



Book of the Short Papers

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Computing Highest Density Regions with Copulae

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Abstract

We investigate the problem of deriving highest density regions (HDRs) from multivariate data samples. We are interested in estimating minimum volume sets that contain a given probability. In the case of unknown distribution probabilities f , the problem involves their estimation, which may be challenging in multidimensional settings. Motivated by the ubiquitous role of copula modelling in modern statistics, we explore their use in the context of HDR estimation. Rather than directly estimating the multivariate f , we propose to estimate the marginals and their dependence structure, i.e., the copula structure, separately. We evaluate this new method, using both a parametric and a nonparametric approach, in a number of synthetic experiments and considering a real dataset.

Keywords: Highest density regions, Copula modelling, Kernel density estimation

1. Introduction

A ubiquitous problem in statistics is to derive statistical intervals or *regions* (in the multivariate setting) for population parameters or other unknown quantities. Given a random sample of data, they provide a way to quantify the uncertainty about a quantity of interest, or simply a way to summarize the information contained in a distribution. In this work, we are interested in statistical *regions* for summarizing probability distributions and we focus on one approach to addressing this problem: *highest density regions* (HDRs, 1). As the name suggests, an HDR specifies the set of points of highest density: the density for every point inside the region is greater than that for every point outside it. More specifically, as we will better discuss in Section 2, the concrete problem is to estimate minimum volume sets of the form $R(f_\alpha) = \{\mathbf{x}: f_{\mathbf{X}}(\mathbf{x}) \geq f_\alpha\}$, such that $P(\mathbf{X} \in R(f_\alpha)) \geq 1 - \alpha$, where $f_{\mathbf{X}}$ is the probability distribution of the variable of interest $\mathbf{X} \in \mathbb{R}^d$ and $1 - \alpha$, with $\alpha \in (0, 1)$, a prespecified coverage probability. In principle, HDRs can be derived for any probability distribution and their scope can be widely different. The following are possible applications of HDRs.

Forecasting The goal is to obtain a “prediction region” for a set of observable variables in order to inform any required action (for illustrative examples, see e.g., 1; 2);

Anomaly detection The goal is to detect abnormal observations from a sample: if a data point does not belong to a region of normal or concentrated data, then it is regarded as anomalous (see e.g., 3);

Unsupervised or semi-supervised classification Identify areas or clusters with a relatively high concentration of a given phenomenon, e.g., areas with remarkably high coronavirus incidence (4).

Such regions are of interest in Bayesian analysis as well, in the formulation of *highest posterior density regions* and *credibility regions* (5; 6). In that context, they are based on a posterior distribution.

Because of their flexibility “to convey both multimodality and asymmetry in the forecast density”, HDRs are argued to be a “more effective summary of the forecast distribution than other common forecast regions” (1). However, to build an accurate HDR, one needs to know (or accurately estimate) the

underlying probability distribution. Methods for estimating f such as the kernel density estimator (KDE, 7) or the local likelihood approach (8) work very well for unidimensional problems, but they may be inefficient for multidimensional problems (9). For example, the bandwidth selection in KDE, recognized as the most crucial and difficult step (see e.g., Chapter 2 in 10), has no definite and unique solution. Further, high-dimensional data pose challenges also from the algorithmic/computational perspective. Altogether, these aspects hamper the ability to derive an appropriate HDR.

The scope of this work is to propose an alternative approach to build HDRs using *copulae* so as to overcome the direct estimation of the multivariate f . Specifically, copulae allow to relax the estimation of multivariate random vectors, by separately estimating the marginals and their dependence structure, i.e., the copula model (11). Motivated by the ubiquitous role of copula modelling in modern multivariate statistics, specifically multivariate density estimation, we explore its use the context of HDR estimation.

2. Problem Setting: Highest Density Regions

Assume we have access to a sample $\mathbf{s}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ of independent and identically distributed (iid) observations, drawn from a probability measure \mathbb{P} . Each data point can be multidimensional, that is $\mathbf{x}_i \in \mathbb{R}^d$, with $d \geq 1$. We denote by $x_i^{(j)}$ the j -th coordinate of \mathbf{x}_i , for $j = 1, \dots, d$ and $i = 1, \dots, n$. For simplicity, we restrict our analysis to bivariate data points with $d = 2$, and we focus on continuous random variables $\mathbf{X} = (X^{(1)}, X^{(2)}) \in \mathbb{R}^2$. Let $f_{\mathbf{X}}$ denote the probability density function (PDF) of \mathbf{X} and $F_{\mathbf{X}}$ its cumulative density function (CDF). Then, given a coverage probability $1 - \alpha$, with $\alpha \in (0, 1)$, the $100(1 - \alpha)\%$ HDR is defined as the subset $R(f_\alpha)$ of the sample space of \mathbf{X} such that:

$$R(f_\alpha) \doteq \{\mathbf{x}: f_{\mathbf{X}}(\mathbf{x}) \geq f_\alpha\}, \quad (1)$$

where f_α is the largest constant such that $P(\mathbf{X} \in R(f_\alpha)) \geq 1 - \alpha$.

It follows from the definition that the boundary of an HDR consists of those values of the sample space with equal density. Hence a plot of a bivariate HDR is a form of contour plot. One of the most distinctive properties of HDRs is that, of all regions of probability coverage $100(1 - \alpha)\%$, the HDR has the smallest region possible in the sample space. Clearly, an HDR always contains the global mode, and in the case of multimodal distributions, it often consists of several disjoint subregions, each containing a local mode. This provides useful information which is “masked” by other types of statistical regions.

To estimate an HDR for \mathbf{X} according to Eq. (1), one needs to know the density function $f_{\mathbf{X}}$. If this is known, the typical way to compute HDRs is the density quantile approach (1), which is based on the following rationale. Let $\mathbf{Y} = f_{\mathbf{X}}(\mathbf{X})$ be the random variable obtained by transforming \mathbf{X} by $f_{\mathbf{X}}$ (bounded and continuous in \mathbf{x}). Consider a set of independent observations from the distribution of \mathbf{X} , say $\mathbf{s}_m = \{\mathbf{x}_1, \dots, \mathbf{x}_m\}$. It follows that independent observations from the distribution of \mathbf{Y} can be obtained as $\{f_{\mathbf{X}}(\mathbf{x}_1), \dots, f_{\mathbf{X}}(\mathbf{x}_m)\}$. Consider now the ordered sample $\{f_{(1)}, \dots, f_{(m)}\}$ with $f_{(j)}$ the j -th largest of $f_{\mathbf{X}}(\mathbf{x}_i)$, $i = 1, \dots, m$, so that $f_{(j)}$ is the (j/m) sample quantile of \mathbf{Y} . Then, given a constant $\alpha \in [0, 1]$, and denoted with $\lfloor \cdot \rfloor$ the floor operator, we have that:

$$\hat{f}_\alpha \doteq f_{\lfloor \alpha m \rfloor} \rightarrow f_\alpha, \quad \text{and} \quad R_m(\hat{f}_\alpha) \doteq \{\mathbf{x}: f_{\mathbf{X}}(\mathbf{x}) > \hat{f}_\alpha\} \rightarrow R(f_\alpha), \quad \text{as } m \rightarrow \infty.$$

Basically, the HDR can be derived based on the sample quantile of $\mathbf{Y} = f_{\mathbf{X}}(\mathbf{X})$.

However, in most real-world scenarios, the density function is unknown. If we have access to a sample of iid observations $\mathbf{s}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$, then we can estimate it, and subsequently obtain an estimate of the $100(1 - \alpha)\%$ HDR by using the again the density quantile approach with

$$\hat{R}_n(\hat{f}_\alpha) \doteq \{\mathbf{x}: \hat{f}(\mathbf{x}) > f_{\lfloor \alpha n \rfloor}\}, \quad (2)$$

where \hat{f} is a possibly consistent estimator of f .

Note that for small n it may not be possible to get a reasonable density estimate. Besides, with few observations and no prior knowledge of the underlying density function, there seems little point in attempting to summarize the sample space. In higher dimensions, the difficulty of selecting an appropriate region is even greater due to the density estimation challenges (see e.g., 9; 10).

3. Using Copulae for Deriving HDRs

A general d -dimensional copula $C : [0, 1]^d \rightarrow [0, 1]$ is a joint cumulative density function whose d marginals are uniform over $[0, 1]$. Consider, without major loss of generality, the bivariate case $d = 2$, with $F_{\mathbf{X}}$ the joint CDF of the random vector $\mathbf{X} = (X^{(1)}, X^{(2)})$, and $F_{X^{(1)}} = F_1$ and $F_{X^{(2)}} = F_2$ its marginals. Then, it follows from the *probability-integral transform* (12) that the joint distribution of (F_1, F_2) is a copula, say $C_{\mathbf{X}}$, and its expression can be derived by noting that

$$C_{\mathbf{X}}(u^{(1)}, u^{(2)}) = \mathbb{P}(F_1(X^{(1)}) \leq u^{(1)}, F_2(X^{(2)}) \leq u^{(2)}) = F_{\mathbf{X}}(F_1^{-1}(u^{(1)}), F_2^{-1}(u^{(2)})).$$

Letting $u^{(j)} \doteq F_j(x^{(j)})$, $j = 1, 2$, this yields the following result due to Sklar (13):

$$F_{\mathbf{X}}(x^{(1)}, x^{(2)}) = C_{\mathbf{X}}(F_1(x^{(1)}), F_2(x^{(2)})), \quad \forall \mathbf{x} = (x^{(1)}, x^{(2)}) \in \mathbb{R}^2.$$

In summary, we can decompose the bivariate CDF $F_{\mathbf{X}}$ into a composition of the two marginal distribution functions and a two-dimensional copula $C_{\mathbf{X}}$. $C_{\mathbf{X}}$ is the copula of $F_{\mathbf{X}}$ and describes the dependence structure of F_1 and F_2 . We refer to (11) for book-length treatment of the foregoing ideas.

In case the bivariate distribution has density f , and if this is available, it holds further that

$$f_{\mathbf{X}}(x^{(1)}, x^{(2)}) = c_{\mathbf{X}}(F_1(x^{(1)}), F_2(x^{(2)}))f_1(x^{(1)})f_2(x^{(2)}),$$

with c being the copula density and f_1 and f_2 the marginal densities. The main advantage of this representation over the one involving the joint PDF is that an estimate of $f_{\mathbf{X}}$ can be obtained by estimating the marginals and the copula density separately, evading potential high-dimensional data challenges (see e.g., 14). Furthermore, copulae offer a flexible framework that can capture complex dependency structures.

If \hat{c} is an estimate of the copula density, we propose to estimate the $100(1 - \alpha)\%$ HDR as

$$\hat{R}_n(\hat{f}_\alpha) = \{\mathbf{x} : \hat{c}_{\mathbf{X}}(\hat{F}_1(x^{(1)}), \hat{F}_2(x^{(2)}))\hat{f}_1(x^{(1)})\hat{f}_2(x^{(2)}) > f_{\lfloor \alpha n \rfloor}\},$$

with \hat{f}_j and \hat{F}_j consistent estimators of the marginals f_j and F_j , $j = 1, 2$. While here, for the sake of space, we focus on the bivariate case, we emphasize that the approach can be easily extended to higher dimensions, as copulae naturally apply to multidimensional contexts (see e.g., *vine copula* methods; 14).

4. Empirical Evaluation

Simulation studies We start with simulation studies, considering the following four data-generation scenarios, with constant parameters fixed at $\mu_1 = 0, \mu_2 = 1, \sigma_1 = \sigma_2 = 2$, and $w_1 = 1 - w_2 = 0.7$ over an increasing number of sample sizes (from 50 to 10,000). For copula specifications, we refer to (11).

SC1: Gaussian marginals \mathcal{N} – Gaussian copula C^{Gauss}

$$f_1 = \mathcal{N}(\mu_1, \sigma_1), \quad f_2 = \mathcal{N}(\mu_2, \sigma_2), \quad C = C_{\rho=0.7}^{\text{Gauss}}$$

SC2: Gaussian \mathcal{N} & Student t marginals – Clayton copula C^{Clay}

$$f_1 = \mathcal{N}(\mu_1, \sigma_1), \quad f_2 = t_{\nu=10}, \quad C = C_{\alpha=2}^{\text{Clay}}$$

SC3: Gaussian \mathcal{N} & Gaussian mixture marginals – Student t copula C^t

$$f_1 = \mathcal{N}(\mu_1, \sigma_1), \quad f_2 = w_1\mathcal{N}(\mu_2, \sigma_2) + w_2\mathcal{N}(\mu_2 + 10, \sigma_2), \quad C = C_{\rho=0.4, \nu=6}^t$$

SC4: Gaussian \mathcal{N} mixture marginals – Gaussian copula C^{Gauss}

$$f_1 = w_1\mathcal{N}(\mu_1, \sigma_1) + w_2\mathcal{N}(\mu_1 + 10, \sigma_1), \quad f_2 = w_1\mathcal{N}(\mu_2, \sigma_2) + w_3\mathcal{N}(\mu_2 + 10, \sigma_2), \quad C = C_{\rho=0.7}^{\text{Gauss}}$$

For each scenario, we evaluate the following three methods.

Method1: Direct estimation of the bivariate density We use the nonparametric KDE (7), and consider the asymptotically optimal solution proposed in (15) for the bandwidths selection.

Method2: Indirect fully-parametric copula-based estimation of the bivariate density For the estimation of the marginals, we consider the true data-generation processes models (with no misspecification) and maximum likelihood fitting. For the copula model, we perform both model selection (with the AIC criterion) and parameter estimation (with maximum likelihood estimation).

Method3: Indirect fully-nonparametric copula-based estimation of the bivariate density For the marginal densities, we use the standard KDE. For the copula model, we use a KDE approach with the *transformation local likelihood estimator* of (16). We use the R KDECOPLA package, adopting the method with quadratic polynomials and nearest-neighbor bandwidths (17).

To quantify the performance of the methods in the simulation study, we call *positive* those points which should be outside the region and *negative* the others. Let FP, TP, FN and TN be, respectively, the number of false positive, true positive, false negative, and true negative points. Well-established measures of inefficiency are the False Negative (Positive) Rates (FNR and FPR), and the Total Error Rate (ER):

$$\text{FNR} = \frac{FN}{FN + TP}; \quad \text{FPR} = \frac{FP}{FP + TN}; \quad \text{ER} = \frac{FN + FP}{FN + FP + TN + TP}.$$

All methods are evaluated based on $\alpha = 0.05$, that is a coverage probability of 95%.

Results As depicted in Figure 1, the three methods lead to slightly different results, with the two copula-based approaches outperforming the direct KDE (Method1). Compared to the nonparametric Method3, the parametric copula-based approach (Method2) shows the lowest ER across all different scenarios and sample sizes, with an exception for the largest sample sizes, where the difference is negligible.

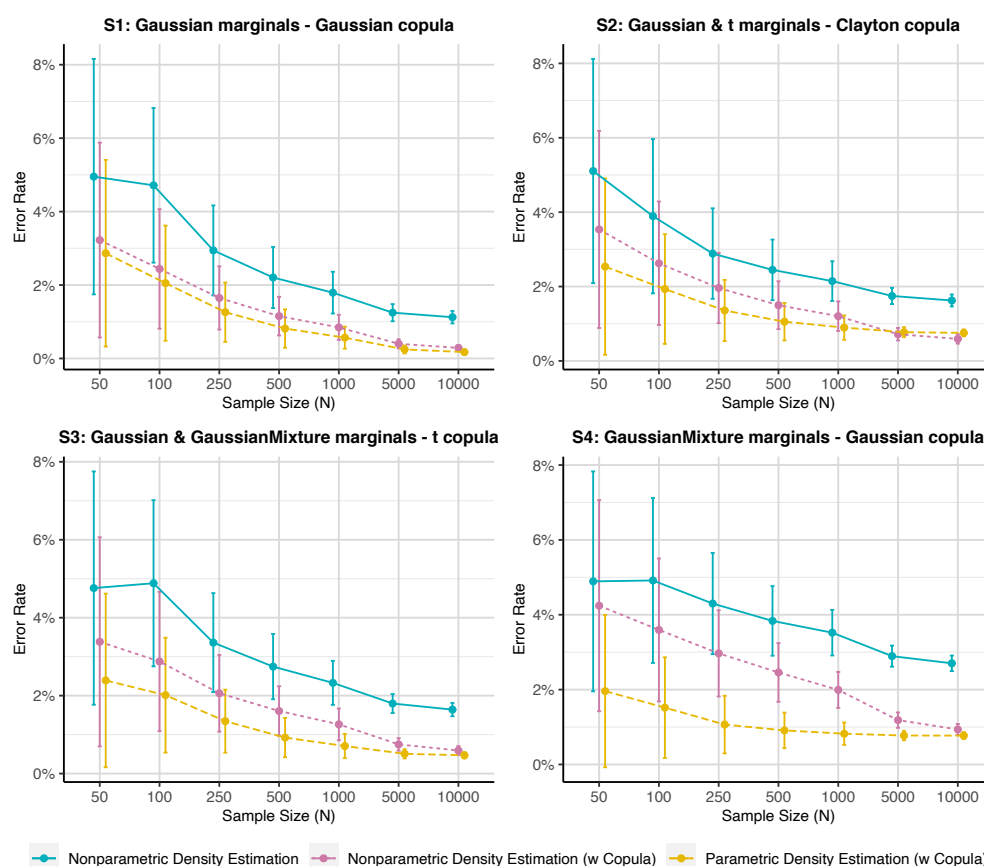


Figure 1: Total error rate (mean and error bars (mean \pm SD), averaged across 10^4 MC samples) of the three compared methods across the different scenarios and for different sample sizes.

Looking at the FPR and FNR, results are very similar across different scenarios and we only discuss scenario S2. As displayed in Figure 2, Method1 has the best FPR performance, with a value close to 0. Rather than being a result of optimal performance, this is due to the fact almost or all data points were classified as highest density points, with no *positives* detected. This is also reflected in its FNR, highlighting a low ability to correctly place *positives* outside the HDR. The two copula-based approaches result in overall better performances, with a slight superiority of the parametric Method2. This was expected as simulation schemes consisted of only parametric copula families, and there is no misspecification.

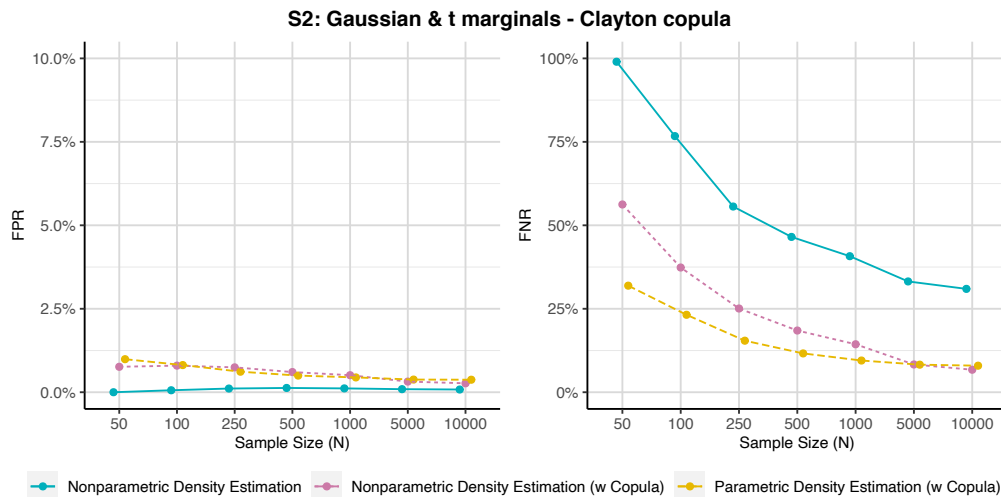


Figure 2: FPR and FNR (averaged across 10^4 MC samples) of the three compared methods for different sample sizes, relatively to scenario S2.

Application to MAGIC Data We apply the proposed methods for constructing a HDR for the joint distribution of two variables from the MAGIC dataset (<https://archive.ics.uci.edu/ml/datasets/MAGIC+Gamma+Telescope>). The data simulate the registration of high-energy gamma particles in a ground-based atmospheric Cherenkov gamma telescope. We focus on gamma observations (overall $n = 12,332$), and consider the two variables “fConc1” and “fM3Long”. In such a case (as deduced from Figure 3), the parametric approach is inappropriate for both the estimation of the marginal distribution and, more importantly, the copula model. Thus, we illustrate the derived HDR using the nonparametric Method1 and Method3 only. While in absence of the underlying truth it is not possible to reliably evaluate the two methods, it seems that the copula-based approach (Method3; right plot), more sensibly excludes the tail data points (which may be expected to have a lower density) from the HDR.

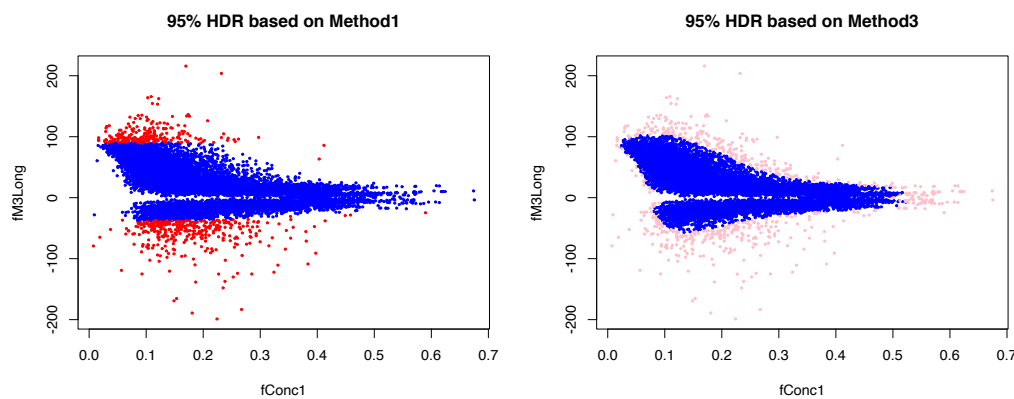


Figure 3: 95% HDR for two variables from the MAGIC dataset with Method1 and Method2.

5. Concluding Remarks

In this work, we proposed an alternative strategy for deriving HDRs in multivariate contexts using *copulae*, and evaluated both a parametric and a nonparametric approach. Compared to traditional kernel density estimation, the copula-based HDR resulted in lower missclassification errors in a number of simulation scenarios and possibly in real data. Although in this work we focused on the bivariate case ($d = 2$), we expect to see remarkable advantages over an increased number of variables $d > 2$. In fact, the extension of the common KDE to high dimensions has proven challenging in terms of both computational efficiency and statistical inference. We aim to pursue such a direction in future work, exploring, e.g., the use of vine copulae to construct flexible dependence models for an arbitrary number of variables using only bivariate building blocks.

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