

Shape-Adaptive Kernel Density Estimation

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Abstract

Kernel density estimation has gained popularity in the past few years. Generally the methods use symmetric kernels, even though the data of which the density is estimated are not necessarily spread equally in all dimensions. To account for this asymmetric distribution of data we propose the use of shape adaptive kernels: kernels whose shape changes to fit the spread of the data in the local neighborhood of the point whose density is estimated. We compare the performance of the shape adaptive kernels on simulated datasets with known density fields.

Results

Conclusion

1 Introduction

Estimating densities with kernels has been fairly popular of late; in the medical field it has been used to predict dose-volume histograms, which are instrumental in the determination of radiation doses [7]. Ecologists have applied it to explore the habitats of seabirds [6]. Ferdosi et al. [4] have described it as “a critical first step in making progress in many areas of astronomy.” Within this discipline density estimation is, among other things, used to estimate the density of the cosmic density field, which is required for the reconstruction of the large-scale structure of the universe.

Formally the aim of density estimation is to find the probability density $f(\mathbf{x})$ in the d -dimensional Euclidean space underlying N points $\mathbf{x}_1, \dots, \mathbf{x}_N$, that have been selected independently from $f(\mathbf{x})$.

Kernel density estimation methods approximate $f(\mathbf{x})$ by placing bumps, referred to as kernels, on the different observations and summing these bumps to arrive at a final density estimate. This paper is concerned with a method to make the shape of the kernels adaptive to their local neighborhood. Before introducing the process used to determine the form of the kernel we first review the different symmetric kernel density estimation methods.

The Parzen approach [8] is one of the simplest kernel density estimation methods. It approximates the density of some pattern \mathbf{x} according to:

$$\hat{f}(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N h^{-d} K\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right). \quad (1)$$

The shape of the used bumps is determined by the

kernel function $K(\bullet)$, their width by the bandwidth h . The Parzen approach requires the kernel to be a probability density function, i.e. $K(\mathbf{x}) \geq 0$ and $\int K(\mathbf{x}) = 1$ [9]. The bandwidth directly influences the result of the density estimation process; a too small bandwidth results in a density estimate with spurious fine structures, whereas kernels that are too wide can oversmooth the density estimate. Kernel estimators, such as the Parzen approach, that use kernels of the same width for all \mathbf{x}_i , are called fixed-width estimators.

One downside of fixed-width methods is that the peakedness of the kernel is not data-responsive. Consequently in low density regions the density estimate will have peaks at the few sample points and be too low elsewhere. Whereas in areas with high density the Parzen estimate is spread out, as the sample points are more densely packed together[2]. Adaptive-width methods address this disadvantage of the fixed-width methods by allowing the width of the kernel to vary per data point. For example the estimator introduced by Breiman, Meisel, and Purcell uses the distance between \mathbf{x}_i and the k -nearest neighbor of \mathbf{x}_i , denoted by $D_{i,k}$, to determine the width of the kernel:

$$\hat{f}(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N (\alpha \cdot D_{i,k})^{-d} K_G\left(\frac{\mathbf{x} - \mathbf{x}_i}{\alpha \cdot D_{i,k}}\right). \quad (2)$$

In this equation K_G is used to represent a Gaussian kernel, and α is a multiplicative constant. The values of both α and k can be determined with a minimization algorithm on a goodness of fit statistic. Comparing Equation (1) with (2) one finds that the bandwidth h of the Parzen estimator is defined as

$\alpha \cdot D_{i,k}$ in Equation (2). The factor $D_{i,k}$ depends on the local neighborhood of \mathbf{x}_i , in low density regions this factor is large, and the kernel spreads out due to its high bandwidth. In areas with relatively many data points the converse occurs.

Silverman [9] shows that the minimization procedure used by Breiman, Meisel, and Purcell implicitly uses a k -NN pilot estimate. If pilot estimates, denoted by $\tilde{f}(\bullet)$, are used explicitly, the density estimation process becomes:

- (i) Compute pilot densities with some estimator that ensures that $\forall i \tilde{f}(\mathbf{x}_i) > 0$.
- (ii) Define local bandwidths γ_i as

$$\gamma_i = \left(\frac{\tilde{f}(\mathbf{x}_i)}{\text{GM}(\tilde{f}(\mathbf{x}_0), \dots, \tilde{f}(\mathbf{x}_N))} \right)^{-\beta}, \quad (3)$$

where GM denotes the geometric mean and the sensitivity parameter β must lie in the range $[0, 1]$.

- (iii) Compute the adaptive kernel estimate as

$$\hat{f}(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N (h \cdot \gamma_i)^{-d} K\left(\frac{\mathbf{x} - \mathbf{x}_i}{h \cdot \gamma_i}\right) \quad (4)$$

with K integrating to unity.

Since the pilot densities computed in step (i) do not need to be sensitive to the fine details of the pilot estimate a convenient method, e.g. the Parzen approach, can be used to estimate them [9]. The local bandwidths, computed in step (ii), depend on the exponent β . The higher this value is the more sensitive the local bandwidths are to variations in the pilot densities. Choosing $\beta = 0$ reduces Equation (4) to a fixed-width method. In the literature two values of β are prevalent. Breiman, Meisel, and Purcell [2] argue that choosing $\beta = 1/d$ ensures that the number of observations covered by the kernel will be approximately the same in all areas of the data. Whereas Silverman [9] favors $\beta = 1/2$ independent of the dimension of the data, as this value results in a bias that can be shown to be of a smaller order than that of the fixed-width kernel estimate.

One disadvantage of the Breiman estimator is its computational complexity. This is partially due to the use of a Gaussian kernel. Because of the infinite base of this kernel an exponential function has to be evaluated N times to estimate the density of one data point. Wilkinson and Meijer [10] address this in their Modified Breiman Estimator (MBE) by replacing the Gaussian kernel with a spherical Epanechnikov kernel in both the computation of the pilot

densities and in the final density estimate. This kernel is defined as

$$K_E(\mathbf{x}) = \begin{cases} \frac{d+2}{2c_d} (1 - \mathbf{x} \cdot \mathbf{x}) & \text{if } \mathbf{x} \cdot \mathbf{x} < 1 \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

where c_d denotes the volume of the d -dimensional unit sphere [3]. It should be noted that the kernel defined in Equation (5) does not have unit variance. This can be corrected by multiplying the bandwidth, h , with the square root of the variance of K_E , i.e. $\sqrt{5}$. There are two advantages to using this kernel, firstly it is computationally much simpler than the Gaussian kernel, in part due to its finite base, and secondly it is optimal in the sense of the Mean Integrated Square Error (MISE) [3]. One downside of this kernel is that it is not continuously differentiable. This is irrelevant when computing the pilot densities, however for the final densities it is a trade off between a continuously differentiable density estimate and a density estimator that has a low computational complexity. Wilkinson and Meijer [10] compute the global bandwidth according to

$$h = \sigma \cdot N^{-1/(d+4)} \left(\frac{8(d+4) \cdot (2\sqrt{\pi})^d}{c_d} \right)^{\frac{1}{d+4}}, \quad (6)$$

where σ represents the square root of the average of the variances of the different dimensions. The final densities are estimated with Equation (4), using the general and local bandwidths estimated with Equation (6) and (3), respectively.

Ferdosi et al. [4] consider the application of density estimation on large datasets, i.e. sets with more than 50 000 points with the dimension of the data points ranging from ten to hundreds of elements. They use the MBE, but introduce a computationally less complex method to estimate the bandwidth. First an intermediate bandwidth for each dimension l of the data is computed with

$$h_l = \frac{P_{80}(l) - P_{20}(l)}{\log N}, \quad l = 1, \dots, d, \quad (7)$$

where $P_{20}(l)$ and $P_{80}(l)$ are the twentieth and eightieth percentile of the data in dimension l , respectively. From these intermediate bandwidths the minimum is used as h .

Although the widths of the kernels of the discussed adaptive-width methods are sensitive to the data, the shapes of the kernels depend only on its definition. To further increase the responsiveness of the estimator to the data we propose the use of shape-adaptive kernels; not only the width but also

the shape of these kernels is steered by the local neighborhood of the data.

A possible disadvantage of these shape-adaptive kernels is that in regions where the density of sample points is low, the number of data points is insufficient to reliably compute the shape of the kernel. Therefore we let the amount of influence exerted by the local data on the shape of the kernel depend on the number of data points in the local neighborhood.

This paper is organized as follows. Section 2 introduces the proposed shape-adaptive kernels. The experiment used to investigate the performance of these kernels is discussed in Section 3, the results are presented in Section 4. They are discussed in Section 5, and the reached conclusion can be found in Section 6.

2 Method

We use shape adaptive kernels in combination with the Modified Breiman Estimator introduced by Wilkinson and Meijer [10], the resulting estimator is henceforth also referred to as the shape-adaptive Modified Breiman Estimator (saMBE). For its lower computational complexity we use the method introduced by Ferdosi et al. [4], defined in Equation (7), to compute the general bandwidth. Pilot densities are computed according to Equation (1), with an Epanechnikov kernel. Since using $\beta = 1/2$ in Equation (3) results in a final density approximation with a lower mean squared error than using $\beta = 1/d$. We use the first when computing the local bandwidths. The final density estimate is computed according to:

$$\hat{f}(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N \frac{1}{\det(\mathbf{H}_i)} K_{\mathcal{E}}(\mathbf{H}_i^{-1}(\mathbf{x} - \mathbf{x}_i)). \quad (8)$$

The shape of the kernel $K_{\mathcal{E}}(\bullet)$ is determined by the bandwidth matrix \mathbf{H}_i [5]. If $\mathbf{H}_i = h \cdot \gamma_i \cdot \mathbb{I}_{d \times d}$, Equation (8) reduces to Equation (4).

For each data point \mathbf{x}_i that is used in the density estimation of some pattern \mathbf{x}_j , the bandwidth matrix is determined according to these steps:

- (i) Find $C_{\mathbf{x}_i}$, the k -nearest neighbors of \mathbf{x}_i .
- (ii) Compute Σ , the unbiased covariance matrix of the local neighborhood $C_{\mathbf{x}_i}$.
- (iii) Determine \mathbf{H}_i by scaling Σ with

$$s = h \cdot \gamma_i \left(\prod_{l=1}^d \lambda_l \right)^{-\frac{1}{d}} \quad (9)$$

where $\lambda_1, \dots, \lambda_d$ are the eigenvalues of Σ .

Step (i) determines the local neighborhood of \mathbf{x}_i with a k -nearest neighbors search in a KD-tree [1], with Euclidean distance as the distance metric. We follow Silverman's [9] recommendation of choosing $k = \sqrt{N}$. To ensure that Σ is nonsingular we also need $k > d$, therefore

$$k = \max \left(\left\lfloor \sqrt{N} \right\rfloor, d \right) + 1.$$

Using a KD-tree for the k -nearest neighbors search instead of the naive implementation, significantly improves the time complexity of finding \mathbf{H}_i . The downside of using a space partitioning tree is that $C_{\mathbf{x}_i}$ is an approximation of the actual neighborhood, as long as k is rather large the use of an approximation instead of the exact k -nearest neighbors should not impact the final kernel result strongly. We use k -NN rather than a fixed-radius neighborhood to ensure that, independent of the sparsity of the data, the kernel shape is always based on a reasonable number of data points.

The basis shape of the kernel is determined in step (ii). The covariance matrix ensures that the major axis of the kernel has the same direction as the maximum variance of the data.

The scaling factor computed in step (iii) ensures that the kernels used in the density estimation of different patterns have a comparable domain. Equation (9) scales the bandwidth matrix in such a way that the volume of the ellipsoid defined by the eigenvectors and values of \mathbf{H}_i is equal to that of the eigenellipsoid of the bandwidth matrix that is implicitly used in Equation (4).

3 Experiment

We contrast the performance of the shape-adaptive and the symmetric Modified Breiman Estimator on simulated datasets with known density fields. This allows us to test how well the proposed method can recover simple density distributions in comparison to an existing method. We distinguish two types of datasets: datasets consisting of a single Gaussian distribution and noise, defined in Section 3.1 and datasets containing multiple Gaussian distributions embed in noise, these sets are presented in Section 3.2.

To quantify the performance of the estimators we use the mean squared error (MSE):

$$\text{MSE}(\hat{f}(\bullet)) = \frac{1}{N} \sum_{j=1}^N (\hat{f}(\mathbf{x}_j) - f(\mathbf{x}_j))^2.$$

3.1 Datasets with a Single Gaussian

Figure 1 shows a scatter plot representation of the datasets containing a single Gaussian distribution defined in Table 1.

The Gaussian components of these datasets progress from a sphere, i.e. dataset S_1 , to an increasingly more elongated ellipsoid. This makes it possible to investigate the influence of how strongly elongated the distribution is on the density estimate. The first dataset is a simple spherical Gaussian distribution centered in a uniform random background. The covariance matrix of the Gaussian component in S_2 is created from S_1 by squaring one of the eigenvalues of the covariance matrix, and taking the square root of the other two eigenvalues, without changing the eigenvectors. The resulting covariance matrix defines an eigenellipse with the same volume as the one defined by S_1 . The Gaussian component of dataset S_3 changes the shape of the eigenellipse of the Gaussian component by lengthening one of the minor axes, and shortening the other. The Gaussian component in S_4 is spread out more along the y-axis and less along the z-axis, than the Gaussian component in dataset S_3 .

We expect the Modified Breiman Estimator and its shape-adaptive cousin to perform comparably on dataset S_1 , since due to the symmetric shape of the Gaussian distribution no advantage should be gained by using a shape-adaptive kernel. As the Gaussian distribution is more and more elongated, the advantage of using saMBE should become more pronounced.

3.2 Datasets with Multiple Gaussians

Table 2 defines the datasets that consist of uniform random noise and multiple Gaussian distributions, a scatter plot representation of these sets is shown in Figure 2. Dataset M_1 consists of two Gaussian distributions, that are unlikely to overlap, embedded in noise, the first Gaussian component is significantly denser than the second. The procedure outlined in Section 3.1 for the creation of dataset S_2 was used to derive dataset M_2 from set M_1 . Dataset M_3 embeds four non-overlapping Gaussians, with eigenspheres with notably differencing radii, in the uniform random background. The last dataset, M_4 , is a variation on M_3 , created with method that was used for the definition of dataset S_2 from S_1 .

We expect to find hardly any difference in performance between the classifiers on dataset M_1 and M_3 . Given the shape of the Gaussian distributions embedded in dataset M_2 and M_4 we hypothesize that

saMBE outperforms MBE on these sets.

Ferdosi et al. [4] found that the Modified Breiman Estimator resulted in lower integrated squared errors if fewer Gaussian distributions were present in the datasets. Since the presented datasets are comparable to those used by Ferdosi et al. we expect to find the same influence of the number of distributions on the error.

4 Results

This section presents the results of the experiments described in Section 3. We compare the performance of the two estimators on each dataset with the mean squared error and visually with plots. All plots associated with a single dataset have the same domain and range, to allow for easy comparison of the results within a dataset. The horizontal axis is used to represent the known densities, its range is such that each known density can be shown. The estimated densities are shown on the vertical axis, the length of these axes is such that they are long enough to represent every estimated density for that dataset, independent of the used estimator. The black line in each plot illustrates the line all points would lie on if a perfect estimator was used, i.e. the line $x = x$. The colors of the points in these plot correspond to the colors of the elements of the datasets in Tables 1 and 2.

Section 4.1 presents the results of the datasets that contain a single Gaussian, in Section 4.2 the results of the datasets that consist of noise and multiple Gaussian distributions are presented.

4.1 Datasets with a Single Gaussian

This section compares the performance of the Modified Breiman Estimator and a shape-adaptive variant on dataset that contain one Gaussian, i.e. dataset S_1 , S_2 , S_3 , and S_4 .

Where to find table and MSE?

Discuss MSE and Plot

Difference between noise and gaussian?

Discuss MSE and Plot

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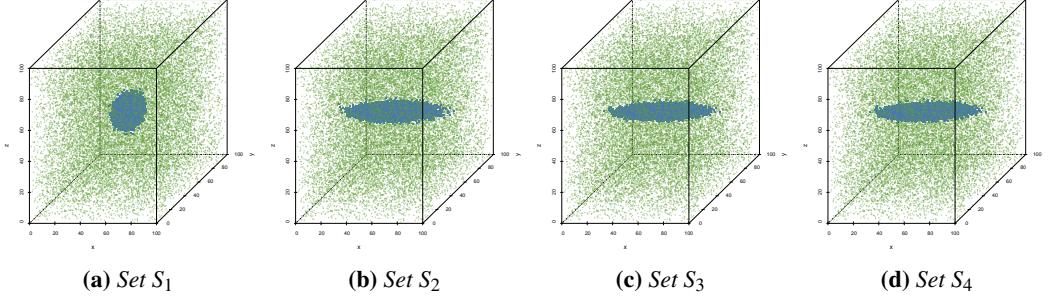


Figure 1: Scatter plot representation of the datasets defined in Table 1. The used colors correspond to those associated with the different components in Table 1.

Set	Component	Number	Distribution
S_1	■ Trivariate Gaussian	4.0×10^4	$\mathcal{N}([50, 50, 50], \text{diag}(11))$
	● Uniform random background	2.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$
S_2	■ Trivariate Gaussian	4.0×10^4	$\mathcal{N}([50, 50, 50], \text{diag}([11, \sqrt{11}, \sqrt{11}]))$
	● Uniform random background	2.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$
S_3	■ Trivariate Gaussian	4.0×10^4	$\mathcal{N}([50, 50, 50], \text{diag}([11, 2 * \sqrt{11}, 1/2\sqrt{11}]))$
	● Uniform random background	2.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$
S_4	■ Trivariate Gaussian	4.0×10^4	$\mathcal{N}([50, 50, 50], \text{diag}([11^2, 11, 1]))$
	● Uniform random background	2.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$

Table 1: The datasets containing a single Gaussian distribution embed in uniform noise. The column ‘Number’ indicates for each component the number of patterns sampled from it. $\mathcal{N}(\mu, \Sigma)$ denotes a Gaussian distribution with mean μ and covariance matrix Σ . A diagonal matrix with the values x_1, \dots, x_d on the diagonal is represented as $\text{diag}([x_1, \dots, x_d])$, a scalar matrix with x on the diagonal is shown as $\text{diag}(x)$. $\mathcal{U}(a, b)$ denotes a uniform distribution with its minimum and maximum set to a and b , respectively. The second column presents the symbol used to represent this component in plots throughout the paper.

Set	Component	Number	Distribution
M_1	■ Trivariate Gaussian 1	2.0×10^4	$\mathcal{N}([25, 25, 25], \text{diag}(5))$
	▲ Trivariate Gaussian 2	2.0×10^4	$\mathcal{N}([45, 45, 45], \text{diag}(11))$
	● Uniform random background	2.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$
M_2	■ Trivariate Gaussian 1	2.0×10^4	$\mathcal{N}([25, 25, 25], \text{diag}([5^2, \sqrt{5}, \sqrt{5}]))$
	▲ Trivariate Gaussian 2	2.0×10^4	$\mathcal{N}([45, 45, 45], \text{diag}([\sqrt{11}, \sqrt{11}, 11^2]))$
	● Uniform random background	2.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$
M_3	■ Trivariate Gaussian 1	2.0×10^4	$\mathcal{N}([24, 10, 10], \text{diag}(2))$
	▲ Trivariate Gaussian 2	2.0×10^4	$\mathcal{N}([33, 70, 40], \text{diag}(10))$
	◆ Trivariate Gaussian 3	2.0×10^4	$\mathcal{N}([90, 20, 80], \text{diag}(1))$
	* Trivariate Gaussian 4	2.0×10^4	$\mathcal{N}([60, 80, 23], \text{diag}(5))$
	● Uniform random background	4.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$
M_4	■ Trivariate Gaussian 1	2.0×10^4	$\mathcal{N}([24, 10, 10], \text{diag}([4, \sqrt{2}, \sqrt{2}]))$
	▲ Trivariate Gaussian 2	2.0×10^4	$\mathcal{N}([33, 70, 40], \text{diag}([\sqrt{10}, \sqrt{10}, 100]))$
	◆ Trivariate Gaussian 3	2.0×10^4	$\mathcal{N}([90, 20, 80], \text{diag}(1))$
	* Trivariate Gaussian 4	2.0×10^4	$\mathcal{N}([60, 80, 23], \text{diag}([25, \sqrt{5}, \sqrt{5}]))$
	● Uniform random background	4.0×10^4	$\mathcal{U}([0, 0, 0], [100, 100, 100])$

Table 2: The datasets with multiple Gaussian distributions embedded in uniform noise. This table has the same structure and uses the same notation as Table 1.

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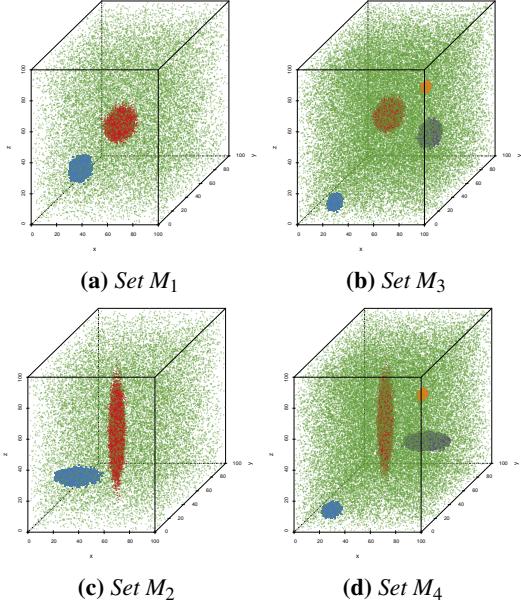


Figure 2: Scatter plot representation of the datasets defined in Table 2, the colors used for the different components correspond to those in Table 2.

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Set	Estimator	
	MBE	saMBE
M_1	0.000	0.000
M_2	0.000	0.000
M_3	0.000	0.000
M_4	0.000	0.000

Table 4: The mean squared error of the known densities and the densities as estimated by the Modified Breiman Estimator (MBE) and the shape-adaptive MBE (saMBE), respectively, for the datasets containing a single Gaussian.

Discuss MSE and Plot

Difference between noise and gaussians?

General observation?

What is the influence of the density of Gaussian?

Rewrite caption

Set	Estimator	
	MBE	saMBE
S_1	0.000	0.000
S_2	0.000	0.000
S_3	0.000	0.000
S_4	0.000	0.000

Table 3: The mean squared error of the known densities and the densities as estimated by the Modified Breiman Estimator (MBE) and the shape-adaptive MBE (saMBE), respectively, for the datasets containing a single Gaussian.

General observation

What is the influence of elongatedness on the density estimate?

4.2 Datasets with Multiple Gaussians

In this section we present the results of the two estimators on dataset M_1, M_2, M_3, M_4 , i.e. the datasets that contain more than one Gaussian.

Discuss MSE and Plot

Difference between noise and gaussians?

5 Discussion

This section first discusses the results of the density estimation of dataset with a single Gaussian, in Section 5.1, Section 5.2 discusses the results of applying the density estimators on datasets with multiple Gaussian components.

5.1 Datasets with a Single Gaussian

The difference in results between the Modified Breiman Estimator and its shape adaptive variant on dataset S_1, S_2, S_3, S_4 raise several questions. This section attempts to answer them.

5.2 Datasets with Multiple Gaussians

What does this section do?

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General Discussion

6 Conclusion

Further research: If the k-nearest neighbor is more than some distance x away from x_i the identity matrix, or better, move between the fixed-width kernel and the shape-adaptive kernel based on the distance of the k-nearest neighbor.

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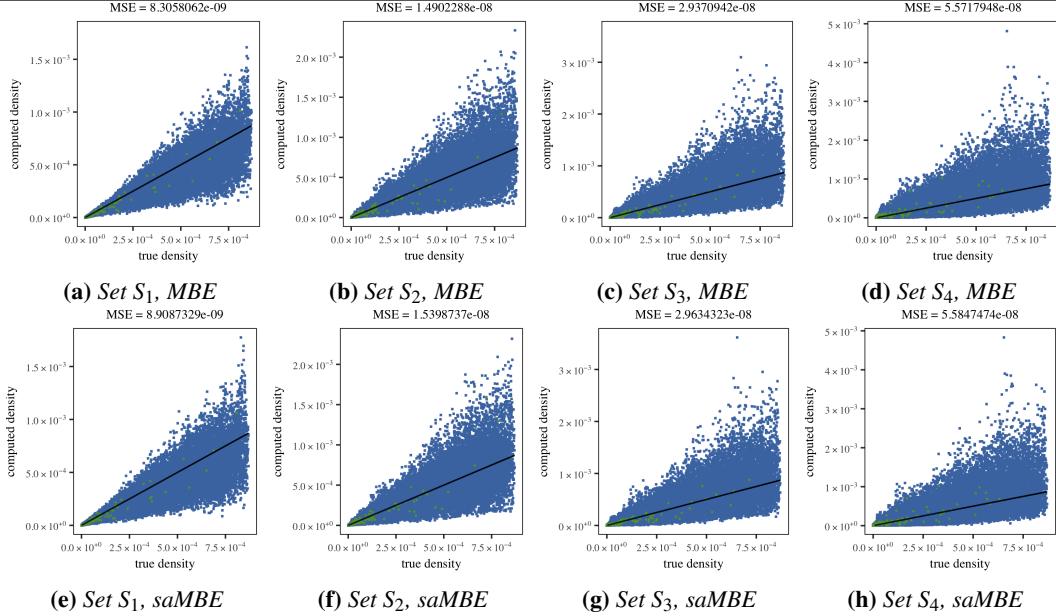


Figure 3: Comparative plots for dataset S_1 , S_2 , S_3 , and S_4 .

Determine the optimal value of k .

References

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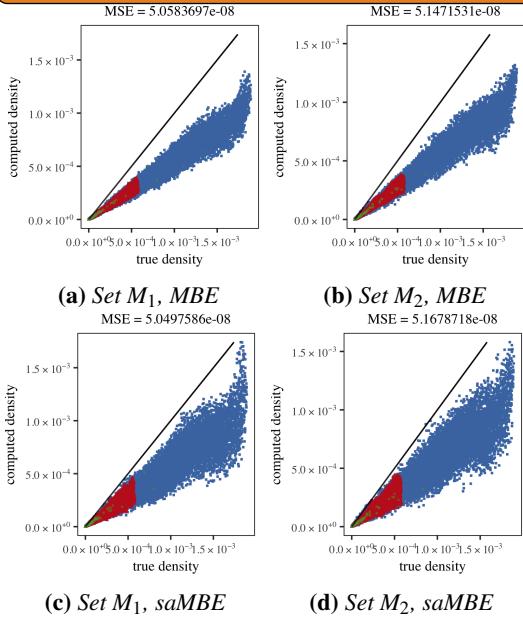


Figure 4: Comparative plots for dataset M_1 and M_2 .

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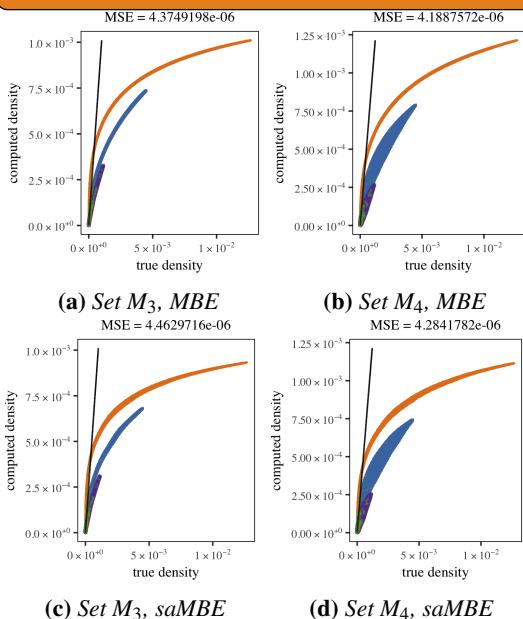


Figure 5: Comparative plots for dataset M_3 and M_4 .