```
> h5<-h.mcv(x = x, deriv.order = 0, kernel = "gaussian")
> h5
Call:        Modified Cross-Validation
Derivative order = 0
Data: x (45 obs.);     Kernel: Gaussian
Min MCV = 0.01147959;   Bandwidth 'h' = 0.6800521

> h5<-h.mcv(x = x, deriv.order = 1, kernel = "gaussian")
> h5
Call:        Modified Cross-Validation
```

```
Derivative order = 1
Data: x (45 obs.);      Kernel: gaussian
Min MCV = 0.008113091;  Bandwidth 'h' = 0.7643845

> h5<-h.mcv(x = x, deriv.order = 2, kernel = "gaussian")
> h5
Call:           Modified Cross-Validation
Derivative order = 2
Data: x (45 obs.);      Kernel: gaussian
Min MCV = -0.009132536; Bandwidth 'h' = 0.8226816

> h5<-h.mcv(x = x, deriv.order = 3, kernel = "gaussian")
> h5
Call:           Modified Cross-Validation
Derivative order = 3
Data: x (45 obs.);      Kernel: gaussian
Min MCV = -0.1630683;   Bandwidth 'h' = 0.8788744
```

We note from above that the method of Modified cross-validation (MCV) for bandwidth the kernel estimation and its derivatives by using Data: x (45 obs.); Kernel: Gaussian ; Derivative order = 0, 1,2,3;; Bandwidth 'h' ≥ 0. It corresponds to the lowest value for this criterion Min MCV, large values of (h) produce smooth results because they increase bias and reduce variance ,which affects the degree of smoothing of the estimated curve and its closeness to the true curve.

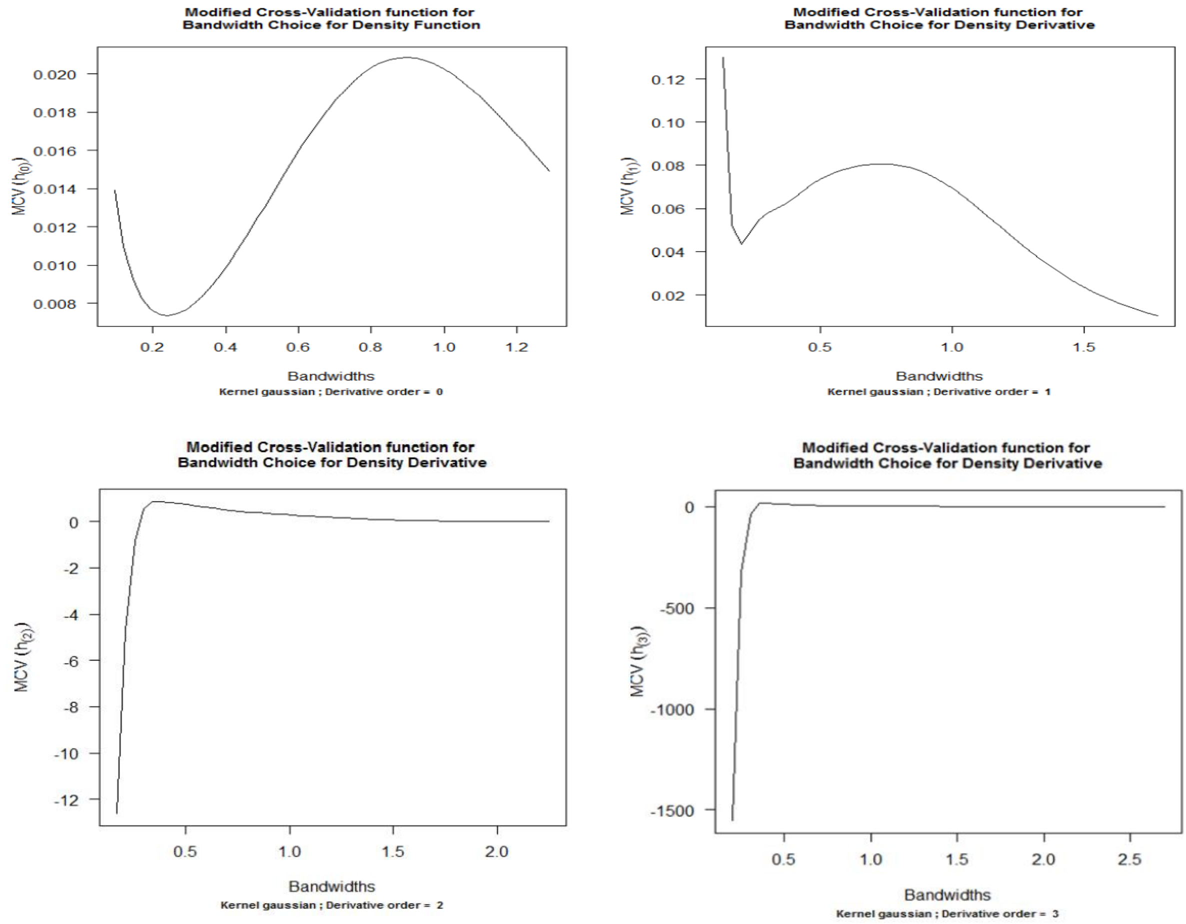

Figure 3. MCV for Bandwidth choice for density derivative

Table 1. Mean square error (MSE) of method of bandwidth

Derivative order = 0,1,2,3	UCV of MSE	CCV of MSE	MCV of MSE
Derivative order = 0	0.341331	0.233340	0.213870
Derivative order = 1	0.329578	0.221652	0.201156
Derivative order = 2	0.294897	0.209815	0.198023
Derivative order = 3	0.207286	0.198732	0.130170

Based on Table 1, the method of Modified cross-validation (MCV) for bandwidth; Derivative order = 0, 1,2,3; is the best method of bandwidth than UCV,CCV which corresponds to the lowest value for this criterion of MSE with derivative order = 3 corresponds to the lowest value from Derivative order = 0,1,2 for this criterion MSE.

4.2. Real life data

Here, we have been considered the real data sets pertaining as given below. The methods and corresponding results in Figures 4-6 are presented. The reported real data set are based on [2] , [12]. The data of failure times (in year) for 45 Patient has the following details:

0.047, 0.115, 0.121, 0.132, 0.164, 0.197,0.203, 0.260, 0.282, 0.296, 0.334, 0.395, 0.458, 0.466, 0.501, 0.507, 0.529, 0.534, 0.540, 0.641,0.644, 0.696, 0.841, 0.863, 1.099, 1.219, 1.271, 1.326, 1.447, 1.485, 1.553, 1.581, 1.589, 2.178,2.343, 2.416, 2.444, 2.825, 2.830, 3.578, 3.658, 3.743, 3.978, 4.003, 4.223

```
x<-c(0.047, 0.115, 0.121, 0.132, 0.164, 0.197,0.203, 0.260, 0.282, 0.296,
+  0.334, 0.395, 0.458, 0.466, 0.501, 0.507, 0.529, 0.534, 0.540, 0.641,0.644,
+  0.696, 0.841, 0.863, 1.099, 1.219, 1.271, 1.326, 1.447, 1.485, 1.553, 1.581,
+  1.589, 2.178,2.343, 2.416, 2.444, 2.825, 2.830, 3.578, 3.658, 3.743, 3.978,
+  4.003, 4.223)
> x
 [1] 0.047 0.115 0.121 0.132 0.164 0.197 0.203 0.260 0.282 0.296 0.334 0.395
[13] 0.458 0.466 0.501 0.507 0.529 0.534 0.540 0.641 0.644 0.696 0.841 0.863
[25] 1.099 1.219 1.271 1.326 1.447 1.485 1.553 1.581 1.589 2.178 2.343 2.416
[37] 2.444 2.825 2.830 3.578 3.658 3.743 3.978 4.003 4.223

> h2<-h.ucv(x = x, deriv.order = 0, kernel = "gaussian")
> h2
Call:       Unbiased Cross-Validation
Derivative order = 0
Data: x (45 obs.);     Kernel: gaussian
Min UCV = -0.339869;    Bandwidth 'h' = 0.2035855

> h2<-h.ucv(x = x, deriv.order = 1, kernel = "gaussian")
> h2
Call:       Unbiased Cross-Validation
Derivative order = 1
Data: x (45 obs.);     Kernel: gaussian
Min UCV = -1.465631;    Bandwidth 'h' = 0.238213

> h2<-h.ucv(x = x, deriv.order = 2, kernel = "gaussian")
> h2
Call:       Unbiased Cross-Validation
Derivative order = 2
```

Data: x (45 obs.);   Kernel: gaussian
Min UCV = -24.23165;   Bandwidth 'h' = 0.2845599
> h2<-h.ucv(x = x, deriv.order = 3, kernel = "gaussian")
> h2
Call: Unbiased Cross-Validation
Derivative order = 3
Data: x (45 obs.);   Kernel: gaussian
Min UCV = -458.7814;   Bandwidth 'h' = 0.3279021.

We note from Figure 4 that the method of Unbiased cross-validation (UCV) for bandwidth the kernel estimation and its derivatives by using real life Data: x (45 obs.); Kernel: Gaussian ; Derivative order = 0, 1,2,3;; Bandwidth 'h' ≥ 0 which corresponds to the lowest value for this criterion Min UCV, large values of (h) produce smooth results because they increase bias and reduce variance ,which affects the degree of smoothing of the estimated curve and its closeness to the true curve.

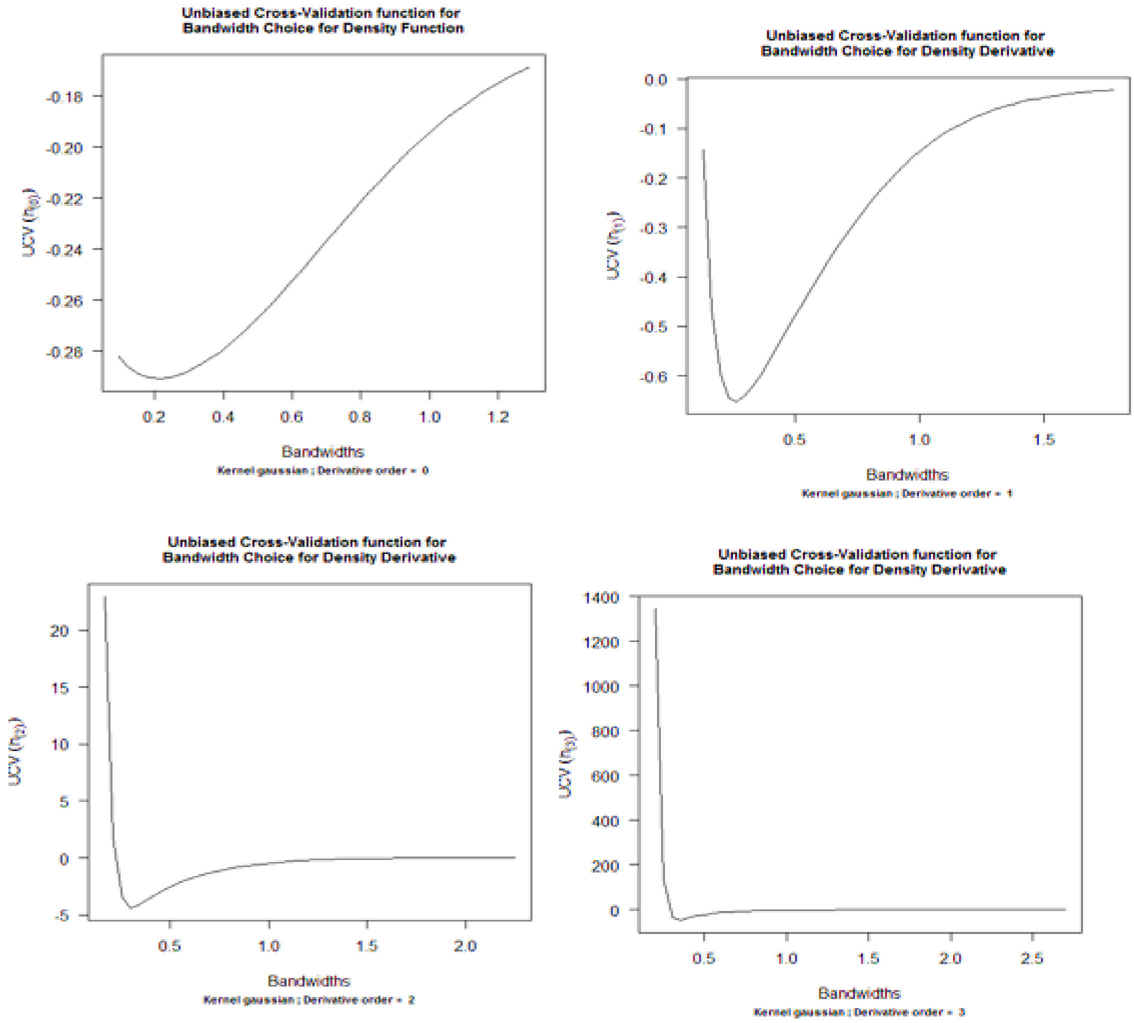

Figure 4. UCV for Bandwidth choice for density derivative
> h4<-h.ccv(x = x, deriv.order = 0, kernel = "gaussian")
> h4
Call: Complete Cross-Validation
Derivative order = 0
Data: x (45 obs.);   Kernel: gaussian
Min CCV = 0.03806313;   Bandwidth 'h' = 0.2011104

> h4<-h.ccv(x = x, deriv.order = 1, kernel = "gaussian")
> h4
Call: Complete Cross-Validation
Derivative order = 1
Data: x (45 obs.); Kernel: gaussian
Min CCV = 0.1769831; Bandwidth 'h' = 0.8465962
> h4<-h.ccv(x = x, deriv.order = 2, kernel = "gaussian")
> h4
Call: Complete Cross-Validation
Derivative order = 2
Data: x (45 obs.); Kernel: gaussian
Min CCV = 0.6411848; Bandwidth 'h' = 1.021682
> h4<-h.ccv(x = x, deriv.order = 3, kernel = "gaussian")
> h4
Call: Complete Cross-Validation
Derivative order = 3
Data: x (45 obs.); Kernel: gaussian
Min CCV = 1.882026; Bandwidth 'h' = 1.188471

We note from Figure 5 that the method of Complete cross-validation (CCV)for bandwidth the kernel estimation and its derivatives by using real life Data: x (45 obs.); Kernel: Gaussian ; Derivative order = 0, 1,2,3;; Bandwidth 'h' ≥ 0. It is based on the lowest value for this criterion Min CCV , large values of (h) produce smooth results because they increase bias and reduce variance,which affects the degree of smoothing of the estimated curve and its closeness to the true curve.

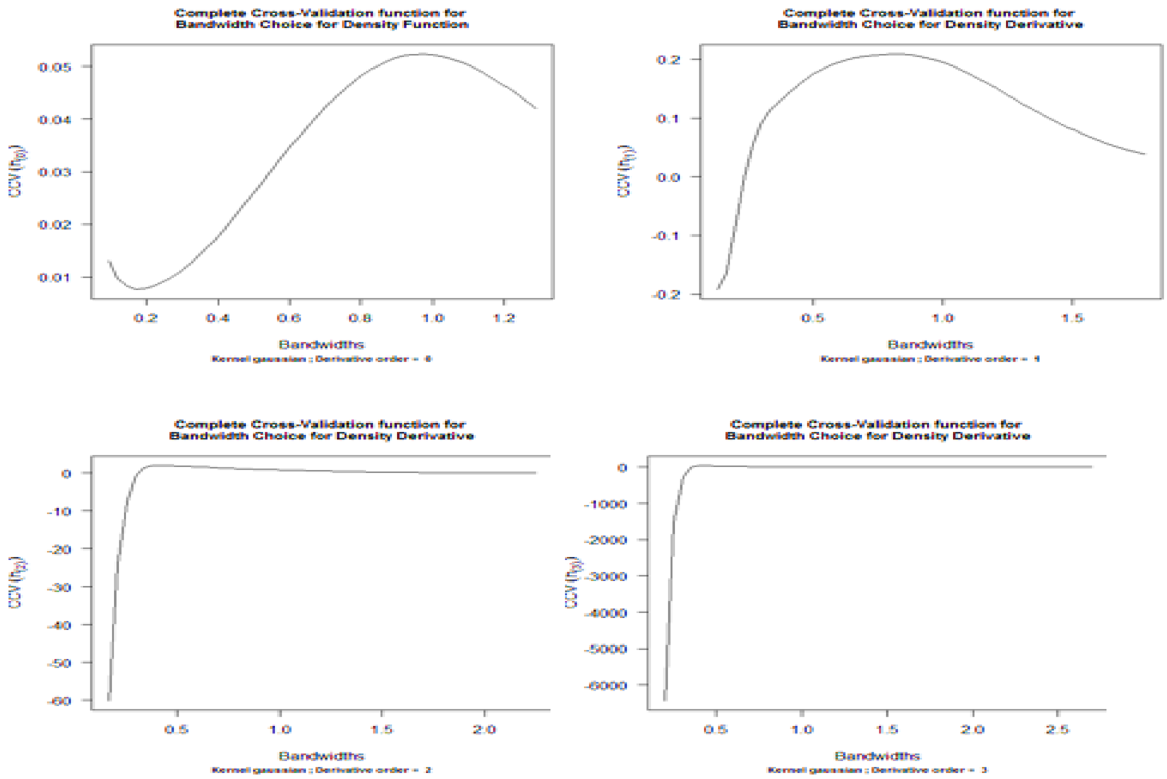

Figure 5. CCV for Bandwidth choice for density derivative.

> h5<-h.mcv(x = x, deriv.order = 0, kernel = "gaussian")
> h5
Call: Modified Cross-Validation
Derivative order = 0
Data: x (45 obs.); Kernel: gaussian

```
Min MCV = 0.01844765;   Bandwidth 'h' = 1.33804
> h5<-h.mcv(x = x, deriv.order = 1, kernel = "gaussian")
> h5
Call:          Modified Cross-Validation
Derivative order = 1
Data: x (45 obs.);      Kernel: gaussian
Min MCV = 0.01577866;   Bandwidth 'h' = 1.698393
> h5<-h.mcv(x = x, deriv.order = 2, kernel = "gaussian")
> h5
Call:          Modified Cross-Validation
Derivative order = 2
Data: x (45 obs.);      Kernel: gaussian
Min MCV = 0.01211543;   Bandwidth 'h' = 2.047737
> h5<-h.mcv(x = x, deriv.order = 3, kernel = "gaussian")
> h5
Call:          Modified Cross-Validation
Derivative order = 3
Data: x (45 obs.);      Kernel: gaussian
Min MCV = 0.007641128; Bandwidth 'h' = 2.380374
```

The above coding stands for modified cross-validation (MCV) for bandwidth the kernel estimation and its derivatives by using real life Data : x (45 obs.); Kernel: Gaussian.

We note that the Method Modified cross-validation (MCV) for bandwidth the kernel estimation and its derivatives by using real life Data: x (45 obs.); Kernel: Gaussian ; Derivative order = 0, 1,2,3; Bandwidth 'h' ≥ 0. It corresponds to the lowest value for this criterion Min MCV, large values of (h) produce smooth results because they increase bias and reduce variance, which affects the degree of smoothing of the estimated curve and its closeness to the true curve.

Table 2. Mean square error (MSE) of method of bandwidth

Derivative order = 0,1,2,3	UCV of MSE	CCV of MSE	MCV of MSE
Derivative order = 0	0.428192	0.349187	0.301872
Derivative order = 1	0.412786	0.3301942	0.3100028
Derivative order = 2	0.328562	0.3001829	0.2561923
Derivative order = 3	0.291817	0.281342	0.2018213

We note Table 2 that the method of Modified cross-validation (MCV) for bandwidth; Derivative order = 0, 1,2,3; is the best method of bandwidth than UCV, CCV which corresponds to the lowest value for this criterion MSE, and the Derivative order = 3 corresponds to the lowest value from Derivative order = 0,1,2 for this criterion MSE. Figure 6 depicts MCV for Bandwidth choice for density derivative.

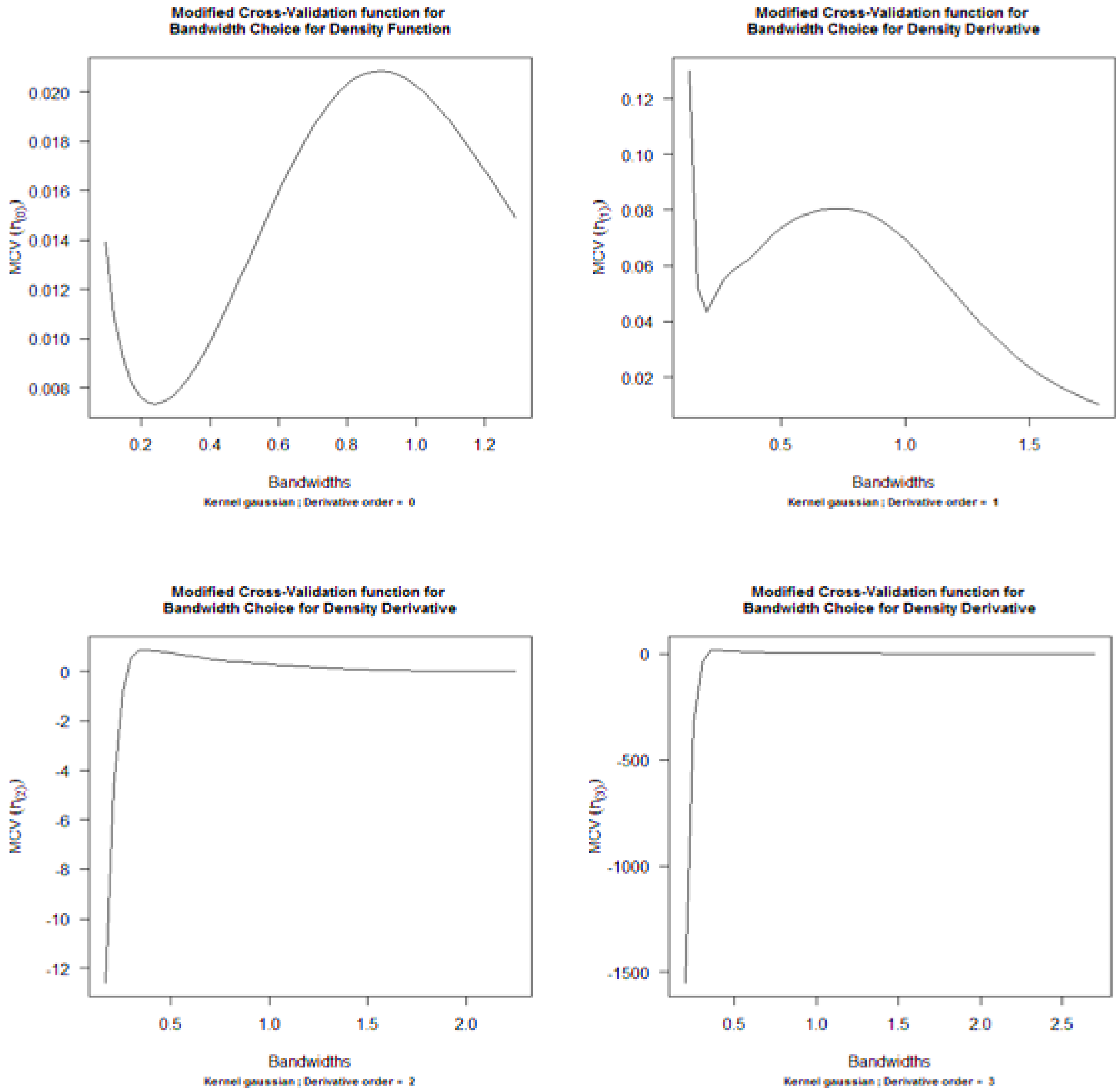

Figure 6. MCV for Bandwidth choice for density derivative

5. Conclusions

In this research, for both the simulated and real-life data sets, we have used in R procedures for bandwidth choice for density derivative including diverse functions based on kedd package introduced by Arsalane Chouaib Guidoum.

Methods for bandwidth the kernel estimation and its derivatives are by using simulated Data: x (45 obs.); Kernel: Gaussian as follows:

1. Min UCV =-0.2835591; Bandwidth 'h' =0.5944787, Derivative order =1; Min UCV =-0.1199174; Bandwidth 'h' = 0.7838137, Derivative order = 2; Min UCV = -0.1093683; Bandwidth 'h' = 0.9782694, Derivative order = 3; Min UCV = -0.1223378;   Bandwidth 'h' = 1.155548.

2. Min CCV = -88037.8; Bandwidth 'h' = 0.1596364, Min MCV = 0.01147959; Bandwidth 'h' = 0.6800521; Derivative order = 1; Min MCV = 0.008113091; Bandwidth 'h' = 0.7643845; Derivative order = 2; Min MCV = -0.009132536; Bandwidth 'h' = 0.8226816; Derivative order = 3 ; Min MCV = -0.1630683; Bandwidth 'h' = 0.8788744.

On the other hands, the methods for bandwidth the kernel estimation and its derivatives by using Real Life Data: x (45 obs.); Kernel: Gaussian, the obtained results are for UCV, CCV and MCV are as follows:
3.Min UCV = -0.340; Bandwidth 'h' = 0.204; Derivative order = 1; Min UCV = -1.466; Bandwidth 'h' = 0.283. Derivative order = 2; Min UCV = -24.232; Bandwidth 'h' = 0.285; Derivative order = 3;Min UCV = -458.781; Bandwidth 'h' = 0.328.
4.Min CCV =0.038; Bandwidth 'h' = 0.201; Derivative order = 1; Min CCV = 0.177; Bandwidth 'h' = 0.847. Derivative order = 2; Min CCV = 0.641; Bandwidth 'h' =1.022; Derivative order =3; Min CCV = 1.882; Bandwidth 'h' = 1.188.
5.Min MCV = 0.018; Bandwidth 'h' = 1.338; Derivative order = 1; Min MCV = 0.016; Bandwidth 'h' = 0.698. Derivative order = 2; Min MCV = -0.012; Bandwidth 'h' = 2.048; Derivative order = 3; Min MCV = 0.008; Bandwidth 'h' = 2.380.
Concisely, the method of Modified cross-validation (MCV) is the best method in term of bandwidth than UCV and CCV which corresponds to the lowest value for this criterion MSE.

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