

## The Derivation of the Efficiency of the Second Order d-dimensional Spherical Kernels

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### *Abstract*

*The focus of this study is on efficiency of the second order spherical kernels. A formula for the efficiency using the epanechnikov kernel as the basis for the optimum based on the fundamentals of Asymptotic Mean Integrated Squared Error (AMISE) is constructed. The resultant expression is a d-dimensional efficiency of the second order spherical kernels*

**Keywords:** Density estimation, spherical kernel, efficiency, Asymptotic mean integrated square error

### 1.0 Introduction

The term density estimation is simply using a random variable  $X$  obtained from an observed data to construct an estimate  $\hat{f}$  of an underlying density function  $f$  [1,2]. The estimation of the unknown density function can be achieved using either the parametric or the nonparametric methods. The parametric methods to density estimation assumes a functional form for the density, and the maximum likelihood technique, for example, can then be used to estimate the unknown parameters. Unless we use the form of the density a priori, assuming a functional form for a density could lead very often to erroneous inference [3].

Sometimes, when the distribution is unknown, then the nonparametric density estimation, like the histogram or the kernel estimator is applied. This approach allows the data to speak for itself [4,5]. The nonparametric methods are flexible and computationally intensive. The trauma associated with the tedious computations in the nonparametric approach has been considerably reduced via the advent of easily fast computing power in the twentieth century [6]. In this work, we concentrate on one class of nonparametric density estimators, namely, the kernel density estimator. This kernel density estimator is a more reliable statistical technique that deals with some of the problems associated with histogram which are discussed in [4,7,8]. Kernel density estimation has found relevance in estimating geographic customer densities [9] and recently in the area of human motion tracking or pattern recognition [10,11,12], for data lying on a d-dimensional torus ( $d \geq 1$ ) [13], in huge computational requirement for large-scale analysis [14,15], and in the area of multivariate cluster sampling kernel approach to multivariate density estimation [16].

A common term in kernel density estimation is the bandwidth or window width which is analogous to the bin width in histogram. The bandwidth determines how much smoothing is done. Generally, a narrow bandwidth implies that more points are allowed and this lead to a better density estimate. This technique, also known as the Parzen window estimator, was studied in the seminal paper by [17], although, the basic idea was independently discussed in [18,19].

For a  $d$ -variate random variable  $X_1, X_2, \dots, X_d$  drawn from a density  $f$  the generalized kernel estimation is given by Wand and Jones [5] as

$$f(\mathbf{x}; H) = n^{-1} \sum_{i=1}^n K_H(\mathbf{x} - \mathbf{X}_i) \quad (1.1)$$

where  $\mathbf{x} = (x_1, x_2, \dots, x_d)^T$  and  $\mathbf{X}_i = (x_{i1}, x_{i2}, \dots, x_{id})^T, i = 1, 2, \dots, n$  In this case  $K(\bullet)$  is assumed to be the multivariate ( $d$ -dimensional) kernel. This kernel is assumed to be a spherical symmetric probability density function.  $H$  is the bandwidth matrix which is symmetric and positive-definite. The scaled and unscaled kernels are related by

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$$K_H(\mathbf{x}) = |H|^{-\frac{1}{2}} K\left(H^{-\frac{1}{2}} \mathbf{x}\right).$$

An equal bandwidth  $h$  in all directions as in (1.1) corresponds to  $H = h^2 I_d$ , where  $I_d$  is the  $d \times d$  identity matrix. This leads to the expression

$$\hat{f}(\mathbf{x}; h) = \frac{1}{nh^d} \sum_{i=1}^n K(h^{-1}(\mathbf{x} - \mathbf{X}_i)) \tag{1.2}$$

The parameterization  $H = h^2 I_d$  can effectively be used if the components of the data vector are commensurate. Two transformation approaches have been suggested to overcome this problem [4,6,20]. These transformations involve either pre-scaling each axis (that is, normalize to unit variance, for instance) or pre-whitening the data (that is, linearly transform to have unit covariance matrix). A detailed study of this can be found in [21]. The transformation guarantees the use of the form involving single bandwidth as in (1.2).

Many of the studies in density estimation have been centred on the univariate kernel density estimators [4]. The focus of this paper, however, is on the multivariate settings with emphasis on the generalized expression for the efficiency of the second-order  $d$ -dimensional spherical kernels using the epanechnikov kernel as the basis for the optimum. The choice of epanechnikov kernel is based on the fact that it minimizes MISE. Other kernels are not that suboptimal [5]. The efficiency concept is used in kernel density estimation to analyse the effect of second-order multivariate kernels so that an appropriate kernel can be chosen.

The choice of (1.2) is that it enables one to obtain closed form expressions for the optimal bandwidth and the asymptotic mean integrated squared error (AMISE). Hence the generalized expression for the efficiency of second-order  $d$ -dimensional

kernel is derived. Throughout this paper,  $\int$  is the shorthand for  $\int_{\mathcal{R}^d}$ .

The concept of efficiency in kernel density estimation has not received much attention and as such literature in this area is quite scanty. The efficiency for univariate kernels popularized by [4] is the efficiency of other kernel function relative to the epanechnikov kernel when using other kernel function. This represents the ratio of sample sizes necessary to obtain the same minimum AMISE (for a given kernel function) when using the epanechnikov as when using any other kernel. In the case of multivariate kernels [5] based their approach on the ratio of spherically symmetric kernel relative to the product kernel. A new computational approach for the efficiency of second-order multivariate product kernels was developed by [22]. The epanechnikov kernel was used as a theoretical underpinning for deriving the efficiency formula. Thus, in this work, the generalized efficiency of the second-order  $d$ -dimensional spherical kernels is derived. This work is motivated by the works of [4,5,22].

The rest of the paper is organized as follows. In section 2, we introduce AMISE for the  $d$ -dimensional kernel which is very germane to the derivation of the proposed efficiency formula. Section 3 is dedicated to the derivation of the proposed efficiency of the second-order  $d$ -dimensional spherical kernel. Section 4 finally concludes with brief discussion on further study.

## 2.0 The Amise for the Multivariate Kernel Density Estimator

To have a good understanding of the performance of the Kernel Density Estimator (KDE), a measure of distance is needed. Though several criteria abound in the literature for measuring this distance, but one common criterion that can be used to achieve this, which can be manipulated easily, is the Integrated Squared Error (ISE), otherwise known as the  $L_2$ -norm. The

ISE between the estimate  $\hat{f}(\mathbf{x})$  and the actual density  $f(\mathbf{x})$  is given by

$$ISE\{\hat{f}(\mathbf{x}), f(\mathbf{x})\} = \int \{\hat{f}(\mathbf{x}) - f(\mathbf{x})\}^2 d\mathbf{x} \tag{1.3}$$

Equation (1.3) can be averaged over the realized  $n$  points to obtain the MISE which is defined as

$$MISE\{\hat{f}(\mathbf{x}), f(\mathbf{x})\} = E \int (\hat{f}(\mathbf{x}) - f(\mathbf{x}))^2 d\mathbf{x} \tag{1.4}$$

This equation (1.4) is a measure of the average performance of the KDE, averaged over the support of the density and the different realized  $n$  points. Thus, from [5], the expression (1.4) can be written as a sum of integrated square bias and integrated variance of  $\hat{f}_H(\mathbf{x})$ . That is,

$$MISE\{\hat{f}_H(\mathbf{x}), f(\mathbf{x})\} = \int (E\{\hat{f}_H(\mathbf{x})\} - f(\mathbf{x}))^2 d\mathbf{x} + \int Var\{\hat{f}_H(\mathbf{x})\} d\mathbf{x} \tag{1.5}$$

This last expression (1.5) is cumbersome to solve analytically, so we resort to an asymptotic large sample approximation for this expression (1.5) which is usually derived via the Taylor's series expansion referred to as the Asymptotic Mean Integrated Squared Error (AMISE).

Based on the assumption that the kernel function is symmetric about the origin (i.e.,  $\int \mathbf{w}k(\mathbf{w})d\mathbf{x} = \mathbf{0}$ ) and has finite second moment (i.e.,  $\int \mathbf{w}\mathbf{w}^T k(\mathbf{w})d\mathbf{w} = \mu_2 I_d$ ), where  $\mathbf{0}$  is a  $d \times 1$  vector of zeros and  $\mu_2 = \int w_i^2 k(\mathbf{w})d\mathbf{w}$  is independent of  $i$  [23,4]. Then, setting  $H = h^2 I_d$ , the AMISE between the actual density and the estimate can be shown to be

$$AMISE(\hat{f}_h(\mathbf{x}), f(\mathbf{x})) = \frac{R(k)}{nh^d} + \frac{1}{(2!)^2} \mu_2(k)^2 h^4 \int (\nabla^2 f(\mathbf{x}))^2 d\mathbf{x} \quad (16)$$

where  $R(k) = \int k(\mathbf{x})^2 d\mathbf{x}$ ,  $\nabla^2 f(\mathbf{x}) = \sum_{i=1}^n \frac{\partial^2 f(\mathbf{x})}{\partial x_i^2}$  and  $\mu_2(k) = \int x_1^2 k(\mathbf{x})d\mathbf{x}$

From the AMISE expression the optimal bandwidth  $h_{AMISE}$  can be obtained by differentiating (1.6) wrt the bandwidth  $h$  and setting it to zero, we have

$$h_{opt} = \left\{ \frac{dn^{-1} R(k)}{\mu_2(k) R(\nabla^2 f(\mathbf{x}))} \right\}^{\frac{1}{d+4}} \quad (1.7)$$

Substituting (1.7) into (1.6), it can be shown that the minimum AMISE for the  $d$ -dimensional kernels is

$$AMISE(\hat{f}_h(\mathbf{x}), f(\mathbf{x})) = \left( \frac{d+4}{4d} \right) \times \left\{ \mu_2(k)^{2d} (dR(k)^4) \times \left( \int (\nabla^2 f(\mathbf{x}))^2 d\mathbf{x} \right)^d n^{-4} \right\}^{\frac{1}{d+4}} \quad (1.8)$$

The expression (1.7) is a closed form solution for the bandwidth which minimizes the expression for the AMISE obtained in (1.8). Moreover, observe that the optimal bandwidth is of order  $n^{-\frac{1}{d+4}}$  and the optimal AMISE is of order  $n^{-\frac{4}{d+4}}$ . The detailed derivations of equations (1.7) and (1.8) respectively are found in [5,22].

### 3.0 Efficiency for the Second Order $D$ -Dimensional Spherical Kernels

In this section, the AMISE expression so derived is used to develop the generalized expression for the efficiency of second order multivariate kernels.

One way of obtaining the multivariate forms of any univariate kernel, apart from the other method discussed in [22] is by using the spherical symmetric kernel method which is given by [5] as;

$$k^s(\mathbf{x}) = \frac{\kappa^s\{\mathbf{x}^T \mathbf{x}\}}{\int \kappa^s\{\mathbf{x}^T \mathbf{x}\}d\mathbf{x}} \quad (3.1)$$

where  $\kappa$  is a univariate symmetric kernel.

The efficiency of the univariate symmetric kernel defined by [4] is

$$Eff(k) = \left\{ \frac{C(k_e)}{C(k)} \right\}^{\frac{5}{4}} \quad (3.2)$$

where  $C(k) = \left\{ \int x_1^2 k(\mathbf{x})d\mathbf{x} \right\}^{\frac{2}{5}} \left\{ \int k(\mathbf{x})^2 d\mathbf{x} \right\}$  is any given kernel constant under discussion and

$C(k_e) = \left\{ \int x_1^2 k_e(\mathbf{x})d\mathbf{x} \right\}^{\frac{2}{5}} \left\{ \int k_e(\mathbf{x})^2 d\mathbf{x} \right\}$  is the epanechnikov kernel constant.

An inspiration is drawn from (3.2) so that the general expression for the efficiency of multivariate kernels based on the spherical approach is now defined as

$$Eff(k^s(\mathbf{x})) = \left\{ \frac{C_d^2(k_e^s)}{C_d^2(k^s)} \right\}^{\frac{d+4}{4}} \quad (3.3)$$

where  $C_d^2(k^s) = \left\{ \int x_1^2 k^s(\mathbf{x}) d\mathbf{x} \right\}^{\frac{2d}{d+4}} \left\{ \int k^s(\mathbf{x})^2 d\mathbf{x} \right\}^{\frac{4}{d+4}}$  is the  $d$ -dimensional spherical form of any given second order kernel constant and  $C_d^2(k_e^s) = \left\{ \int x_1^2 k_e^s(\mathbf{x}) d\mathbf{x} \right\}^{\frac{2d}{d+4}} \left\{ \int k_e^s(\mathbf{x})^2 d\mathbf{x} \right\}^{\frac{4}{d+4}}$  is the  $d$ -dimensional spherical form of the epanechnikov kernel constant.

**Theorem1.** If equation(3.3) holds, then the efficiency for the second order  $d$  -dimensional kernel is

$$Eff [k^s(\mathbf{x})] = \left[ \frac{5d\Gamma(d/2)}{2(d+4)\Gamma(d/2)} \right]^{\frac{d}{2}} \left[ \frac{d(d+2)\Gamma(d/2)}{(d+4)5^{d/2}\pi^{d/2}} \right] \left[ \left( \int x_1^2 k^s(\mathbf{x}) d\mathbf{x} \right)^{\frac{d}{2}} \left( \int k^s(\mathbf{x}) d\mathbf{x} \right)^{-1} \right]$$

**Proof:**

The univariate epanechnikov kernel as defined in [4] is

$$K(x) = \frac{3}{4\sqrt{5}} \left( 1 - \frac{x^2}{5} \right), \quad -\sqrt{5} \leq x \leq \sqrt{5}$$

Hence, the multivariate version using (3.1) is

$$k_e^s(\mathbf{x}) = \frac{d(d+2)\Gamma(d/2) \left[ 5 - (x_1^2 + x_2^2 + \dots + x_d^2) \right]}{4 \times 5^{\frac{d+2}{2}} \pi^{d/2}} \tag{3.4}$$

The expression (3.4) and the subsequent derivations are made possible by [23] who gave the polar coordinates in  $d$  - dimension. From (2.1), set

$$C_d^2\{k(\mathbf{x})\} = \mu_2(k) \frac{2d}{d+4} R(k)^{\frac{4}{d+4}} = \left\{ \int x_1^2 k(\mathbf{x}) d\mathbf{x} \right\}^{\frac{2d}{d+4}} \left\{ \int k(\mathbf{x})^2 d\mathbf{x} \right\}^{\frac{4}{d+4}} \tag{3.5}$$

Re-write equation (3.5) to reflect (3.3). That is,

$$C_d^2(k_e^s(\mathbf{x})) = \left\{ \int x_1^2 k_e^s(\mathbf{x}) d\mathbf{x} \right\}^{\frac{2d}{d+4}} \left\{ \int k_e^s(\mathbf{x})^2 d\mathbf{x} \right\}^{\frac{4}{d+4}} \tag{3.6}$$

and

$$C_d^2(k^s(\mathbf{x})) = \left\{ \int x_1^2 k^s(\mathbf{x}) d\mathbf{x} \right\}^{\frac{2d}{d+4}} \left\{ \int k^s(\mathbf{x})^2 d\mathbf{x} \right\}^{\frac{4}{d+4}} \tag{3.7}$$

Thus

$$\mu_2(k_e^s(\mathbf{x})) = \int x_1^2 k_e^s(\mathbf{x}) d\mathbf{x} = \int x_1^2 \left[ \frac{d(d+2)\Gamma(d/2) \left[ 5 - (x_1^2 + x_2^2 + \dots + x_d^2) \right]}{4 \times 5^{\frac{d+2}{2}} \pi^{d/2}} \right] d\mathbf{x}$$

$$R(k_e^s(\mathbf{x})) = \int k_e^s(\mathbf{x})^2 d\mathbf{x} = \int \left[ \frac{d(d+2)\Gamma(d/2) \left[ 5 - (x_1^2 + x_2^2 + \dots + x_d^2) \right]}{4 \times 5^{\frac{d+2}{2}} \pi^{d/2}} \right]^2 d\mathbf{x}$$

Thus,

$$C_d^2(k_e^s(\mathbf{x})) = \int x_1^2 \left[ \frac{d(d+2)\Gamma(d/2) \left[ 5 - (x_1^2 + x_2^2 + \dots + x_d^2) \right]}{4 \times 5^{\frac{d+2}{2}} \pi^{d/2}} \right] d\mathbf{x} \tag{3.8}$$

$$\times \int \left[ \frac{d(d+2)\Gamma(d/2) \left[ 5 - (x_1^2 + x_2^2 + \dots + x_d^2) \right]}{4 \times 5^{\frac{d+2}{2}} \pi^{d/2}} \right]^2 d\mathbf{x}$$

Equation (3.8) can be expressed in its Spherical Polar Coordinate and to do this, recognize that the change of variables to spherical polar coordinate consist of the transformation, as contained in [23], from the  $x_1, x_2, \dots, x_d$  coordinates to the  $r\theta_1\theta_2 \dots \theta_{d-1}$  coordinates by

$$\begin{aligned} x_1 &= r \cos \theta_1 \cos \theta_2 \cdots \cos \theta_{d-3} \cos \theta_{d-2} \cos \theta_{d-1} \\ x_2 &= r \cos \theta_1 \cos \theta_2 \cdots \cos \theta_{d-3} \cos \theta_{d-2} \sin \theta_{d-1} \\ &\vdots \\ x_j &= r \cos \theta_1 \cdots \cos \theta_{d-j} \sin \theta_{d-j+1} \\ &\vdots \\ x_d &= r \sin \theta_1 \end{aligned}$$

where  $r$  is the radius, a base angle  $\theta_{d-1}$  ranging over  $(0, 2\pi)$ , and  $d - 2$  angles  $\theta_1, \theta_2, \dots, \theta_{d-2}$  each ranging over  $(-\pi/2, \pi/2)$ . This gives the Jacobian

$$\frac{\partial(x_1, x_2 \cdots x_d)}{\partial(r, \theta_1, \theta_2 \cdots \theta_{d-1})} = \begin{vmatrix} \frac{\partial x_1}{\partial r} & \frac{\partial x_1}{\partial \theta_1} & \cdots & \frac{\partial x_1}{\partial \theta_{d-1}} \\ \frac{\partial x_2}{\partial r} & \frac{\partial x_2}{\partial \theta_1} & \cdots & \frac{\partial x_2}{\partial \theta_{d-1}} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial x_d}{\partial r} & \frac{\partial x_d}{\partial \theta_1} & \cdots & \frac{\partial x_d}{\partial \theta_{d-1}} \end{vmatrix}$$

$$\therefore \frac{\partial(x_1, x_2 \cdots x_d)}{\partial(r, \theta_1, \theta_2 \cdots \theta_{d-1})} = r^{d-1} \cos^{d-2} \theta_1 \cos^{d-3} \theta_2 \cos^{d-4} \theta_3 \cdots \cos \theta_{d-2}$$

Thus

$$\iint \cdots \int f(x_1, x_2 \cdots x_d) dv = \iint \cdots \int f(r \cos \theta_1 \cos \theta_2 \cdots \cos \theta_{d-1}, r \cos \theta_1 \cos \theta_2 \cdots \sin \theta_{d-1}, r \sin \theta_1) \left| \frac{\partial(x_1, x_2 \cdots x_d)}{\partial(r, \theta_1, \theta_2 \cdots \theta_{d-1})} \right| dr, d\theta_1, d\theta_2 \cdots d\theta_{d-1} \tag{3.9}$$

Writing (3.6) in its polar coordinate form, we have

$$C_d^2(k_e^s) = \left\{ \begin{aligned} &\int_0^{2\pi} \int_{-\pi/2}^{\pi/2} \cdots \int_{-\pi/2}^{\pi/2} \int_0^{\sqrt{5}} r^2 \cos^2 \theta_1 \cos^2 \theta_2 \cdots \cos^2 \theta_{d-2} \cos^2 \theta_{d-1} \\ &\times \left[ \frac{d(d+2)\Gamma(d/2)[5 - (x_1^2 + x_2^2 + \cdots + x_d^2)]}{4.5^{\frac{d+2}{2}} \pi^{d/2}} \right] r^{d-1} \cos^{d-2} \theta_1 \cos^{d-3} \theta_2 \cdots \cos \theta_{d-2} \\ &\times dr, d\theta_1, d\theta_2 \cdots d\theta_{d-1} \end{aligned} \right\} \tag{3.10}$$

$$\times \left\{ \begin{aligned} &\int_0^{2\pi} \int_{-\pi/2}^{\pi/2} \cdots \int_{-\pi/2}^{\pi/2} \int_0^{\sqrt{5}} \left[ \frac{d(d+2)\Gamma(d/2)[5 - r^2]}{4.5^{\frac{d+2}{2}} \pi^{d/2}} \right]^2 \\ &\times r^{d-1} \cos^{d-2} \theta_1 \cos^{d-3} \theta_2 \cdots \cos \theta_{d-2} dr, d\theta_1, d\theta_2 \cdots d\theta_{d-1} \end{aligned} \right\}$$

Using the identity relation between the gamma and the beta functions on (3.10), we have

$$C_d^2(k_e^s) = \left[ \frac{5d\Gamma(d/2)}{2(d+4)\Gamma(\frac{d+2}{2})} \right] \left[ \frac{d(d+2)\Gamma(d/2)}{(d+4)5^{d/2} \pi^{d/2}} \right]$$

Hence

$$C_d^2(k_e^s) = \left[ \frac{5d\Gamma(d/2)}{2(d+4)\Gamma(\frac{d+2}{2})} \right]^{\frac{2d}{d+4}} \left[ \frac{d(d+2)\Gamma(d/2)}{(d+4)5^{d/2} \pi^{d/2}} \right]^{\frac{4}{d+4}} \tag{3.11}$$

Substituting (3.11) and (3.7) into the numerator and denominator respectively of (3.5), we obtain.

$$Eff[k^s(\mathbf{x})] = \left[ \frac{5d\Gamma(d/2)}{2(d+4)\Gamma(\frac{d+2}{2})} \right]^{\frac{d}{2}} \left[ \frac{d(d+2)\Gamma(d/2)}{(d+4)5^{d/2} \pi^{d/2}} \right] \times \left[ \left( \int x_1^2 k^s(\mathbf{x}) d\mathbf{x} \right)^{\frac{d}{2}} \left( \int k^s(\mathbf{x}) d\mathbf{x} \right)^{-1} \right] \tag{3.12}$$

Equation (3.12) is the generalized efficiency of the second-order  $d$ -dimensional kernels using the spherical method.

#### 4.0 Conclusion

In this paper, an expression has been developed for the efficiency of second-order  $d$ -dimensional spherical kernels. This was achieved by using the epanechnikov kernel as the basis for the optimum which was based on the fundamentals of the AMISE for the  $d$ -dimensional kernels. Our future work would include the relatively straightforward but more involved extension of the current procedure to handle the  $d$ -dimensional spherical forms of some second-order polynomial kernels that would be considered in this work. Consequent upon this the efficiency (in terms of the numerical values) of some of the second-order polynomial kernels would be obtained and as a result enable us to see if there would be any loss or gain in efficiency as the dimension increases.

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