

Derivative and Evaluation of the Exact Mean Hellinger Distance in the Kernel Density Estimation

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Abstract. The Mean Integrated Square Error (MISE) and the Mean Hellinger Distance (MHD) are two measures of error to evaluate the kernel density estimator. The exact MISE was derived by Marron and Wand (1992). In this investigation we will derive an exact formula for the MHD. Also, using simulations and several mixture of normal densities, we will compare and study the relationships among the exact MHD, it is asymptotic, the MISE and it is asymptotic.

1 Introduction

Let X_1, X_2, \dots, X_n be a random sample from the unknown probability density function $f(x)$. The well known kernel density estimator for $f(x)$ is given by:

$$\hat{f}(x, h) = n^{-1} \sum_{i=1}^n k_h(x - X_i),$$

where k is a kernel function and h is the bandwidth. The k is usually a chosen to be a symmetric function such that $\int k(x)dx = 1$. Several techniques are proposed to select the bandwidth, part of them can be found in Wand and Jones (1994), Jones, Marron and Sheather (1996) and Mugdadi and Jetet (2010). There are several measures of error criterion to evaluate the estimator $\hat{f}(x)$ among them the Mean Integrated Square Error (MISE) and the Mean Hellinger Distance (MHD) of $\hat{f}(x)$, where.

$$MISE(\hat{f}(x)) = \int E(\hat{f}(x; h) - f(x))^2 dx,$$

and the

$$MHD\{\hat{f}(x; h)\} = E \int \{\hat{f}^{1/2}(x; h) - f^{1/2}(x)\}^2 dx.$$

More details about these two measures of error can be found in Wand and Jones (1994) and Ahmad and Mugdadi (2006) respectively. During this study, we will derive a closed formula for the exact $MHD\{\hat{f}(\cdot; x)\}$, then we will perform comparisons among the MISE, MHD, the approximate MISE and the approximate MHD .

The Exact MSE and MISE calculations were first performed by Fryer (1976) and Deheuvels (1977) for estimation of normal densities. Marron and Wand (1992) extended the MISE calculations to the case of normal mixture densities and they derived a exact formula for the MISE. In this investigation we derive a exact formula for the MHD

2 The Exact MHD

First we will derive some preliminary results in order to derive the closed form formula for the $MHD(\hat{f}(x))$. We will assume the pdf f to be $N(0, \sigma^2)$ and the kernel function to be $N(0, 1)$. Also, the notation $\phi_\sigma(x) = (2\pi\sigma^2)^{-1/2} \exp(-x^2/2\sigma^2)$ will be used to denote the $N(0, \sigma^2)$ density. Then $\phi_\sigma(x - \mu)$ is the density of the $N(\mu, \sigma^2)$ distribution. Consider the expectation of $\hat{f}(x)$ at $x \in \mathfrak{R}$.

$$\begin{aligned}
 E\hat{f}(x; h) &= E \left\{ \frac{1}{m} \sum_{i=1}^m K_h(x - x_i) \right\} \\
 &= \int K_h(x - y) f(y) dy \\
 &= (K_h * f)(x) \\
 &= \int \phi_h(y - x) \phi(x) dy \\
 &= \phi_{(h^2+1)^{1/2}}(x).
 \end{aligned}$$

Also the Multinomial Theorem which will be used later is give by:

$$(x_1 + x_2 + \dots + x_m)^n = \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{n}{k_1 \ k_2 \ \dots \ k_m} x_1^{k_1} x_2^{k_2} \dots x_m^{k_m}.$$

Theorem

Assume we have a data from $N(0, \sigma^2)$ and the kernel is $N(0, 1)$, then the exact MHD for the kernel density estimator can be written as:

$$\begin{aligned}
 MHD(\hat{f}(x)) &= 21 - 2\sigma_1(2\pi^3)^{1/4} \phi_{(\sigma_1^2)^{1/2}}(0) \\
 &\cdot 2 \sum_{n=0}^{\infty} [c(n) \sum_{j=1}^n (-1)^j \frac{1}{(cm)^{n-j}} \\
 &\cdot \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{n-j}{k_1, \dots, k_m}].
 \end{aligned}$$

where $c(n) = \frac{(-1)^n (2n)!}{(-2n)n!2^{4n}}$

Proof

The MHD expression can be written as:

$$\begin{aligned}
 MHD\{\hat{f}(x; h)\} &= E \int \{\hat{f}^{1/2}(x; h) - f^{1/2}(x)\}^2 dx \\
 &= \int E\{\hat{f}(x; h) + f(x) - 2\hat{f}^{1/2}(x; h)f^{1/2}(x)\} dx \\
 &= \int [E\hat{f}(x; h) + f(x) - 2E\{\hat{f}^{1/2}(x; h)\}f^{1/2}(x)] dx \\
 &= \int \phi_{(h^2+1)^{1/2}}(x) dx + 1 \\
 &\quad - 2 \int E\{\hat{f}^{1/2}(x; h)\} f^{1/2}(x) dx \\
 &= 2 - 2I.
 \end{aligned}$$

In order to find the expression for $E\{\hat{f}^{1/2}(x; h)\}$ we will use the fact: $\sqrt{1+x} = \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{(-2n)n!2^{4n}} x^n$ for $|x| < 1$

Let $u = \hat{f}(x; h) - 1 = \lambda - 1$, $A(n, m, j) = \binom{n}{j} (-1)^j \frac{1}{(cm)^{n-j}}$ and $c(n) = \frac{(-1)^n (2n)!}{(-2n)n!2^{4n}}$,

where

$$\begin{aligned} \lambda &= \hat{f}(x; h) = \frac{1}{m\sqrt{2\pi h^2}} \sum_{i=1}^m e^{\frac{-1}{2h^2}(x-x_i)} \\ &= \frac{1}{cm} \sum_{i=1}^m \lambda_i, \end{aligned}$$

$\lambda_i = e^{\frac{-1}{2h^2}(x-x_i)}$ and $c = \frac{1}{\sqrt{2\pi h^2}}$. Then

$$\begin{aligned} \sqrt{1+u} &= \sqrt{1+\lambda-1} = \sqrt{\lambda} = \sqrt{\hat{f}(x; h)} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{(-2n)n!2^{2n}} (\lambda-1)^n \\ &= \sum_{n=0}^{\infty} c(n)(\lambda-1)^n. \end{aligned}$$

Therefore we can write

$$\begin{aligned} E\sqrt{\hat{f}(x; h)} &= E \sum_{n=0}^{\infty} c(n)(\lambda-1)^n \\ &= \sum_{n=0}^{\infty} c(n)E\{(\lambda-1)^n\}. \end{aligned} \tag{2.1}$$

Consider

$$\begin{aligned} E\{(\lambda-1)^n\} &= E \left\{ \sum_{j=1}^n \binom{n}{j} (-1)^j \lambda^{n-j} \right\} \\ &= \sum_{j=1}^n \binom{n}{j} (-1)^j E\{\lambda^{n-j}\} \\ &= E \left\{ \binom{n}{0} \lambda^n - \binom{n}{1} \lambda^{n-1} + \right. \\ &\quad \left. \dots + \binom{n}{j} \lambda^{n-j} (-1)^j + \dots + (-1)^n \right\}. \end{aligned} \tag{2.2}$$

Note that

$$\begin{aligned} \lambda^{n-j} &= \frac{1}{m^{n-j}} \left(\sum_{i=1}^m \frac{\lambda_i}{c} \right)^{n-j} \text{ and let } n-j = l \\ \lambda^l &= \frac{1}{(cm)^l} \left(\sum_{i=1}^m \lambda_i \right)^l. \end{aligned}$$

Using the multinomial theorem we can write

$$\begin{aligned} \lambda^l &= \frac{1}{(cm)^l} [(\lambda_1 + \lambda_2 + \dots + \lambda_m)^l] \\ &= \frac{1}{(cm)^l} \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = l}} \binom{l}{k_1 \ k_2 \ \dots \ k_m} \lambda_1^{k_1} \lambda_2^{k_2} \dots \lambda_m^{k_m}. \end{aligned}$$

Now consider

$$\begin{aligned} \lambda_1^{k_1} \lambda_2^{k_2} \dots \lambda_m^{k_m} &= [e^{-(x-x_1)^2/2h^2}]^{k_1} \dots [e^{-(x-x_m)^2/2h^2}]^{k_m} \\ &= e^{-k_1(x-x_1)^2/2h^2} \dots e^{-k_m(x-x_m)^2/2h^2} \\ &= e^{-\sum_{i=1}^n k_i(x-x_i)^2/2h^2} . \end{aligned}$$

Therefore

$$\lambda^l = \frac{1}{(cm)^l} \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{l}{k_1, k_2, \dots, k_m} e^{-\sum k_i(x-x_i)^2/2h^2} . \tag{2.3}$$

Now plug-in (2.3) in to (2.2) and we can write

$$\begin{aligned} E\{(\lambda - 1)^n\} &= E \left\{ \binom{n}{0} \lambda^n - \binom{n}{1} \lambda^{n-1} + \dots + A(n, m, j) \right. \\ &\quad \times \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{n-j}{k_1, k_2, \dots, k_m} e^{-\sum k_i(x-x_i)^2/2h^2} \\ &\quad \left. + \dots + (-1)^n \right\} . \end{aligned} \tag{2.4}$$

Therefore,

$$\begin{aligned} &E \left\{ A(n, m, j) \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{n-j}{k_1, k_2, \dots, k_m} e^{-\sum k_i(x-x_i)^2/2h^2} \right\} \\ &= A(n, m, j) \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{n-j}{k_1, k_2, \dots, k_m} E \left\{ e^{-\sum k_i(x-x_i)^2/2h^2} \right\} \\ &= A(n, m, j) \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{n-j}{k_1 \dots k_m} \\ &\quad \cdot \int e^{-\sum k_i(x-x_i)^2/2h^2} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy . \end{aligned} \tag{2.5}$$

Consider the integral part of (2.5)

$$\begin{aligned} \int e^{-\sum k_i(x-x_i)^2/2h^2} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy &= \int e^{-\sum k_i(x-y)^2/2h^2} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy \\ &= \int e^{-l(x-y)^2/2h^2} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy \\ &= \int e^{-l(x-y)^2/2h^2} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy; \quad \sigma_1^2 = h^2/l \\ &= \sqrt{2\pi\sigma_1^2} \int \phi_{\sigma_1}(y-x) \phi_1(y) dy \\ &= \sqrt{2\pi\sigma_1^2} \phi_{(\sigma_1^2+1)^{1/2}}(x) . \end{aligned} \tag{2.6}$$

Thus (2.5) can be written as

$$\binom{n}{j} (-1)^j \frac{1}{(cm)^{n-j}} \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n-j}} \binom{n-j}{k_1 \dots k_m} \sqrt{2\pi\sigma_1^2} \phi_{(\sigma_1^2+1)^{1/2}}(x). \tag{2.7}$$

Therefore using (2.5), (2.7) can be written as

$$E\{(\lambda - 1)^n\} = \sum_{j=1}^n \left\{ \binom{n}{j} (-1)^j \frac{1}{(cm)^{n-j}} \times \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n-j}} \binom{n-j}{k_1 \dots k_m} \sqrt{2\pi\sigma_1^2} \phi_{(\sigma_1^2+1)^{1/2}}(x) \right\}. \tag{2.8}$$

Now plug in (2.7) in to (2.1) to get

$$\begin{aligned} E\sqrt{\hat{f}(x; h)} &= E \sum_{n=0}^{\infty} c(n) (\lambda - 1)^n \\ &= \sum_{n=0}^{\infty} c(n) E\{(\lambda - 1)^n\} \text{ by(1)} \\ &= \sum_{n=0}^{\infty} c(n) \left\{ \sum_{j=1}^n \binom{n}{j} (-1)^j \frac{1}{(cm)^{n-j}} \right. \\ &\quad \left. \times \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n-j}} \binom{n-j}{k_1 \dots k_m} \sqrt{2\pi\sigma_1^2} \phi_{(\sigma_1^2+1)^{1/2}}(x) \right\}. \end{aligned}$$

Therefore,

$$\begin{aligned} \int E\sqrt{\hat{f}(x; h)} f^{1/2}(x) dx &= \int \left[\sum_{n=0}^{\infty} c(n) \left[\sum_{j=1}^n \binom{n}{j} (-1)^j \frac{1}{(cm)^{n-j}} \right. \right. \\ &\quad \left. \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n-j}} \binom{n-j}{k_1 \dots k_m} \sqrt{2\pi\sigma_1^2} \right. \\ &\quad \left. \left. \phi_{(\sigma_1^2+1)^{1/2}}(x) [\phi(x)]^{1/2} \right] \right] dx \end{aligned}$$

Consider

$$\begin{aligned} \int \phi_{(\sigma_1^2+1)^{1/2}}(x) \phi_{\sqrt{2}}(x) dx &= (8\pi)^{1/4} \phi_{(\sigma_1^2+1+2)^{1/2}}(0) \\ &= (8\pi)^{1/4} \phi_{(\sigma_1^2+3)^{1/2}}(0). \end{aligned}$$

Hence we can write

$$\begin{aligned} \int E\sqrt{\hat{f}(x; h)} f^{1/2}(x) dx &= \sum_{n=0}^{\infty} c(n) \left[\sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}} \binom{n-j}{k_1, \dots, k_m} \right. \\ &\quad \left. \cdot \sqrt{2\pi\sigma_1^2} (8\pi)^{1/4} \phi_{(\sigma_1^2+3)^{1/2}}(0) \right]. \end{aligned}$$

Thus, the exact MHD can be written as

$$2[1 - 2\sigma_1(2\pi^3)^{1/4}\phi_{(\sigma_1^2)^{1/2}}(0) \cdot \sum_{n=0}^{\infty} [c(n) \sum_{j=1}^n (-1)^j \frac{1}{(cm)^{n-j}} \cdot \sum_{\substack{k_1, k_2, \dots, k_m \geq 0 \\ k_1 + k_2 + \dots + k_m = n}}^n \binom{n-j}{k_1, \dots, k_m}]]$$

3 A Comparison among MISE, AMISE, MWHD and AMWHD

AMISE provides an easier analysis of the variance-bias trade off. Also provides a closed form expression for the optimal bandwidth, which will be denoted by h_{AMISE} .

$$h_{AMISE} = \left[\frac{R(k)}{\mu_2(k)^2 R(f'') n} \right]^{1/5}$$

The optimal bandwidth is calculated for the densities Standard normal distribution, Bimodal normal, Kurtotic Normal, Skewed normal, and Skewed Bimodal Normal (see Marron and Wand (1992)). Here the kernel k is taken to be the standard normal. For this kernel $R(k) = (2\pi^{1/2})^{-1}$ and $\mu_2(k) = 1$. Also $R(f'')$ must be calculated for each density. For the standard normal density, $R(f'') = 3(8\pi^{1/2})^{-1}$; for the bimodal density $R(f'') = 2\pi^{-1/2}(19e^{-4} + 3)$; for the kurtotic normal density $R(f'') = 7387.1498\pi^{-1}$; for the skewed normal density $R(f'') = 4.9087\pi^{-1}$; and for the skewed bimodal normal density $R(f'') = 9.811288\pi^{-1}$.

Tables 1 to 5 give the values of h_{AMISE} , also the tables give the MWHD and AMWHD and MISE and AMISE values when each corresponding value of h is used to create the kernel density estimate for f .

Sample size	h_{AMISE}	MWHD	AMWHD	MISE	AMISE
10	0.6683771	0.006482034	0.013189350	0.02577320	0.05275742
20	0.5818561	0.004003377	0.007575295	0.01607537	0.03030118
30	0.5365341	0.003102222	0.005476795	0.01248757	0.02190718
40	0.5065351	0.002529913	0.004350864	0.01021333	0.01740346
50	0.4844261	0.002192208	0.003639549	0.00883057	0.01455819
60	0.4670801	0.001930302	0.003145593	0.00778131	0.01258237
70	0.4528996	0.001716971	0.002780642	0.00692164	0.01112257
80	0.4409644	0.001582848	0.002498915	0.00637497	0.00999566
90	0.4306982	0.001437614	0.002274204	0.00578314	0.00909681
100	0.4217174	0.001342390	0.002090372	0.00539959	0.00836148
500	0.3056522	0.000415497	0.000576829	0.00166825	0.00230731
1000	0.2660857	0.000259514	0.000331301	0.00104108	0.00132520

Table 1. Asymptotic analysis for the standard normal density.

Sample size	h_{AMISE}	MWHD	AMWHD	MISE	AMISE
10	0.5265108	0.010778400	0.016743180	0.03846808	0.06697270
20	0.4583542	0.006461690	0.009616430	0.02432821	0.03846572
30	0.4226521	0.004722364	0.006952498	0.01814435	0.02780999
40	0.3990205	0.003865223	0.005523189	0.01497321	0.02209275
50	0.3816043	0.003290934	0.004620211	0.01280267	0.01848085
60	0.3679400	0.002841681	0.003993161	0.01114893	0.01597265
70	0.3567694	0.002545817	0.003529876	0.00999479	0.01411950
80	0.3473676	0.002319659	0.003172239	0.00911578	0.01268896
90	0.3392804	0.002097948	0.002886981	0.00828693	0.01154792
100	0.3322058	0.001957106	0.002653615	0.00772051	0.01061446
500	0.2407760	0.000584756	0.000732254	0.00233156	0.00292901
1000	0.2096077	0.000355834	0.000420569	0.00142127	0.00168227

Table 2. Asymptotic analysis for the Bimodal normal density.

Sample size	h_{AMISE}	MWHD	AMWHD	MISE	AMISE
10	0.10086960	0.07199216	0.08739462	0.24313800	0.34957850
20	0.08781210	0.04307696	0.05019503	0.14415660	0.20078010
30	0.08097224	0.03114141	0.03629006	0.10697630	0.14516020
40	0.07644488	0.02463330	0.02882947	0.08520769	0.11531790
50	0.07310825	0.02035942	0.02411619	0.07186512	0.09646476
60	0.07049043	0.01754922	0.02084317	0.06279939	0.08337267
70	0.06835036	0.01546181	0.01842495	0.05559269	0.07369979
80	0.06654913	0.01367891	0.01655818	0.04971318	0.06623274
90	0.06499978	0.01253516	0.01506922	0.04579358	0.06027687
100	0.06364443	0.01142401	0.01385111	0.04205413	0.05540446
500	0.04296321	0.00386062	0.00410372	0.01497229	0.01641491
1000	0.03740165	0.00226801	0.00235697	0.00888610	0.00942788

Table 3. Asymptotic analysis for the Kurtotic normal density.

Sample size	h_{AMISE}	MWHD	AMWHD	MISE	AMISE
10	0.2314282	0.024798690	0.038091560	0.08646607	0.15236630
20	0.2014700	0.014579360	0.021877860	0.05299060	0.08751143
30	0.1857770	0.010463400	0.015817280	0.03898160	0.06326912
40	0.1753898	0.008247085	0.012565530	0.03112176	0.05026212
50	0.1677345	0.007001383	0.010511210	0.02655518	0.04204485
60	0.1617283	0.006062104	0.009084642	0.02311910	0.03633857
70	0.1568183	0.005385616	0.008030644	0.02058424	0.03212258
80	0.1526857	0.004881074	0.007217002	0.01875771	0.02886801
90	0.1491310	0.004482127	0.006568025	0.01727130	0.02627210
100	0.1460213	0.004093811	0.006037106	0.01580647	0.02414842
500	0.1058278	0.001177494	0.001666001	0.00465622	0.00666400
1000	0.0921284	0.000673826	0.000956866	0.00268084	0.00382746

Table 4. Asymptotic analysis for the Skewed normal density.

Sample size	h_{AMISE}	MWHD	AMWHD	MISE	AMISE
10	0.4025223	0.014796730	0.021900560	0.05166863	0.08760223
20	0.3504160	0.008645617	0.012578570	0.03221991	0.05031427
30	0.3231214	0.006456072	0.009094067	0.02449353	0.03637627
40	0.3050549	0.005102752	0.007224490	0.01966709	0.02889796
50	0.2917400	0.004335389	0.006043370	0.01682776	0.02417348
60	0.2812935	0.003800738	0.005223170	0.01479806	0.02089268
70	0.2727535	0.003394171	0.004617179	0.01329518	0.01846872
80	0.2655657	0.003112582	0.004149380	0.01218742	0.01659752
90	0.2593830	0.002829565	0.003776254	0.01112178	0.01510501
100	0.2539744	0.002577683	0.003471004	0.01012707	0.01388402
500	0.1840755	0.000784913	0.000957809	0.00313287	0.00383123
1000	0.1602470	0.000461089	0.000550117	0.00184370	0.00220046

Table 5. Asymptotic analysis for the Skewed Bimodal normal density.

Many insights can be gained from the analysis of Tables 1 through 5. First, focus on the error criterion. In each table the AMWHD is approaching the exact MWHD and the AMISE is approaching exact MISE as the sample size gets larger. This is no surprise because the AMWHD and the AMISE are large sample approximations to the exact MWHD and exact MISE respectively. In addition, the exact MWHD, AMWHD, exact MISE and AMISE become smaller as the sample size increases, which means the kernel density estimator is becoming more accurate and performs better. One would expect $\hat{f}(x)$ to give a better picture of $f(x)$ with large sample sizes since there is more data present.

Next focus on the values of h in each table. As the sample size increases, the bandwidth decreases. In other words, less smoothing is needed with larger sample sizes. Again, this is attributed to the fact that more information about the true density is present.

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