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ABSTRACT

Recently, distribution element trees (DETs) were introduced as an accurate and computationally efficient method for density estimation. In this work, we demonstrate that the DET formulation promotes an easy and inexpensive way to generate random samples similar to a smooth bootstrap. These samples can be generated unconditionally, but also, without further complications, conditionally using available information about certain probability-space components. This article is accompanied by the R codes that were used to produce all simulation results. Supplementary material for this article is available online.

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Sampling

1. Introduction

In many statistical problems, resampling methods such as cross-validation—used, for example, for the evaluation of regression models, jackknife—applied for estimator bias reduction (Leger, Politis, and Romano 1992; Chernick 2012), or bootstrap methods (Efron 1979) are applied. Bootstrapping is, for example, applied to determine—based on an available ensemble of n independent and identically distributed samples $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ that stem from an unknown d -dimensional probability density $p(\mathbf{x})$ with $\mathbf{x} \in \Omega$ —the distribution of an estimator (Hinkley 1988). The resulting distribution can be further used to evaluate standard errors and confidence intervals, or for hypothesis testing.

The basic concept behind the bootstrap is the use of simulated bootstrap ensembles $\mathbf{x}_1^*, \mathbf{x}_2^*, \dots, \mathbf{x}_n^*$ that are, in the case of the standard bootstrap, generated from the empirical distribution function $p_n(\mathbf{x}) = \frac{1}{n} \sum_{j=1}^n \delta(\mathbf{x} - \mathbf{x}_j)$ with the Dirac function δ . Alternatively, bootstrap ensembles may be obtained from a parametric model (parametric bootstrap) or from a smoothed density resulting typically from kernel density estimation (KDE; Hesterberg 2015) (smoothed bootstrap). Based on the available ensemble and the simulated bootstrap ensembles, the properties of a statistical quantity, for example, a parameter estimator, can be extracted. The standard and smoothed bootstraps enable this extraction by means of Monte Carlo simulation without further parametric assumptions about the underlying distribution $p(\mathbf{x})$, which renders both bootstraps particularly useful. Under certain conditions, Silverman and Young (1987) have demonstrated that the smoothed bootstrap leads to parameter estimates at reduced mean square errors compared to the standard bootstrap. Hall, DiCiccio, and Romano (1989) have shown that the smoothed bootstrap has an improved error convergence for increasing n over the standard bootstrap, when the statistical quantity of interest involves the probability density such as when estimating quantiles. Moreover, smoothed boot-

strapping is advantageous when applied for optimal bandwidth selection in KDE (Leger, Politis, and Romano 1992; Taylor 1989).

In addition to existing density estimation methods such as KDE (e.g., Silverman 1998; Botev, Grotowski, and Kroese 2010; Scott 2015) or mixture-based approaches (e.g., Ferguson 1973; Neal 2000; Wang and Wang 2015), we recently introduced a new nonparametric density estimator that is based on distribution element trees (DETs; Meyer 2018a). Here, the d -dimensional probability space Ω is decomposed into m disjoint cuboids C_k with $\Omega = \bigcup_{k=1}^m C_k$. The density inside cuboid k is given by

$$p_k(\mathbf{x}) = \begin{cases} \frac{n(C_k)}{n} \prod_{i=1}^d p[x_i | \theta_i(C_k)] & \forall \mathbf{x} \in C_k, \\ 0 & \text{otherwise,} \end{cases} \quad (1)$$

and can be viewed as a simplest building block or atom of the DET estimator

$$\hat{p}(\mathbf{x}) = \sum_{k=1}^m p_k(\mathbf{x}) \quad \forall \mathbf{x} \in \Omega \quad (2)$$

of the unknown density $p(\mathbf{x})$. In cuboid density (1), $n(C_k)$ counts the number of samples $\mathbf{x}_j \in C_k$ with $j \in \{1, 2, \dots, n\}$ and $p[x_i | \theta_i(C_k)]$ is a marginal polynomial density for component x_i of the d -dimensional probability space Ω (e.g., Meyer 2018a, Eqs. (3) and (4)). The density parameter vector $\theta_i(C_k)$ is estimated from the $n(C_k)$ samples in C_k . The cuboids C_k and their densities $p_k(\mathbf{x})$, that form a so-called distribution element (DE), are resulting from a tree-like subdivision process with cuboids (tree nodes) being divided into subcuboids (tree branches). Subdivisions are determined by a goodness-of-fit test that evaluates locally the compatibility of density (1) with the samples contained in C_k . This subdivision criterion resolves

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termination issues of earlier tree-based methods (e.g., Wong and Ma 2010; Ram and Gray 2011; Jiang et al. 2016) and leads to a highly adaptive estimator with a density that is either piecewise constant, piecewise linear, etc., depending on the DE order or more precisely the order of $p[x_i|\theta_i(C_k)]$. The performance of the DET estimator was evaluated in a series of test cases of different dimensionality involving Gaussian mixtures as well as other densities including discontinuous ones. The linear DET estimator was found to be more accurate and computationally efficient than existing tree-based approaches such as density trees (Ram and Gray 2011) and limited-lookahead optional Pólya trees (Wong and Ma 2010; Jiang et al. 2016). Moreover, compared to the highly cited adaptive KDE of Botev, Grotowski, and Kroese (2010), that is based on the solution of a nonlinear diffusion partial differential equation (PDE) and a fix-point iteration involving a linear diffusion PDE, the linear DET estimator displayed equal or superior mean integrated square error (MISE) convergence rates and scaled favorably in terms of computational costs for increasing n .

In this work, we are making use of the structure of the DET estimator given by Equations (1) and (2) to formulate a smooth bootstrap that allows for the simulation of (un)conditional samples. The underlying formulation is outlined in Section 2 followed by exemplary simulations presented in Section 3.

2. Formulation

In the smoothed bootstrap resulting from KDE, a sample is generated by (I) drawing a sample from the available ensemble and by (II) adding noise to it, as implied by the kernel located at the selected sample (Efron 1979, Eq. (3.11); Scott 2015, Sec. 3.9.1). Given the DET estimator (2), samples can be generated based on a similar two-step procedure, as is outlined in a first step for the unconditional case in the following section.

2.1. Unconditional Generation

Given DET estimator (2), the probability mass for a sample to reside in cuboid C_k is given by

$$\int_{C_k} p_k(\mathbf{x})d\mathbf{x} = \frac{n(C_k)}{n} \int_{C_k} \prod_{i=1}^d p[x_i|\theta_i(C_k)]d\mathbf{x} = \frac{n(C_k)}{n} \prod_{i=1}^d \int_{x_{i,l}^k}^{x_{i,u}^k} p[x_i|\theta_i(C_k)]dx_i = \frac{n(C_k)}{n}, \tag{3}$$

where, Equation (1) was introduced in the first step,

$$\int_{C_k} \dots d\mathbf{x} = \int_{x_{1,l}^k}^{x_{1,u}^k} \int_{x_{2,l}^k}^{x_{2,u}^k} \dots \int_{x_{d,l}^k}^{x_{d,u}^k} \dots dx_d \dots dx_2 dx_1,$$

cuboid k is defined as $C_k = \prod_{i=1}^d [x_{i,l}^k, x_{i,u}^k]$ with lower and upper bounds $x_{i,l}^k$ and $x_{i,u}^k$, respectively, and the last step in expression (3) is based on the normalization condition of the marginal densities, that is, $\int_{x_{i,l}^k}^{x_{i,u}^k} p[x_i|\theta_i(C_k)]dx_i = 1$.

Therefore, to generate a random sample \mathbf{x}^* based on an existing DET estimator, first, we randomly pick a DE C_k according to the probability masses $n(C_k)/n$. Inside the selected C_k , components x_i are statistically independent (see Equation (1)). The x_i^* are thus generated in a second step based on uniformly distributed random numbers $y_i^* \in [0, 1]$ and the inverse cumulative distribution functions (CDF) of the marginal densities $p[x_i|\theta_i(C_k)]$ as $x_i^* = P^{(-1)}[y_i^*|\theta_i(C_k)]$. For the constant and linear marginal densities considered in our earlier work (Meyer 2018a), the inverse CDFs are available in analytical form.

2.2. Conditional Generation

In a next step, a sample \mathbf{x}^* shall be generated under the condition that components $x_{q+1}, x_{q+2}, \dots, x_d$ with $1 \leq q \leq d$ take known prescribed values. Here, $q = d$ corresponds to the unconditional case discussed in the previous section, whereas with $q = 1$ all but one, or more precisely, all but the first component of \mathbf{x}^* are known. It is pointed out that the ordering of components x_i with known components following unknown components serves the sole purpose of a simplified notation. The conditional density of the remaining random components x_1, x_2, \dots, x_q is then given by

$$p(\mathbf{x}'|\mathbf{x}^c) = \frac{p(x_1, x_2, \dots, x_q | x_{q+1}, x_{q+2}, \dots, x_d)}{p(x_{q+1}, x_{q+2}, \dots, x_d)} = \frac{p(\mathbf{x}')}{p(\mathbf{x}^c)}, \tag{4}$$

where

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}' \\ \mathbf{x}^c \end{pmatrix}, p(\mathbf{x}^c) = \int_{x_{1,l}}^{x_{1,u}} \int_{x_{2,l}}^{x_{2,u}} \dots \int_{x_{q,l}}^{x_{q,u}} p(\mathbf{x}) dx_q \dots dx_2 dx_1$$

is a normalization constant, and $x_{i,l}$ and $x_{i,u}$ are the lower and upper bounds, respectively, of component x_i of the probability space Ω . Similarly to derivation (3) in the unconditional case, the probability mass for a sample to reside in cuboid C_k —with C_k honoring condition

$$x_i \in [x_{i,l}^k, x_{i,u}^k] \forall i \in \{q + 1, q + 2, \dots, d\}, \tag{5}$$

which accounts for the known prescribed components—is given by

$$\begin{aligned} & \int_{x_{1,l}^k}^{x_{1,u}^k} \int_{x_{2,l}^k}^{x_{2,u}^k} \dots \int_{x_{q,l}^k}^{x_{q,u}^k} p(\mathbf{x}'|\mathbf{x}^c) dx_q \dots dx_2 dx_1 \\ &= \frac{1}{p(\mathbf{x}^c)} \int_{x_{1,l}^k}^{x_{1,u}^k} \int_{x_{2,l}^k}^{x_{2,u}^k} \dots \int_{x_{q,l}^k}^{x_{q,u}^k} p(\mathbf{x}) dx_q \dots dx_2 dx_1 \\ &= \frac{1}{p(\mathbf{x}^c)} \int_{x_{1,l}^k}^{x_{1,u}^k} \int_{x_{2,l}^k}^{x_{2,u}^k} \dots \int_{x_{q,l}^k}^{x_{q,u}^k} \frac{n(C_k)}{n} \prod_{i=1}^d p[x_i|\theta_i(C_k)] dx_q \dots dx_2 dx_1 \\ &= \frac{1}{p(\mathbf{x}^c)} \frac{n(C_k)}{n} \prod_{i=q+1}^d p[x_i|\theta_i(C_k)] \prod_{i=1}^q \int_{x_{i,l}^k}^{x_{i,u}^k} p[x_i|\theta_i(C_k)] dx_i \\ &= \frac{1}{p(\mathbf{x}^c)} \frac{n(C_k)}{n} \prod_{i=q+1}^d p[x_i|\theta_i(C_k)]. \end{aligned} \tag{6}$$

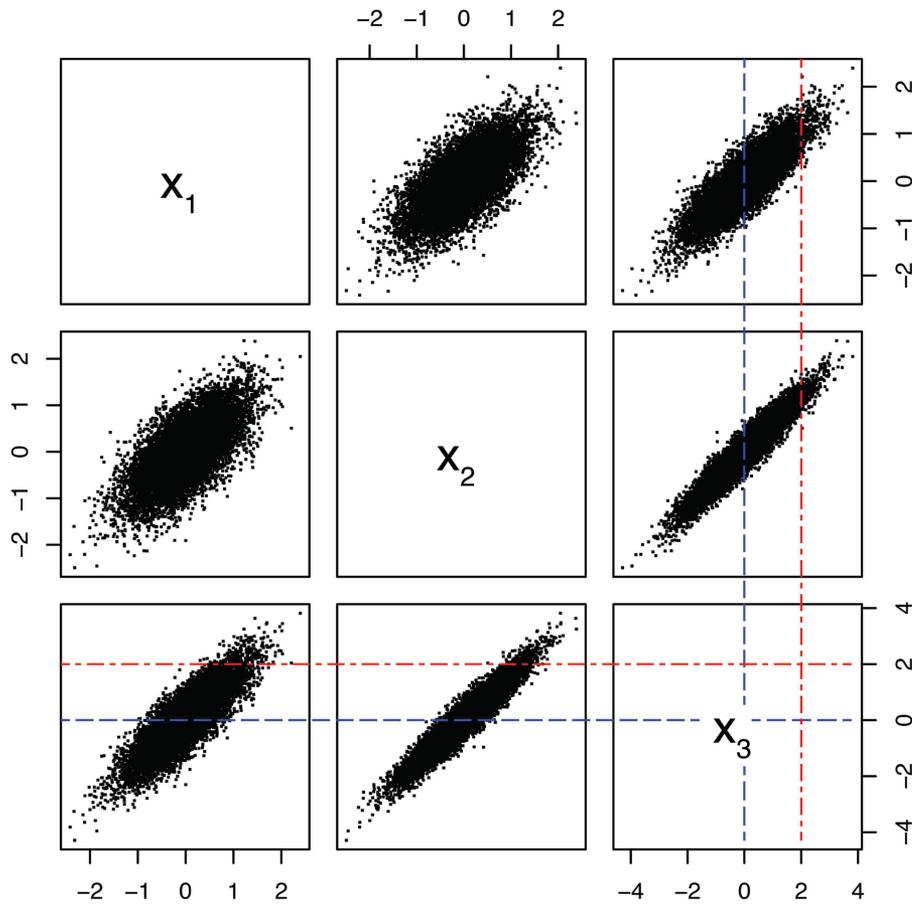


Figure 1. The ensemble with 10^6 samples resulting from the Gaussian density (7) is shown in x_1 - x_2 - x_3 probability space. Conditioning x_1 - x_2 -planes at $x_3 = 0$ (blue dashed) and 2 (red dash-dotted) are provided as well.

This result is based on Equations (1), (2), and (4). Therefore in the conditional case, the probability masses from the unconditional case $n(C_k)/n$ are modified by the constant $1/p(\mathbf{x}^c)$ and a factor. The latter involves the marginal DE densities evaluated at the prescribed values and thus differs among the DEs that intersect with the conditions \mathbf{x}^c or more precisely satisfy condition (5).

In summary, to generate a sample \mathbf{x}^* with components $x_{q+1}, x_{q+2}, \dots, x_d$ prescribed, the cuboids or DEs satisfying condition (5) are identified and one DE from this set is randomly picked according to the probabilities (6). Based on the marginal densities of the selected DE, components x_1, x_2, \dots, x_q of \mathbf{x}^* are determined in a second step based on uniformly distributed random numbers $y_1^*, y_2^*, \dots, y_m^*$ and inverse CDFs like in the unconditional case (see last paragraph of the previous section). Given the tree-based arrangement of the DEs introduced in our earlier work (Meyer 2018a, sec. 2.2), the DEs that honor condition (5) can be identified efficiently. To this end, we start at the tree root (cuboid corresponding to Ω) and navigate along branches keeping track of cuboids that satisfy condition (5).

3. Simulations

As an illustration of the outlined (conditional) DET-based sample generation method, we provide three different examples involving linear DEs.

3.1. Trivariate Gaussian

The first case deals with an available ensemble with $n = 10^6$ samples that stems from the Gaussian density

$$p(\mathbf{x}) = \frac{\exp\left[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{C}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right]}{\sqrt{(2\pi)^d \det(\mathbf{C})}} \quad (7)$$

with $d = 3$, $\mathbf{x} = (x_1, x_2, x_3)^\top$, mean vector $\boldsymbol{\mu} = (0, 0, 0)^\top$, and arbitrarily chosen covariance matrix

$$\mathbf{C} = \begin{pmatrix} 0.35 & 0.25 & 0.5 \\ 0.25 & 0.4 & 0.6 \\ 0.5 & 0.6 & 1 \end{pmatrix}.$$

The degree of statistical dependence among the components x_i is illustrated in Figure 1, where the available ensemble is depicted. Given the data and using the DET implementation (Meyer 2018b), a linear DET was constructed with equal-size cuboid splits (for details see Meyer 2018a, sec. 2.2.1). Cross-sections at $x_3 = 0$ and 2 of the resulting density estimate are compared in Figure 2 against the reference density (7). Based on the DET and using the previously outlined methodology, 10^5 samples \mathbf{x}^* were resampled under the condition that $x_3 = 0$ or 2. The resulting conditional densities $p(x_1^*, x_2^* | x_3)$, estimated again with a linear DET, are depicted in Figure 2. One can observe that at $x_3 = 0$, where the marginal density $p(x_3)$ is larger (like the local sample frequency) compared to $p(x_3 = 2)$, the statistical error is locally smaller in the DET estimator used

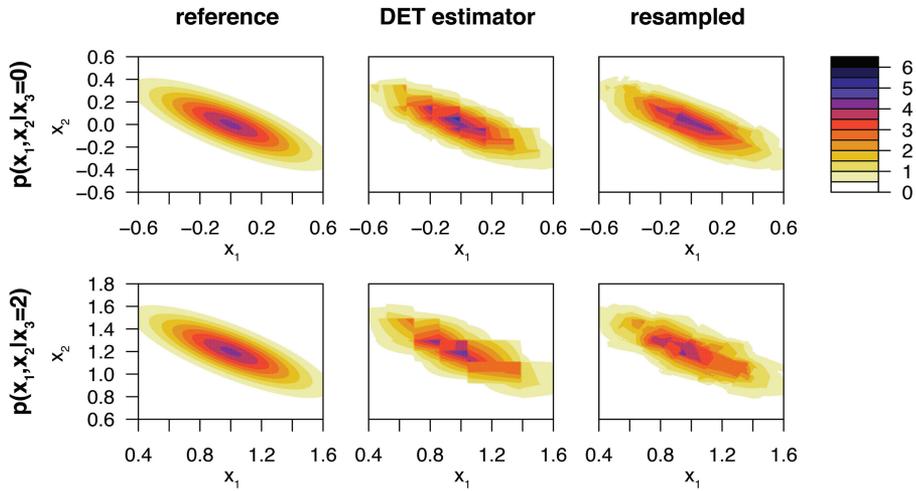


Figure 2. Conditional density and density estimates of $p(x_1, x_2|x_3)$ resulting from the joint Gaussian (7) (left column), the DET estimator (center) resulting from the ensemble with 10^6 samples $(x_1^*, x_2^*, x_3^*)^\top$, and the DET estimator (right) based on 10^5 resampled $(x_1^*, x_2^*)^\top$ conditional on x_3 are shown. Densities and density estimates for $x_3 = 0$ and 2 are depicted in the top and bottom rows, respectively.

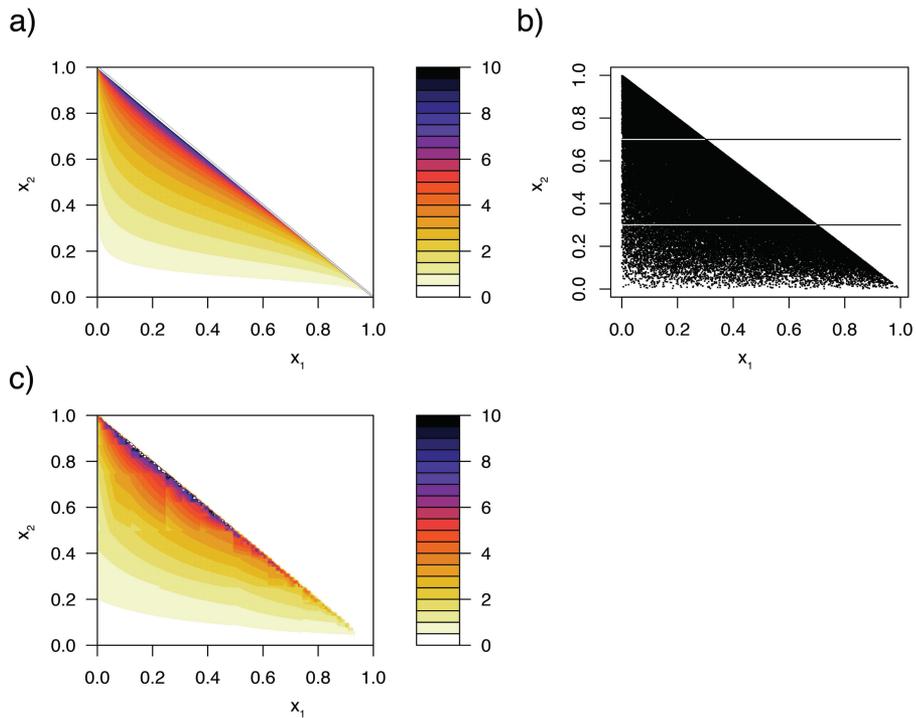


Figure 3. (a) Bivariate Dirichlet density (8) with parameters $\alpha_1 = 1.25, \alpha_2 = 2$, and $\alpha_3 = 0.75$, and (b) the corresponding ensemble with $n = 10^5$ samples \mathbf{x}^* . The horizontal lines mark conditioning locations at $x_2 = 0.3$ and 0.7 . (c) Linear DET estimator resulting from the data shown in panel (b).

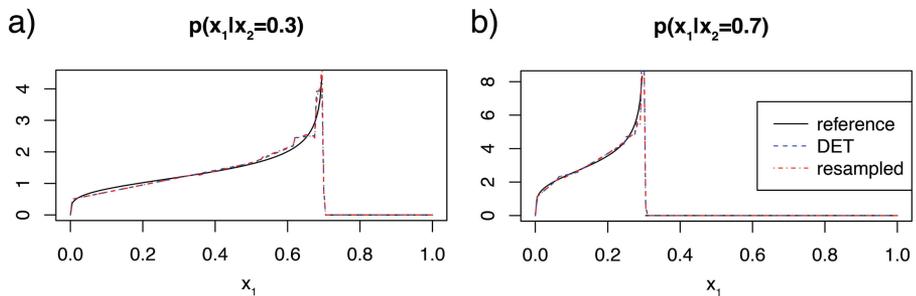


Figure 4. Conditional density and density estimates of $p(x_1|x_2)$ resulting from the Dirichlet density (8) (black solid), the DET estimator (blue dashed) resulting from an ensemble with 10^5 samples $(x_1^*, x_2^*)^\top$, and the DET estimator (red dash-dotted) based on 10^5 resampled x_1^* conditional on x_2 are shown. Densities and density estimates for $x_2 = 0.3$ and 0.7 are depicted in panels (a) and (b), respectively.

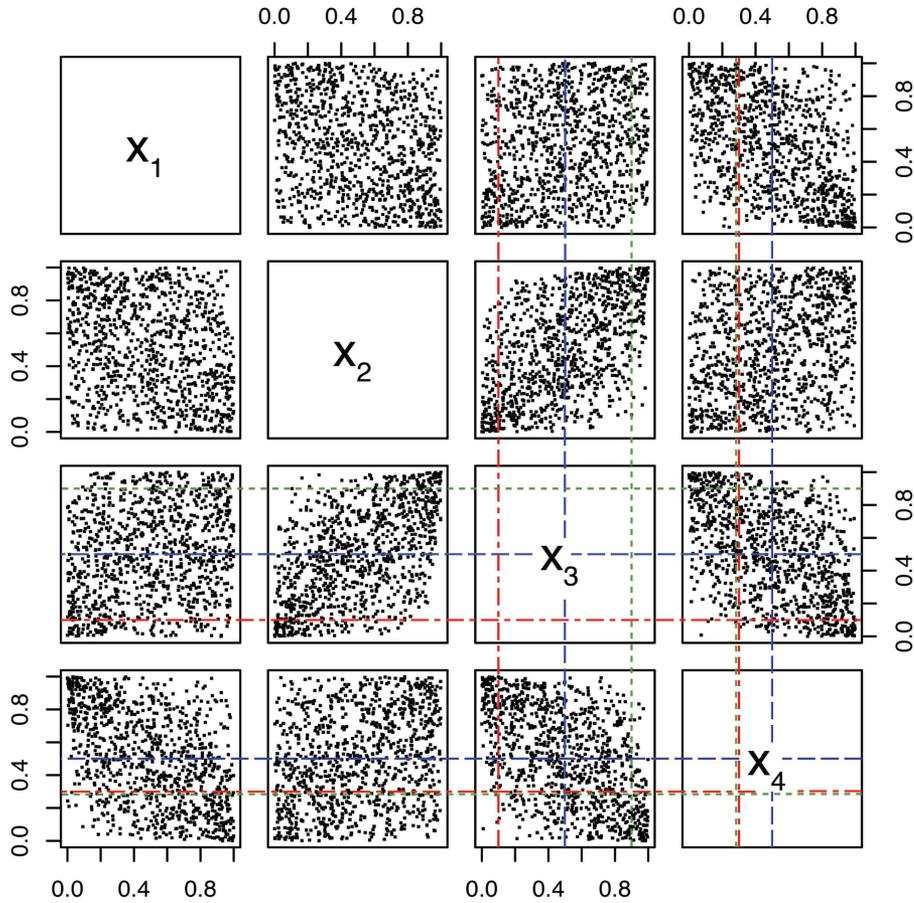


Figure 5. An ensemble with 10^3 samples stemming from copula density (9) is shown in x_1 - x_2 - x_3 - x_4 probability space. Conditioning x_1 - x_2 -planes at $(x_3, x_4) = (0.5, 0.5)$ (blue dashed), $(0.1, 0.3)$ (red dash-dotted), and $(0.9, 0.3)$ (green dotted) are depicted as well.

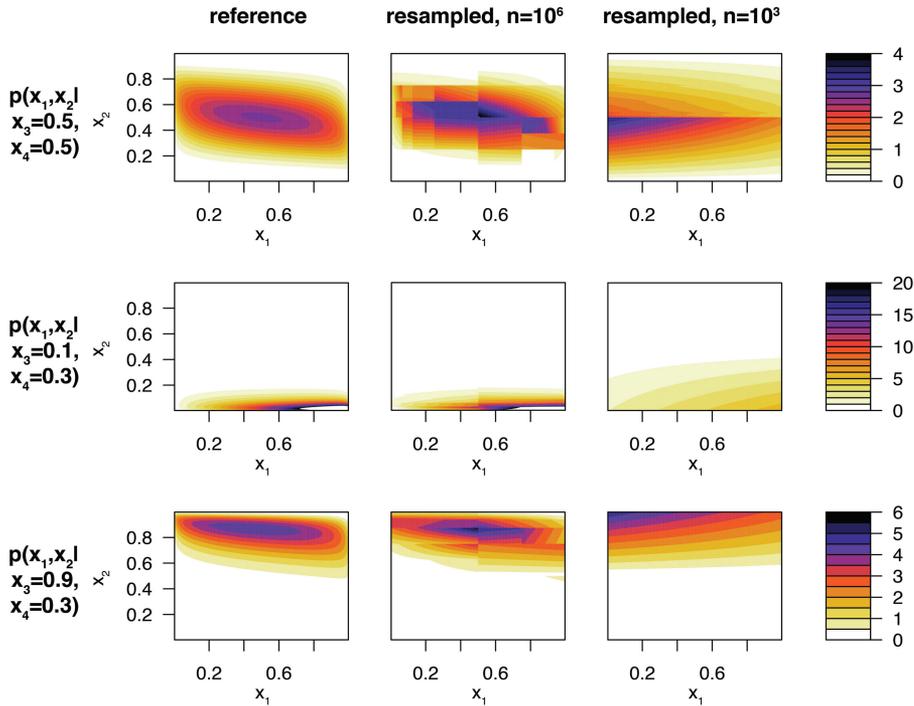


Figure 6. Conditional density and density estimates of $p(x_1, x_2 | x_3, x_4)$ resulting from the copula density (9) (left column) and DET estimators (center and right) obtained from ensembles with 10^3 bootstrap samples $(x_1^*, x_2^*)^T$ resampled conditionally on x_3 and x_4 as indicated (rows). For the central column, the DET estimator for resampling was computed based on an available ensemble with 10^6 samples, while for the right column 10^3 samples were used.

for resampling, and consequently the agreement between the reference density (first column in Figure 2) and the resulting resampled data (last column) is better.

3.2. Bivariate Dirichlet Distribution

In a second case, the bivariate Dirichlet density

$$p(x_1, x_2) = \begin{cases} \frac{x_1^{\alpha_1-1} x_2^{\alpha_2-1} (1-x_1-x_2)^{\alpha_3-1} \Gamma(\alpha_1 + \alpha_2 + \alpha_3)}{\Gamma(\alpha_1)\Gamma(\alpha_2)\Gamma(\alpha_3)} & \forall x_1 \geq 0 \vee x_2 \geq 0 \\ & \vee 1-x_1-x_2 \geq 0, \\ 0 & \text{otherwise,} \end{cases} \quad (8)$$

with parameters $\alpha_1 = 1.25$, $\alpha_2 = 2$, and $\alpha_3 = 0.75$ is considered. This parameter set leads, differently to the previous Gaussian case, to a discontinuity along the line $x_2 = 1 - x_1$ as is depicted in Figure 3(a), where density (8) is plotted. To further illustrate the resampling method outlined in Section 2, an ensemble with $n = 10^5$ samples stemming from the Dirichlet density (8) and shown in Figure 3(b) was used as a basis, and the linear DET estimator depicted in Figure 3(c) was constructed. Estimates of the conditional density $p(x_1|x_2)$ for $x_2 = 0.3$ and 0.7 resulting from the DET are plotted in Figure 4 (blue dashed lines) and can be compared with the conditional densities derived from reference density (8). Based on the DET estimator, ensembles with 10^5 samples x_1^* were resampled given the condition $x_2 = 0.3$ or 0.7 . DET-based density estimates from the resampled data are provided in Figure 4 as well (red dash-dotted lines) and compare well against the reference density (8) (black lines). A closer look at the DET estimators, that is, the one from the available ensemble $\mathbf{x}^* = (x_1^*, x_2^*)^\top$ (blue dashed) and the DET from the conditionally resampled x_1^* data (red dash-dotted), illustrates that the resampled data emulates as expected the underlying DET given by the blue dashed lines.

3.3. Four-Dimensional Copula

Finally, conditional simulations involving a four-dimensional Gauss copula shall be presented. The copula density is given by

$$p(x_1, x_2, x_3, x_4) = \frac{1}{\sqrt{\det(\mathbf{R})}} \exp \left\{ -\frac{1}{2} \begin{bmatrix} \Phi^{(-1)}(x_1) \\ \vdots \\ \Phi^{(-1)}(x_4) \end{bmatrix}^\top (\mathbf{R}^{-1} - \mathbf{I}) \begin{bmatrix} \Phi^{(-1)}(x_1) \\ \vdots \\ \Phi^{(-1)}(x_4) \end{bmatrix} \right\} \quad (9)$$

where $\Phi^{(-1)}$ is the inverse of the standard normal CDF, \mathbf{I} is the identity matrix, and the randomly selected correlation matrix \mathbf{R} is defined as

$$\mathbf{R} = \begin{pmatrix} 1 & -0.344 & 0.141 & -0.486 \\ -0.344 & 1 & 0.586 & 0.244 \\ 0.141 & 0.586 & 1 & -0.544 \\ -0.486 & 0.244 & -0.544 & 1 \end{pmatrix}.$$

Matrix \mathbf{R} depicts different extents of correlation among the components x_i with $i = 1, \dots, 4$. To assess the performance of the DET-based bootstrap with sparse data, original ensembles with $n = 10^3$ and $n = 10^6$ samples \mathbf{x}^* were considered.

In Figure 5, the smaller ensemble is depicted together with three sets of conditions involving components x_3 and x_4 (lines). These sets explore different forms of the conditional density $p(x_1, x_2|x_3, x_4)$ as is shown in the first column of Figure 6. The depicted $p(x_1, x_2|x_3, x_4)$ serve as references for DET estimates (second and third columns) that were computed from bootstrap samples $(x_1^*, x_2^*)^\top$, which in turn were resampled conditional on x_3 and x_4 . The bootstrap samples in the second column of Figure 6 resulted from DETs based on original ensembles with 10^6 samples \mathbf{x}^* , while in the third column only 10^3 samples \mathbf{x}^* were used as a basis. For all three condition sets (rows), the agreement between the resampled data $(x_1^*, x_2^*)^\top$ (or more specifically its DET estimates) and the reference density $p(x_1, x_2|x_3, x_4)$ is better for the large original ensemble (central column). Nevertheless, the modes in $p(x_1, x_2|x_3, x_4)$ are captured reasonably well given an original ensemble with just 10^3 samples.

The presented simulations, including DET generation and resampling, were performed with the R scripts listed in Section 3.3. All scripts make use of the detpack library that is available on CRAN (Meyer 2018b). An equivalent library for Matlab is available on the MathWorks File Exchange (Meyer 2018c).

Supplementary Materials

The following R scripts are contained in the supplementary package `detrnd_test.zip`:

- `detrnd_test_1.R` script for the trivariate Gaussian case discussed in Section 3.1
- `detrnd_test_2.R` script for the bivariate Dirichlet case discussed in Section 3.2
- `detrnd_test_3.R` script for the four-dimensional copula case discussed in Section 3.3

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