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A modified intersection of confidence intervals approach in the multivariate data density estimation

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Data density estimation provides estimates of the probability function from which a set of data is drawn. It is better to estimate density from the data, hence the variable bandwidth approach. One of the popular approach in density estimation is the multivariate kernel density estimation (MKDE). It is a nonparametric estimation approach which requires a kernel function and a bandwidth. This work focuses on a proposed modified intersection of confidence intervals ($MICI_H$) approach in the multivariate data density estimation. It is based on the intersection of confidence intervals (ICI). It is an attempt to correct the problem of discontinuities and boundary value problem in the density to be constructed. The quality of the estimates obtained of the proposed approach showed some improvements over the existing methods in kernel density estimation. This is seen in the lower asymptotic mean integrated error (AMISE) and a relative rate of convergence in the approach.

Keywords: density; estimator; bandwidth; multivariate; optimal.

1. Introduction

Data density estimation provides estimates of the probability function from which a set of data is drawn. Density is better estimated from the data set. In density estimation, the true density is unknown. One of the popular approaches is the multivariate kernel density estimation. It is a nonparametric estimation approach which requires a kernel function and a bandwidth (window size or smoothing parameter H). When we consider the variable window sizes on the multivariate cluster kernel density estimation (MCKDE) and the intersection of confidence interval (ICI) approaches for estimating densities, we identified points for improvements, so that the methods could be adaptive to the multivariate kernel density estimation (MKDE). In most cases, the above methods could lead to under-fitting of the data set density, an indication that the methods are often less optimal result. See Bowman and Azzalini (1997) and Zhang and Chan (2011). In this presentation, a data-driven approach that requires only the knowledge of the use of pilot plots and the bandwidth sizes from the data set with a view to correcting the identified problems, while aiming for lower asymptotic mean integrated squared error (AMISE) and faster rates of convergence in the approaches is proposed. The aim of this study is basically on how to fit density to observations in the multivariate data sets.

The multivariate kernel density estimator that we are going to study is a direct extension of the univariate kernel estimator. Let $X_1, ..., X_n$ denote a d-variate random sample having a density f. We shall use the notation $X_i = (X_{i1}, ..., X_{in})^T$ to denote the Xi and a generic vector $X \in \mathcal{R}^d$ has the representation $x = (x_1, ..., x_d)^T$. The d-variate random sample $X_1, ..., X_n$ drawn from f the kernel estimator evaluated at x is given by:

$$\hat{f}(X, H) = \frac{1}{n} \sum_{i=1}^{n} K_H(x - X_i) \tag{1.1}$$

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where n is the sample size, and H is a symmetric positive definite d x d matrix called the bandwidths, the smoothing parameters or the bandwidth matrix, and $K_H(x) = |H|^{-\frac{1}{2}} K(H^{-\frac{1}{2}}x)$, |.| stands for the determinant of H and K is d-variate kernel satisfying $\int k(x)dx = 1$ which is a regularity condition, where the integral is over $\mathcal{R}^d$ unless stated otherwise. However, in choosing kernel to use, the gaussian kernel

$$K(u) = \frac{1}{\sqrt{2\pi}} exp(-\frac{u^2}{2})$$

is a popular choice among many kernels. Silverman, (1986), Bowman and Azzalini (1997), Kathovnik and Shmulevich (2002). However, the matrix H is a smoothing parameter. It specifies the 'width' of the kernel around each sample point X_i.

When we consider the works on variable bandwidths sizes in the average cluster approach and the intersection of confidence interval (ICI) methods applied to MKDE, one is tasked with how sensitive these methods are, and the errors committed using these methods? What are the effects when we extend them to multivariate kernel density? These questions led to the reasons for their modifications. We identified areas for improvements, so that the methods could be more adaptive. This work is basically concerned with a method of achieving adaptive multivariate kernel density estimation. The aim of this study includes how to fit density to data sets.

2. Literature Review

There exist some methods of estimating bandwidths in the multivariate kernel density. Some of these methods use a fixed window width. However, approaches that uses varied window widths in the course of density estimation which seems adaptive are few. A review of available variable methods showed basically that the cross-validation, the plug-in bandwidths approaches or any subjective method (which are fixed smoothing approaches). See Doung and Hazelton (2005) and Dicu and Stanga (2013). There is the cluster and the average cluster approach by Wu and Tsai (2004), Wu et al (2007) and Ogbeide et al (2016) which are more data sensitive are often used. The window width controls the smoothness of the fitted density curve. The true density is unknown.

$$H_{AMISE} = agr \min_{h \in H} AMISE(H)$$

According to Wand and Jones (1995) and Horova et al (2008), they asserted that it was better to estimate optimal MISE element-wise. They further asserted that the ideal optimal bandwidth selector that is point-wise adaptive is given by

$$H_{AMISE} = agr \min_{h \in H} AMISE(H) \tag{2.1}$$

where agr is partition optimal evaluation of bandwidths from the data. See Horova et al (2008). So we shall adopt point-wise adaptive bandwidth procedures in estimating densities, where H is equivalent to the selection of optimal h_{ij} in $\{H_1, ..., H_n\}$. In order to correct the problem of over fitting and under fitting of the data density as the case may be as observed in Dicu and Stanga (2013) and Ogbeide et al (2016), hence, the modifications of the ICI approach to density estimation. This modified approach adjusts the amount of bandwidths using some idea from the kernel nearest neighbour estimation of the density to the multivariate data. Its smoothing parameter would be a n x d dimensional matrix obtained from forming relevant number of clusters in an information matrix. The Euclidean distance would be used to form bandwidths.

3. Methodology

In this section, the proposed method of estimating densities is presented. This method is the modified intersection of confidence intervals ($MICI_H$) approach. The $MICI_H$ procedure is basically a minimization of $AMISE(H_i)$ with respect to H, where it is equivalent to the selection of optimal h_{ij} in $\{H_1, ..., H_n\}$

Our data driven bandwidth matrix selector $\hat{H}$ is point-wise data adaptive base selection approach. Its density uses a pilot plot in order to address identified problem(s). Equation (3.2.1) is proposed,

$$\hat{H}_{AMISE} = agr \min_{H_{D_j} \in H} AMISE(H) \tag{3.1}$$

Assume that

$$H = \{H_1 \leq H_2 \leq ...H_n\} \tag{3.2}$$

is a finite collection of window sizes, starting with a smallest $h_{ij} \in H$ and we determine a sequence of confidence intervals given by

$$D_{ij} = [\underline{L}_{ij}, \underline{U}_{ij}], i = 1, ...n, j = i, ...d$$

$$\underline{L}_{ij} = \hat{f}_{H_{ij}}(X_i) - \beta.std\{\hat{f}_{H_{ij}}(X_i)\} \tag{3.3}$$

$$\underline{U}_{ij} = \hat{f}_{H_{ij}}(X_i) - \beta.std\{\hat{f}_{H_{ij}}(X_i)\}$$

Each h_{ij} corresponding to a value in $H_{ij} \in H$, We assume the data at hand is normally distributed. Subjecting the data to normality, we propose $\beta = 1.06$ via normal reference rule. See Scott (1992).
Next compute,

$$H_{opt_{ij}}(X_{ij}) = \left[\frac{abs}{v}[\underline{L}_{ij}, \underline{U}_{ij}]\right] \tag{3.4}$$

where

$$abs[\underline{L}_{ij}, \underline{U}_{ij}] = |[\underline{L}_{ij}, \underline{U}_{ij}]| = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{d}|\underline{L}_{ij} - \underline{U}_{ij}|^2}$$

See Gray (1997) for lengths and distances' details. Subjectively we adopt $v = 2$, considering pilot plots. Where v is a positive real number. The $MICI_H$ procedure is based on consideration of the intersection of the adjusted intervals D_{ij} , $1 \leq i \leq d$. So, we use the bandwidth sizes $H_{opt_{i-1}}(X)$ where

$$H_{opt_{ij}}(X) = \left[\frac{abs}{2}[\underline{L}_{ij}, \underline{U}_{ij}]\right] \quad \text{with} \quad H_{opt_i}(X) \leq H_{opt_{i-1}}(X) \tag{3.5}$$

where $H = (h_{ij}) = \begin{pmatrix} h_{11} & h_{12} & \ldots & h_{1d} \\ h_{21} & h_{22} & \ldots & h_{2d} \\ . & . & \ldots & . \\ . & . & \ldots & . \\ . & . & \ldots & . \\ h_{n1} & h_{n2} & \ldots & h_{nd} \end{pmatrix}$

Consequently, substituting bandwidths h_{ij} from equation (3.5) into the kernel density estimator

$$\hat{f}_{H_i}(X, H) = \frac{1}{n}\sum_{i=1}^{n} K_H(x - X_i)$$

to obtain the density estimates. Thus, we proposed an algorithm.

Algorithm 1

The algorithm involves the following steps:

Step 1: $\underline{L}_{ij} \Leftarrow -\infty$, $\underline{U}_{ij} \Leftarrow -\infty$, $j = 1, 2, \cdots, n$

Step 2: while $(\underline{L}_{ij} \leq \underline{U}_{ij})$ and $(i \leq j)$ do

Step 3: $\underline{L}_{ij} \Leftarrow \hat{f}_{H_{ij}}(X_i) - \beta.std\{\hat{f}_{H_{ij}}(X_i)\}$

Step 4: $\underline{U}_{ij} \Leftarrow \hat{f}_{H_{ij}}(X_i) + \beta.std\{\hat{f}_{H_{ij}}(X_i)\}$

Step 5: $\underline{L}_{ij} \Leftarrow max[\underline{L}, \underline{L}_{ij}], \underline{U}_{ij} \Leftarrow min[\underline{U}, \underline{U}_{ij}]$

Step 6: $i \Leftarrow i + 1$

Step 7: $H_{opt_{ij}}(X) = \left[\frac{abs}{2}[\underline{L}_{ij}, \underline{U}_{ij}]\right]$

Step 8: do $i \Leftarrow i + 1$

Step 9: $H_{opt_i}(X) \leq H_{opt_{i-1}}(X)$

Step 10: Compute h_{ij} in H $\in H_i$

Step 11: end while $(i = n)$.

4. Results

4.1 *Application/Results*

We present estimates based on mode related expectation adaptive maximization (MEAM) imputation approach. Here we use the data of Rubin and Little (2002, Pg 310, exercise 14.7) on a survey of 20 graduates of a university class five year after graduation with missing data of race (White or Others) and income (in Dollar). 1 represents male, 2 represents female. 1 represents white race, 2 represents the other race and - represents missing observations. The results are presented in the Appendix.

The calculated bandwidth selections errors and convergence rate from the data set with missing observation in Rubin and Little (2002, Pg 310) are given in Table 4.4 in the Appendix. The relative errors, h^* (which is the error in relation to the fixed optimal bandwidth value), and the convergence rates of methods are also calculated therein.

Table 4.4 showed that there are reduced relative errors, h^* (which is the error in relation to the fixed optimal bandwidth value) and $AMISE^*$ in the proposed methods. The proposed method has faster convergence rates compared to other versions. That is, the $MICI_H$ have lower error propagation and faster convergence rates when used to estimates the Little and Rubin (2002) data with fixed optimal H, MCKDE and the MMCKDE approaches. The estimated bandwidth selection errors and convergence rates from the data set with missing observation in Rubin and Little (2002, Pg 310) data, via the various methods favour the use of the $MICI_H$ approach over the other approaches. This is because its bandwidth errors are smaller as well as having higher convergence rate. The MMCKDE has some improvement over the MCKDE approach. These can be seen in Table 4.3 and Table 4.4. Generally, the AMISE shows the difference between the "true density" and the estimated density. The AMISE for $MICI_H$ is smaller than that of MMCKDE and MCKDE approaches.

The graphical displays (see Appendix) from the various approaches have identifiable differences from Figures 1a-2d, using the fixed H, MCKDE, MMCKDE and $MICI_H$ for the dataset in Little and Rubin (2002) page 310. The $MICI_H$ did not indicate under fitting for the dataset. The application of the modified intersection of confidence intervals ($MICI_H$) corrects identified cluster sampling points of discontinuities in the multivariate kernel nearest neighbour density estimates. The $MICI_H$ method which is based on the ICI rule, produces smaller but optimal smoothing parameters extended to the multivariate data set. This is an attempt to achieve reduced error and show more hidden features of the density.

4.2 *Advantages of the proposed $MICI_H$ method*

(1) The $MICI_H$ scheme produces smaller but optimal smoothing parameters. The estimates of the smoothing parameters h_{ih} are smaller in $MICI_H$ scheme when compared to the ICI approach. This contributes significantly to the density estimate by showing more hidden features of the density.

(2) The choice of the smoothing parameters h_{ij} in $H_j \in H$ follows the procedure $H_{opt_j}(X) \leq H_{opt_{j-1}}(X)$ in each coordinate directions. This enables the bandwidth to be controlled such that no new bandwidth h would be larger than the preceeding bandwidths. This ensures that the scheme is adaptive. Otherwise the scheme is done in reversed order. The procedure $H_{opt_i}(X) \leq H_{opt_{i-1}}(X)$ can be seen in step 9 of the proposed algorithm.

(3) This approach provides full bandwidths matrix from the data, (see Table 4.2.) for the multivariate kernel density estimation. This is a better approach because it is data sensitive.

Like in every other improved method, the $MICI_H$ scheme requires only simple but two additional steps when compared to the ICI approach. These additional procedures are in the choice and application of the smoothing parameters to multivariate density estimation. $MICI_H$ and MMCSKDE generate full bandwidths matrices. The cost of these steps brings about the adaptive density to be constructed. So far the Modified Intersection of Confidence Interval ($MICI_H$) approach in estimating density has been presented. Some improvements were seen, when the quality of the density estimates obtained by this approach were compared with other approaches using the mean-squared error criterion.

5. Conclusion

The quality of the proposed approach estimates have shown some improvements when assessed and compared with the estimates obtained using existing approaches. These are seen in the errors generated using these proposed approach. The $MICI_H$ convergence rates compared to some other known approaches when applied to some data sets showed an improvement.

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Appendix

List of tables

Table 4.1: The estimates of data set with missing observation in Rubin and Little (2002, Pg 310) using the MEAM imputation approach.

Case	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Sex	1	1	1	2	2	2	2	2	2	2	2	1	1	2	2	1	1	1	2	2
Race	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2	-	-	-	-	-
$MEAM_{Race}$	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	1	1
Income	25	46	31	05	16	26	08	10	02	-	-	20	29	-	32	-	-	38	15	-
$MEAM_{Income}$	25	46	31	05	16	26	08	10	02	11.1666	11.2380	20	29	37.292	32	34	34.6875	38	15	11.6005

Table 4.2: Estimated bandwidths for the multivariate cluster sampling kernel density estimation (MCKDE), the modified multivariate cluster sampling kernel density estimation (MMCKDE) and $MICI_H$ approaches for data set with missing observation in Rubin and Little (2002, Pg 310).

Data point	Approaches							
X	Fixed H_{Race}	MCKDE Race	MMCKDE Race	$MICI_H$ Race	Fixed H_{Income}	MCKDE Income	MMCKDE Income	$MICI_H$ Income
1	0.2500	0.2500	0.2500	0.2500	5.1500	5.0000	5.0000	5.0000
2	0.2500	0.2500	0.2500	0.2500	5.1500	7.5000	7.5000	5.5000
3	0.2500	0.2500	0.2500	0.2500	5.1500	4.5000	4.5000	4.5000
4	0.2500	0.2500	0.2500	0.2500	5.1500	13.0000	6.5000	6.5000
5	0.2500	0.2500	0.2500	0.2500	5.1500	5.5000	2.7500	4.9300
6	0.2500	0.2500	0.2500	0.2500	5.1500	4.1600	2.0800	4.1600
7	0.2500	0.2500	0.2500	0.2500	5.1500	5.0000	5.0000	4.7900
8	0.2500	0.2500	0.2500	0.2500	5.1500	9.0000	4.5000	4.0500
9	0.2500	0.2500	0.2500	0.2500	5.1500	1.0000	1.0000	2.2100
10	0.2500	0.2500	0.2500	0.2500	5.1500	5.4000	5.4000	4.7000
11	0.2500	1.0000	0.5000	0.2300	5.1500	5.4000	5.4000	4.9000
12	0.2500	0.2500	0.2500	0.2500	5.1500	3.5000	3.5000	3.4500
13	0.2500	0.2500	0.2500	0.2500	5.1500	4.5000	4.5000	3.2500
14	0.2500	0.2500	0.2500	0.2500	5.1500	5.1400	5.1400	4.2700
15	0.2500	0.2500	0.2500	0.2500	5.1500	3.6400	3.6400	3.1200
16	0.2500	0.2500	0.2500	0.2500	5.1500	1.7100	1.7100	2.0300
17	0.2500	1.0000	0.5000	0.2300	5.1500	1.7100	0.8550	1.2200
18	0.2500	0.2500	0.2500	0.2500	5.1500	4.6900	4.6900	4.5300
19	0.2500	0.2500	0.2500	0.2500	5.1500	11.500	5.7500	5.0200
20	0.2500	0.2500	0.2500	0.2500	5.1500	1.0600	1.0600	1.0400
Var	**0.0000**	**0.2812**	**0.1875**	**0.0072**	**0.0000**	**8.003**	**7.7639**	**6.9157**

Table 4.3: Estimated densities for the multivariate cluster sampling kernel density estimation (MCKDE), the modified multivariate cluster sampling kernel density estimation (MMCKDE) and $MICI_H$ approaches from the data set with missing observation in Rubin and Little (2002, Pg 310).

Data point	Density estimates from various bandwidths approaches							
X	Fixed H density Race	MCKDE Race	MMCKDE Race	$MICI_H$ Race	Fixed H Income	MCKDE Income	MMCKDE Income	$MICI_H$ Income
1	0.0414	0.0414	0.0414	0.0414	0.0543	0.0543	0.0543	0.0543
2	0.0414	0.0414	0.0414	0.0414	0.099	0.0981	0.099	0.0993
3	0.0414	0.0414	0.0414	0.0414	0.0674	0.0660	0.0674	0.0674
4	0.0414	0.0414	0.0414	0.0414	0.0109	0.0109	0.0163	0.0171
5	0.0414	0.0414	0.0414	0.0414	0.0348	0.0348	0.0370	0.0382
6	0.0414	0.0414	0.0414	0.0414	0.0565	0.0565	0.0770	0.0830
7	0.0414	0.0414	0.0414	0.0414	0.0177	0.0174	0.0174	0.0172
8	0.0414	0.0414	0.0414	0.0414	0.0301	0.0331	0.0329	0.0331
9	0.0414	0.0414	0.0414	0.0414	0.0042	0.0043	0.0043	0.0044
10	0.0414	0.0414	0.0414	0.0414	0.0231	0.0279	0.0279	0.0281
11	0.0482	0.0488	0.0499	0.0501	0.0267	0.0312	0.0324	0.0332
12	0.0820	0.0820	0.0820	0.082	0.0431	0.0435	0.0554	0.0556
13	0.0820	0.0820	0.0820	0.0820	0.0621	0.0630	0.0630	0.0640
14	0.0820	0.0820	0.0820	0.0820	0.0846	0.0853	0.0867	0.0872
15	0.0820	0.0820	0.0820	0.0820	0.0693	0.0695	0.0695	0.0699
16	0.0414	0.0414	0.0414	0.0414	0.0414	0.0401	0.0267	0.0269
17	0.0414	0.0414	0.0418	0.0421	0.0826	0.0826	0.0826	0.0791
18	0.0414	0.0414	0.0414	0.0414	0.0825	0.0825	0.0825	0.0831
19	0.0414	0.0414	0.0414	0.0414	0.0341	0.0345	0.0347	0.0334
20	0.0414	0.0414	0.0414	0.0414	0.0279	0.0279	0.0257	0.0250
Density sum	**0.9972**	**0.9978**	**0.9993**	**0.9998**	**0.9523**	**0.9601**	**0.9927**	**0.9995**

Table 4.4: Table of bandwidth selections errors and convergence rate from the estimated bandwidths for the race and income using the multivariate cluster sampling kernel density estimation (MCKDE), the modified multivariate cluster sampling kernel density estimation (MMCKDE) and the $MICI_H$ approaches from the data set with missing observation in Rubin and Little (2002).

Approach	Relative error v_e	Variance	δ	h^*	$AMISE^*$	Convergence rate
MCKDE (Race)	0.3000	0.2812	0.5302	0.1637	6.5021×10^{-2}	0.4071
MMCKDE (Race)	0.1000	0.1875	0.4330	0.1091	2.3555×10^{-2}	0.7411
$MICI_H$ (Race)	**0.0080**	**0.0072**	**0.0848**	**0.0041**	5.4365×10^{-3}	**0.9763**
MCKDE (Income)	-0.0097	8.003	2.8289	4.6596	8.9928×10^{-2}	1.0029
MMCKDE (Income)	-0.2085	7.7639	2.7863	4.5204	5.7629×10^{-2}	1.8675
$MICI_H$ (Income)	**-0.2313**	**6.9157**	**2.6297**	**4.0265**	5.0502×10^{-2}	**1.9995**

Graphical densities display

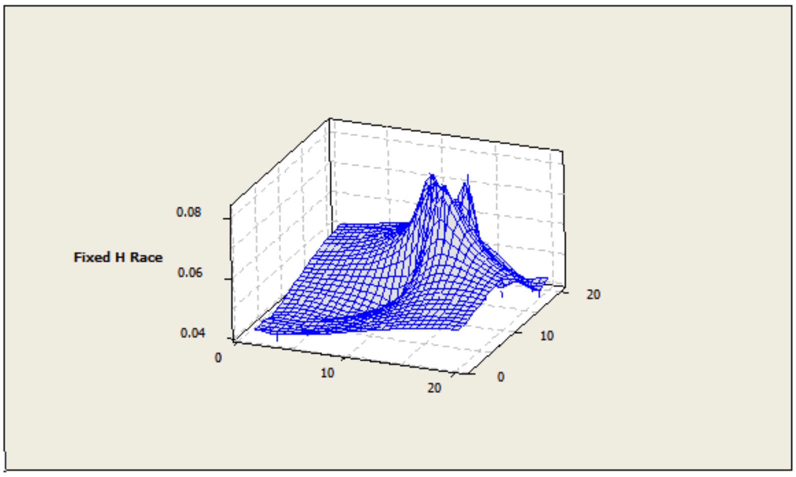

Figure 1a: Graphical density estimates for Race data using the fixed H approach.

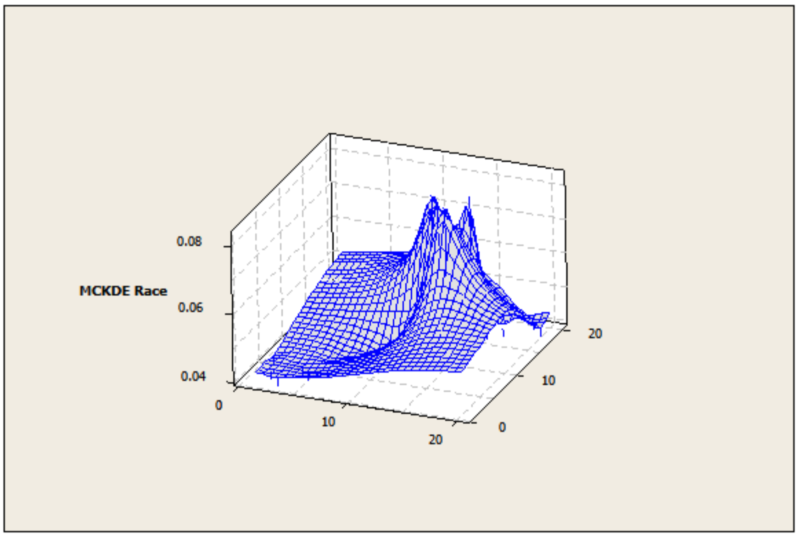

Figure 1b: Graphical density estimates for Race data using the MCKDE approach.

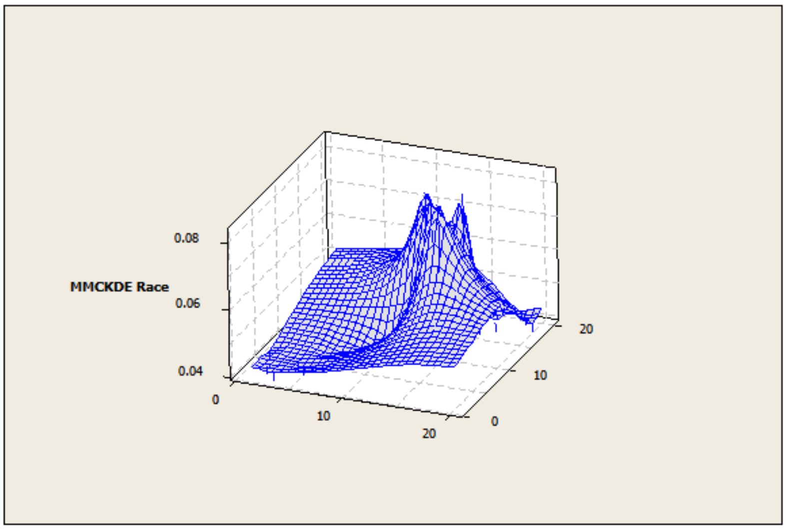

Figure 1c: Graphical density estimates for Race data using the MMCKDE approach.

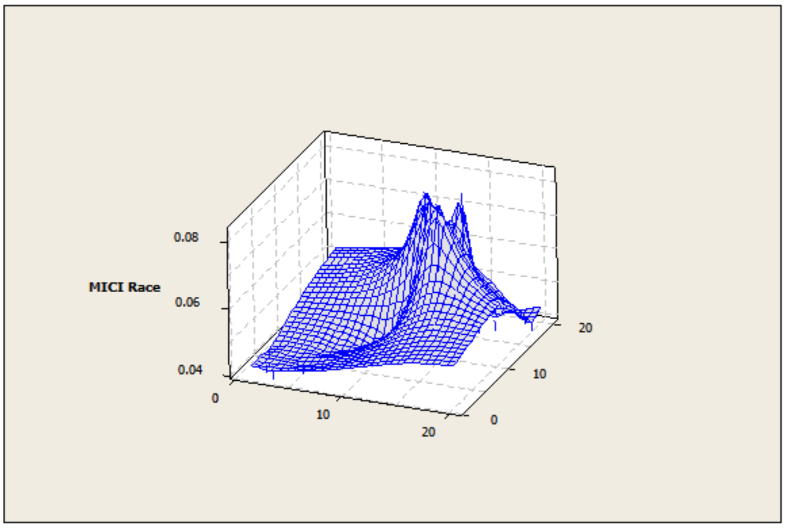

Figure 1d: Graphical density estimates for Race data using the $MICI_H$ approach.

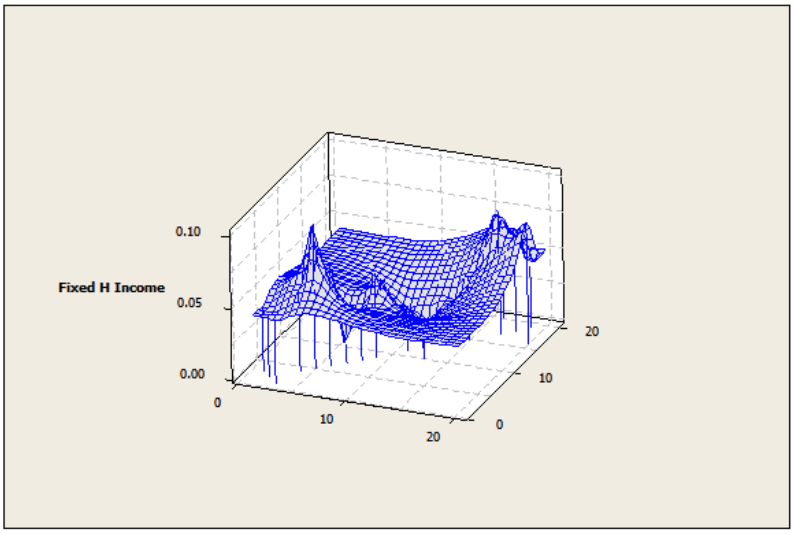

Figure 2a: Graphical density estimates for Income using the fixed H approach.

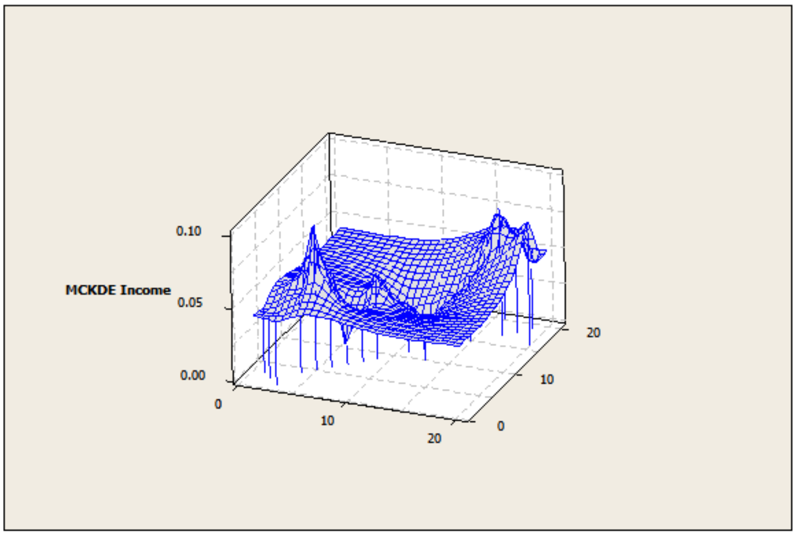

Figure 2b: Graphical density estimates for Income using the MCKDE approach.

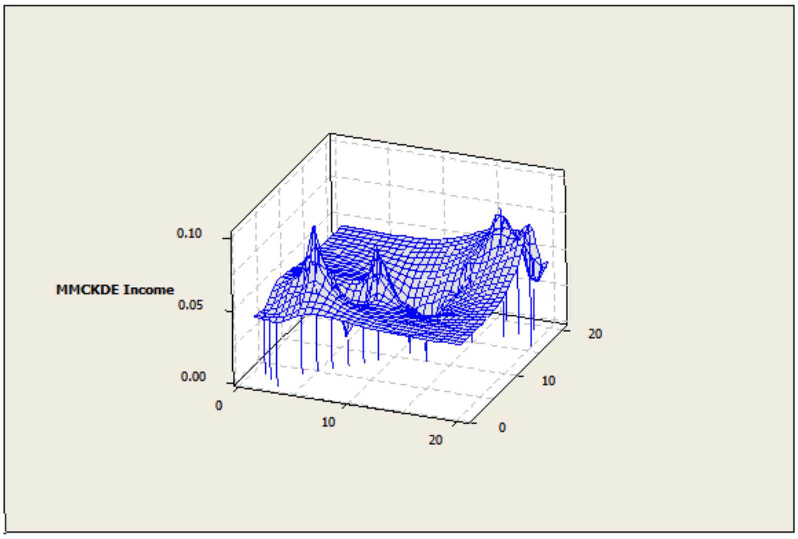

Figure 2c: Graphical density estimates for Income using the MMCKDE approach.

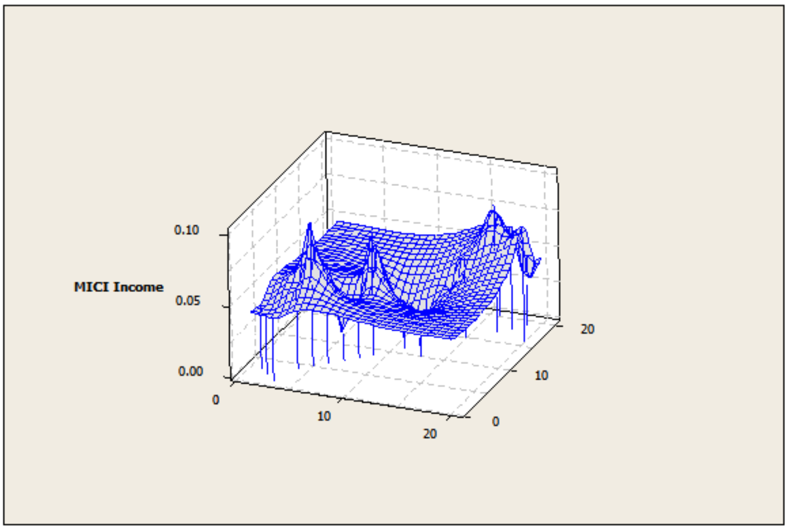

Figure 2d: Graphical density estimates for Income using the $MICI_H$ approach.