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Dependence structure estimation using Copula Recursive Trees

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Abstract

We construct the Copula Recursive Tree (CORT) estimator: a flexible, consistent, piecewise linear estimator of a copula, leveraging the patchwork copula formalization and various piecewise constant density estimators. While the patchwork structure imposes a grid, the CORT estimator is data-driven and constructs the (possibly irregular) grid recursively from the data, minimizing a chosen distance on the copula space. The addition of the copula constraints makes usual denisty estimators unusable, whereas the CORT estimator is only concerned with dependence and guarantees the uniformity of margins. Refinements such as localized dimension reduction and bagging are developed, analyzed, and tested through applications on simulated data.

Keywords: CORT, piecewise linear copula, patchwork copula, density estimation trees, nonparametric estimation, quadratic program, bagging.

1 Introduction

Although the estimation of copula [38, 26, 15] is a wide-treated subject, most performant estimators available in the litterature are based on restricted, parametric estimation.

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Vine copulas[37, 36, 35, 34, 40], although useful in high dimensions, often use parametric models such as archimedean copulas as base building blocks. On one other hand, graphical models [28, 17] assume a gaussian dependence structure and therefore are fast but under restrictive assumptions. Classical nonparametric density estimators such as kernels [23, 45, 46, 47] or wavelets [21, 33, 18] are not suited to satisfy constraints such as the uniformity of margins (one counter-example may be found in [8, 16]). We explore here a specific class of non-parametric copula density estimators with tree-structured piecewise constant densities, and design an estimator that lies in this class, the CORT estimator.

The CORT estimator is based on the *density estimation trees* from [42], which is a treestructured non-parametric density estimator, and on the framwork of *patchwork copulas* from [14, 12, 13]. There already exist several others piecewise constant density estimators: the *cascaded histograms* of [22], the *Dirichlet-based Polya tree* [39], the *distribution element trees* by [31], the *adaptative sparse grids* of [41], the framework of *gaussian mixtures* by [9], the *bayesian sequential partitioning* techniques by [29, 27] with their interesting asymptotic consistency results, and the *Wasserstein compression* techniques provided by [30] are all worth noting in the field of non-parametric piecewise density estimation. But these models are built to estimate densities without taking into account uniformity of margins, and they do not always lead to proper copulas when applied on pseudo-observations or true copula samples.

The CORT estimator has the particularity of being tree-shaped which ensures on one hand that the computation of the estimated density and the distribution function on new data points is fast, and on the other hand that storage of the model is efficient. Thus, it could be used for tasks such as re-sampling a dataset outside of the already existing points, or for compression purposes, when dealing with big-data dependencies. Finally, under mild conditions, the estimator is a proper copula, where classical non-parametric estimators, such as Deheuvel's empirical copula, are not.

This paper is organised as follows. In Section 2 we describe the class of piecewise linear copulas and give some of their properties. In Section 3, we propose an estimation procedure, allowing localized dimension reduction, and we establish a convergence result for this procedure. In Section 4 we deal with ensemble models based on the CORT estimator: Bagging techniques and out-of-bag generalisation statistics are developed in the field of copula density estimation, and applied to the CORT estimator. Finally, Section 5 investigates the performance of the model by applications on some simulated examples, and Section 6 concludes.

2 The piecewise linear copula

Let $X = (X_1, ..., X_d)$ be a multivariate random vector of dimension d. We are interested in the dependence structure between components of X. The concept of copula, whose formalisation is due to [48], allows to study this dependence separately from the marginal distributions. Consider that the distribution function (d.f.) F of the random vector X with marginal d.f.s $F_1, ..., F_d$, and define the function C as:

$$C(\boldsymbol{u}) = F\left(F_1^{-1}(u_1), ..., F_d^{-1}(u_d)\right), \quad \forall \boldsymbol{u} \in [0, 1]^d$$

Then the distribution of the random vector X is characterised by the marginal distributions and the function C, called the copula. Sklar's Theorem [48] states that a copula Csatisfying the previous equality always exists, and that it is uniquely defined provided that the marginal random variables are absolutely continuous. In particular, it is unique if the random vector is continuous. One can easily check that C is the distribution function of a d-dimensional random vector with uniform margins. Furthermore, C defines the whole dependence structure of the random vector and does not contain information about the marginal distributions.

The estimation of the full distribution can then be splitted into the estimation of onedimensional margins, which is a wide-treated subject, and the estimation of the copula. We are here concerned by the estimation of the copula, and we propose to work with a piecewise linear distribution function. In the following, we will define the piecewise linear copulas and then present some of their properties.

2.1 Definition

Let $\mathbb{I} = [0, 1]^d$ be the unit hypercube.

Definition 2.1 (Piecewise linear copula). Let \mathcal{L} be a finite partition of \mathbb{I} into subsets called *leaves*, usually denoted by ℓ . The piecewise linear copula with partition \mathcal{L} and weighs p is defined by its distribution function:

$$\forall \boldsymbol{u} \in \mathbb{I}, \ C_{\boldsymbol{p},\mathcal{L}}(\boldsymbol{u}) = \sum_{\ell \in \mathcal{L}} p_{\ell} \lambda_{\ell}(\boldsymbol{u})$$
(2.1)

where λ denotes the Lebesgue measure of a set, $\lambda_{\ell}(\boldsymbol{u}) = \lambda(\ell)^{-1}\lambda([0, \boldsymbol{u}] \cap \ell)$, and \boldsymbol{p} is a vector of non-negative weights summing to one. The corresponding density, which is piecewise constant, is given by:

$$c_{\boldsymbol{p},\mathcal{L}}(\boldsymbol{u}) = \sum_{\ell \in \mathcal{L}} \frac{p_{\ell}}{\lambda(\ell)} \mathbb{1}_{\boldsymbol{u} \in \ell}$$
(2.2)

where $\mathbb{1}$ is the indicator function.

This type of histogram has already been used, in the case of density estimation, with different construction schemes and bin shapes, e.g with a Voronoï diagram [7, 19] or a Delaunay tessellation [51, 25, 4] as partition, or more trivially with simple sets of hyperboxes [42, 2, 29, 30].

Remark 2.2 (Existence). Depending on the choice of the partition \mathcal{L} and the weights p, the distribution function $C_{p,\mathcal{L}}$ is not always a copula. However, if $\forall \ell \in \mathcal{L}, p_{\ell} = \lambda(\ell)$, then $C_{p,\mathcal{L}}$ is the independence copula. Therefore, for any partition, there exist at least one set of weights making the model a proper copula. On the other hand, a partition that is too complex might not have other solutions: the assumption of uniform leaves and the marginals uniformity constraints restrict the shape of bins. For polytopial non-hyperrectangular leaves, the independence copula is often the only solution.

Before analysing more precisely the copula constraints on such a model, we restrict ourselves to the case of hyper-rectangular leaves, leading to the following definition:

Definition 2.3 (Suitable partition). Let \boldsymbol{a} and \boldsymbol{b} both be in \mathbb{I} . Then, if $\boldsymbol{a} \leq \boldsymbol{b}$ (componentwise), we define the hyper-rectangular leaf $(\boldsymbol{a}, \boldsymbol{b}]$ as $(\boldsymbol{a}, \boldsymbol{b}] = (a_1, b_1] \times ... \times (a_d, b_d]$. We call *suitable* a partition where every leave with strictly positive Lebesgue measure is an hyper-rectangle.

Remark 2.2 is one of the reasons driving the definition of a suitable partition. Remark that it is also why we chosed to extend the *density estimation trees* from [42] instead of another piecewise constant density estimator: this algorithm produces a suitable partition.

If not specified, we consider by default that partitions we are dealing with are suitable. In the next subsection, we propose some properties of this dependence structure.

2.2 Properties

The above formulation of a piecewise linear copula allows to obtain closed-form expressions for classical quantities of interest in copula modeling. We recall some of those quantities and then derive their expression for piecewise linear copulas.

The Kendall τ and Spearman ρ (see [38]) are common dependence measures that can be computed from a copula. They are respectively defined as:

$$\tau = 4 \int C(\boldsymbol{u}) c(\boldsymbol{u}) d\boldsymbol{u} - 1$$
 and $\rho = 12 \int C(\boldsymbol{u}) d\boldsymbol{u} - 3$,

for a copula C and its density c. The piecewise constant expression of the density in the piecewise linear class allows for simple computation of τ and ρ , although the expressions can be somewhat cumbersome. Note that both τ and ρ are always in [-1, 1].

Property 2.4 (Common dependence measures). Let $C_{p,\mathcal{L}}$ be a piecewise linear copula.

its Kendall τ and Spearmann ρ are given in closed form by:

$$\begin{aligned} \tau &= -1 + 2\sum_{\substack{\ell \in \mathcal{L} \\ k \in \mathcal{L}}} \frac{p_{\ell} p_k}{\lambda(\ell) \lambda(k)} \prod_{i=1}^d \left(\left(b_i \wedge d_i - a_i \wedge c_i \right) \left(b_i \wedge d_i + a_i \wedge c_i - 2c_i \right) + 2 \left(d_i - c_i \right) \left(b_i - a_i \wedge d_i \right) \right) \\ \rho &= -3 + 6\sum_{\ell \in \mathcal{L}} p_\ell \prod_{i=1}^d \left(2 - b_i - a_i \right) \end{aligned}$$

where we denote $\ell = (a, b]$ and k = (c, d], and \land denotes the minimum operator.

Proof. We have:

$$\int c_{\boldsymbol{p},\mathcal{L}}(u) C_{\boldsymbol{p},\mathcal{L}}(u) \, du = \sum_{\ell \in \mathcal{L}} \sum_{k \in \mathcal{L}} \frac{p_{\ell} p_k}{\lambda(\ell) \lambda(k)} \int_{\ell} \lambda([0, \boldsymbol{u}] \cap k) \, du$$
$$= \sum_{\ell \in \mathcal{L}} \sum_{k \in \mathcal{L}} \frac{p_{\ell} p_k}{\lambda(\ell) \lambda(k)} \prod_{i=1}^d \int_{\ell_i} \lambda([0, u_i] \cap k_i) \, du_i$$

where ℓ_i denotes the projection of ℓ onto the dimension *i*. Remark that:

$$\lambda([0, u_i] \cap [c_i, d_i]) = \begin{cases} 0, & u_i \le c_i \\ u_i - c_i, & c_i < u_i < d_i \\ d_i - c_i, & d_i \le u_i \end{cases}$$

and hence (dropping the index i on u, a, b, c, d for clarity):

$$\begin{split} \int_{\ell_i} \lambda([0, u] \cap k_i) \, du &= \int_a^b 0 \, \mathbb{1}_{u < c} \, du + \int_a^b (u - c) \, \mathbb{1}_{c < u < d} \, du + \int_a^b (d - c) \, \mathbb{1}_{d < u} \, du \\ &= \int_{a \wedge c}^{b \wedge d} (u - c) \, \mathbb{1}_{c < u < d} \, du + \int_{a \wedge d}^b (d - c) \, \mathbb{1}_{d < u} \, du \\ &= \left(\frac{(b \wedge d)^2}{2} - (b \wedge d)c \right) - \left(\frac{(a \wedge c)^2}{2} - (a \wedge c)c \right) \\ &+ (b(d - c)) - ((a \wedge d)(d - c)) \, . \end{split}$$

The given expression for τ can now be retrieved easily. For ρ , one only needs to derive the integral expression:

$$\begin{split} \int C_{\boldsymbol{p},\mathcal{L}}(u) du &= \sum_{\ell \in \mathcal{L}} \frac{p_{\ell}}{\lambda(\ell)} \int \lambda([0,\boldsymbol{u}] \cap \ell) du \\ &= \sum_{\ell \in \mathcal{L}} \frac{p_{\ell}}{\lambda(\ell)} \prod_{i=1}^{d} \int_{0}^{a_{i}} 0 du_{i} + \int_{a_{i}}^{b_{i}} (u_{i} - a_{i}) du_{i} + \int_{b_{i}}^{1} (b_{i} - a_{i}) du_{i} \\ &= \sum_{\ell \in \mathcal{L}} \frac{p_{\ell}}{\lambda(\ell)} \prod_{i=1}^{d} 0 + \frac{b_{i}^{2} - a_{i}^{2}}{2} - (b_{i} - a_{i})a_{i} + (1 - b_{i})(b_{i} - a_{i}) \\ &= \sum_{\ell \in \mathcal{L}} \frac{p_{\ell}}{\lambda(\ell)} \prod_{i=1}^{d} \frac{1}{2} (b_{i} - a_{i})(2 - b_{i} - a_{i}) \end{split}$$

which concludes the argument since $\lambda(\ell) = \prod_{i=1}^{d} (b_i - a_i).$

Matrices of bivariate dependence measures can be obtained by projection of the partition on couples of dimensions and using the same formula on the projected models.

The above proofs showed that the closed form expression for piecewise linear copulas facilitates some computations. This property will be exploited later, when introducing penalisation techniques. Furthermore, these closed form expressions will be used to assess the performance of the fitting procedure that will be described in the next section. Note that the diagonal section of the copula is also easily computable.

3 Estimation

Suppose that we have a dataset $(u_{i,j})_{n \times d}$ of (pseudo-)observations from an unknown copula C. We seek parameters $(\boldsymbol{p}, \mathcal{L})$ of $c_{\boldsymbol{p}, \mathcal{L}}^{(n)}$, an approximation of c in the piecewise linear copula class, based on these n observations. To find the optimal parameters $(\boldsymbol{p}^*, \mathcal{L}^*)$, we will adopt a two stage mechanism, considering first that the partition \mathcal{L} is known.

3.1 Optimal weights $p_{\mathcal{L}}^*$ knowing the partition \mathcal{L}

Suppose that a partition \mathcal{L} is already constructed, and that we want to contruct weights p to complete the approximation. As was done by [42] (see also [1, 3]), we will use an Integrated Square Error (ISE) loss to build the weights. Given a copula density c, the

ISE of an estimator \hat{c} is the squared L_2 distance to c:

$$I(\hat{c}) = \|\hat{c} - c\|_2^2 = \int (\hat{c}(\boldsymbol{u}) - c(\boldsymbol{u}))^2 d\boldsymbol{u}.$$

We want to approximate the true copula density c by a copula in the piecewise linear copula class, so we are looking for the solution of:

$$\underset{\boldsymbol{p},\mathcal{L}}{\arg\min} \ I(c_{\boldsymbol{p},\mathcal{L}}^{(n)}) = \underset{\boldsymbol{p},\mathcal{L}}{\arg\min} \ \|c_{\boldsymbol{p},\mathcal{L}}^{(n)}\|_{2}^{2} - 2\langle c_{\boldsymbol{p},\mathcal{L}}^{(n)}, c \rangle$$
(3.1)

since $||c||_2^2$ is irrelevant to the minimisation.

Remark 3.1 (Existence of the density). Remark that $\langle c_{\boldsymbol{p},\mathcal{L}}^{(n)}, c \rangle = \mathbb{E}\left(c_{\boldsymbol{p},\mathcal{L}}^{(n)}(U)\right)$, so that, with a slight abuse of notation, we write $\langle c_{\boldsymbol{p},\mathcal{L}}^{(n)}, c \rangle$ even if C does not admit a density.

Since c is unknown, using empirical observations $(u_{i,j})$ from the copula, $\mathbb{E}\left(c_{p,\mathcal{L}}^{(n)}(U)\right)$ can be approximated by $n^{-1}\sum_{i=1}^{n} c_{p,\mathcal{L}}^{(n)}(u_i)$. We then define the empirical loss.

Definition 3.2 (Empirical Integrated Square Error). Given observations from a copula $(u_{i,j})$, define the Empirical Integrated Square Error (EISE) of an estimator \hat{c} of the copula density as:

$$\hat{I}(\hat{c}) = \|\hat{c}\|_2^2 - \frac{2}{n} \sum_{i=1}^n \hat{c}(u_i).$$

We are looking to solve the following problem :

$$\underset{p,\mathcal{L}}{\operatorname{arg\,min}} \quad \hat{I}(c_{\boldsymbol{p},\mathcal{L}}). \tag{3.2}$$

We start by funding the weights $p_{\mathcal{L}}^*$ knowing the partition \mathcal{L} .

Lemma 3.3. Let \mathcal{L} be a partition of \mathbb{I} . Then the weights p, solution of (3.2) are given as the unique solution of the quadratic program with objective:

$$\boldsymbol{p}'\boldsymbol{A}_{\mathcal{L}}\boldsymbol{p} - 2\boldsymbol{p}'\boldsymbol{A}_{\mathcal{L}}\mathbf{f}_{\mathcal{L}}$$
(3.3)

The matrix $A_{\mathcal{L}}$ and the vector $\mathbf{f}_{\mathcal{L}}$ are given by:

$$\begin{aligned} \mathbf{A}_{\mathcal{L}} &= \left(\lambda(\ell)^{-1} \mathbb{1}_{\ell=k}\right)_{\ell \in \mathcal{L}, k \in \mathcal{L}} & (size \ |\mathcal{L}| \times |\mathcal{L}|) \\ \mathbf{f}_{\mathcal{L}} &= \left(\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\mathbf{u}_{i} \in \ell}\right)_{\ell \in \mathcal{L}} & (size \ |\mathcal{L}|) \end{aligned}$$

Where $|\mathcal{L}|$ denotes the cardinal of \mathcal{L} . Note that $A_{\mathcal{L}}$ depends only on the partition and that $\mathbf{f}_{\mathcal{L}}$ represents the empirical frequencies in the leaves.

Proof. Introduce first a new scalar product on $\mathbb{R}^{|\mathcal{L}|}$: $\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\mathcal{L}} = \sum_{\ell \in \mathcal{L}} \frac{x_{\ell} y_{\ell}}{\lambda(\ell)}$. We denote by $\|.\|_{\mathcal{L}}^2$ its associated square norm, and by $d_{\mathcal{L}}$ its associated distance. Note that the associated bilinear symetric endomorphism has matrix $\boldsymbol{A}_{\mathcal{L}}$ (defined above), a diagonal and positive definite matrix.

Using the definition of $A_{\mathcal{L}}$, $\mathbf{f}_{\mathcal{L}}$ and $\langle ., . \rangle_{\mathcal{L}}$, the objective function in (3.2) rewrites:

$$\hat{I}(c_{\boldsymbol{p},\mathcal{L}}) = \|\boldsymbol{p}\|_{\mathcal{L}}^2 - 2\langle \boldsymbol{p}, \mathbf{f}_{\mathcal{L}} \rangle_{\mathcal{L}} = \boldsymbol{p}' \boldsymbol{A}_{\mathcal{L}} \boldsymbol{p} - 2\boldsymbol{p}' \boldsymbol{A}_{\mathcal{L}} \mathbf{f}_{\mathcal{L}}.$$
(3.4)

Then, the unconstrained convex optimisation problem (3.2) corresponds to the projection of $\mathbf{f}_{\mathcal{L}}$ onto $[0,1]^{|\mathcal{L}|}$ (convex, closed), with respect to the norm $\|.\|_{\mathcal{L}}^2$. It has therefore a unique solution $\mathbf{f}_{\mathcal{L}}$, since $\mathbf{f}_{\mathcal{L}}$ is already in $[0,1]^{|\mathcal{L}|}$. \Box

If we set the weights to be equal to the empirical frequencies $\mathbf{f}_{\mathcal{L}}$, this result yields, for the optimisation of \mathcal{L} , a loss of the form:

$$- \|\mathbf{f}_{\mathcal{L}}\|_{\mathcal{L}}^{2} = -\sum_{\ell \in \mathcal{L}} \frac{\mathbf{f}_{\ell}^{2}}{\lambda(\ell)}.$$
(3.5)

which is the loss that was directly used by [42]. But since we are here looking for a copula, we need to include the copula constraints in the optimisation problem (3.2). These constraints are usually stated as in Definition 3.4.

Definition 3.4 (Copula constraints). For a function C from \mathbb{I} to \mathbb{R} to be a copula, denoting μ_C its associated measure, there are three conditions:

$\forall \boldsymbol{u} \in \mathbb{I}, \forall i \in \{1,, d\}, C(u_1,, u_{i-1}, 0, u_{i+1},, u_d) = 0$	(Ground constraint)
$\forall u \in \mathbb{I}, \forall i \in \{1,, d\}, C(1,, 1, u_i, 1,, 1) = u_i$	(Marginal uniformity)
$\forall \boldsymbol{a}, \boldsymbol{b} \in \mathbb{I}, \mu_{C}\left([\boldsymbol{a}, \boldsymbol{b}]\right) \geqslant 0$	(d-increasingness)

Note that, if C is a distribution function of some random variable, the first and third conditions are verified. Denote now by $\mathcal{C}_{\mathcal{L}}$ the subset of $[0,1]^{|\mathcal{L}|}$ containing vectors p such that $C_{p,\mathcal{L}}$ satisfies these constraints, for a given \mathcal{L} . We have the following result:

Lemma 3.5. The set $C_{\mathcal{L}}$ is closed, convex, non-empty and writes:

$$\mathcal{C}_{\mathcal{L}} = \{ \boldsymbol{p} \in \mathbb{R}^{|\mathcal{L}|} : \ \boldsymbol{B}_{\mathcal{L}} \boldsymbol{p} = \boldsymbol{g}_{\mathcal{L}} \ and \ \boldsymbol{p} \ge 0 \}$$

where, denoting $M_{\mathcal{L}}$ the set of middle-points of leaves, the matrix $B_{\mathcal{L}}$ and the vector $g_{\mathcal{L}}$ are given by:

$$\begin{split} \boldsymbol{B}_{1} &= (\lambda_{\ell_{i}}(u_{i}))_{(i,\boldsymbol{u})\in\{1,\dots,d\}\times M_{\mathcal{L}},\ \ell\in\mathcal{L}} & (size\ nd\times |\mathcal{L}|) \\ \boldsymbol{B}_{2} &= (1)_{\ell\in\mathcal{L}} & (size\ 1\times |\mathcal{L}|) \\ \boldsymbol{g}_{1} &= (u_{i})_{(i,\boldsymbol{u})\in\{1,\dots,d\}\times M_{\mathcal{L}}} & (size\ nd) \\ \boldsymbol{B}_{\mathcal{L}} &= (\boldsymbol{B}_{1},\boldsymbol{B}_{2}) & (size\ (nd+1)\times |\mathcal{L}|) \\ \boldsymbol{g}_{\mathcal{L}} &= (\boldsymbol{g}_{1},1) & (size\ (nd+1)) \end{split}$$

Proof. The first constraint of Definition 3.4 is trivially satisfied by our model. We show that the second constraint can be evaluated on only one point per leaf. Remember that the piecewise linear copula is uniformly distributed on each leaf. Hence, for all $i \in \{1, ..., d\}$, if on some point $\boldsymbol{u} = (u_1, ..., u_d)$, $\sum_{\ell \in \mathcal{L}} p_\ell \lambda_{\ell_i}(u_i) = u_i$, then defining \boldsymbol{x} such that $\boldsymbol{u} + \boldsymbol{x}$ is in the same leaf as \boldsymbol{u} will give us that $\sum_{\ell \in \mathcal{L}} p_\ell \lambda_{\ell_i}(u_i + x_i) = u_i + x_i$ since only one leaf is active in the sum. Which means that the marginal uniformity constraint may be evaluated on only one point per leaf, and hence is equivalent to:

$$\forall \ell \in \mathcal{L}, \exists \boldsymbol{u} \in \ell, \forall i \in \{1, ..., d\}, \sum_{\ell \in \mathcal{L}} p_{\ell} \lambda_{\ell_i}(u_i) = u_i.$$

Then, if we choose evaluation points as middle-points of leaves to put the constraints in matrix-vector form, we have the expression $B_1p = g_1$ for these constraints.

Futhermore, we need to force the sum of weights p to be equal to 1 (so that the total mass is 1), giving a last line of ones to $B_{\mathcal{L}}$ and a last value of one to $g_{\mathcal{L}}$. The last constraint is equivalent to positivity of weights, which gives the last part of the wanted expression for $\mathcal{C}_{\mathcal{L}}$. The closure and convexity of $\mathcal{C}_{\mathcal{L}}$ are then obvious, and Remark 2.2 ensures that $\mathcal{C}_{\mathcal{L}}$ is non-empty.

Lemmas 3.3 and 3.5 lead to the following property, summarising the previous ideas.

Property 3.6 (Quadratic program). Let \mathcal{L} be a suitable partition. Then the weights minimizing the empirical integrated square error (3.3) under the copula constraints are the unique solution of the following quadratic program:

$$\underset{p}{\operatorname{arg\,min}} \quad p' A_{\mathcal{L}} p - 2p' A_{\mathcal{L}} \mathbf{f}_{\mathcal{L}}$$

s.t. $B_{\mathcal{L}} p = g_{\mathcal{L}} \text{ and } p \ge 0$

where matrices $A_{\mathcal{L}}, B_{\mathcal{L}}$ and vectors $\mathbf{f}_{\mathcal{L}}, \mathbf{g}_{\mathcal{L}}$ have been defined in Lemmas 3.3 and 3.5.

Proof. Only the existence and the unicity remain to be proved. We have shown that the problem was convex with a non-empty constraint space. Hence, it has a unique solution. \Box

Denoting $P_{\mathcal{L},\mathcal{S}}(\boldsymbol{x})$ the orthogonal projection of a vector \boldsymbol{x} onto a set S regarding the distance $d_{\mathcal{L}}$, the quadratic program from Property 3.6 gives the optimal weights knowing the partition as:

$$\boldsymbol{p}_{\mathcal{L}}^* = P_{\mathcal{L},\mathcal{C}_{\mathcal{L}}}(\mathbf{f}_{\mathcal{L}}).$$

The empirical frequencies $\mathbf{f}_{\mathcal{L}}$, which are the unconstraint solution, can then be used as a good starting point for a solver.

We concentrate in the following on the construction of the partition \mathcal{L} .

3.2 Locally optimal splitting point $x_{\ell,D}^*$

Suppose that we have already a suitable partition \mathcal{L} and associated weights $p_{\mathcal{L}}$ such that $C_{p_{\mathcal{L}},\mathcal{L}}$ is a copula. For a given leaf $\ell \in \mathcal{L}$, denote $L = \ell_1, ..., \ell_k$ a partition of ℓ into k new leaves such that \mathcal{L}_2 , defined by:

$$\mathcal{L}_2 = \mathcal{L} \setminus \{\ell\} \cup L$$

is a new suitable partition. Then we have, as in [42], the following property:

Property 3.7 (Independence of surrogate loss). Define the surrogate loss associated to the additional split from $(\mathbf{p}_{\mathcal{L}}^*, \mathcal{L})$ to $(\mathbf{p}_{\mathcal{L}_2}^*, \mathcal{L}_2)$ as the difference of empirical integrated squared errors:

$$\hat{I}(c_{\boldsymbol{p}^{\boldsymbol{*}}_{\mathcal{L}_{2}},\mathcal{L}_{2}}) - \hat{I}(c_{\boldsymbol{p}^{\boldsymbol{*}}_{\mathcal{L}},\mathcal{L}}).$$

Then the surrogate loss depends only on the partition L and data inside it.

Proof. Indexing the objects of Property 3.6 by the partitions they are constructed on, note that the part of losses corresponding to $\mathcal{L} \setminus \{\ell\}$ cancels out.

This locality of the loss allowed [42] to use a recursive partitioning algorithm to fit the model. We then only perform *simple splits*.

Definition 3.8 (Simple split and splitting dimensions). Denote \boldsymbol{x} a given breakpoint in the leaf ℓ and $\boldsymbol{D} \subseteq \{1, ..., d\}$ the set of splitting dimensions. Then the simple split of ℓ on \boldsymbol{x} with dimensions \boldsymbol{D} is defined as the partition $L(\ell, \boldsymbol{x}, \boldsymbol{D})$ given by:

$$L((\boldsymbol{a},\boldsymbol{b}],\boldsymbol{x},\boldsymbol{D}) = \underset{j \in \boldsymbol{D}}{\times} \{(a_j,x_j],(x_j,b_j]\} \underset{j \in \{1,\dots,d\} \setminus \boldsymbol{D}}{\times} \{(a_j,b_j]\}$$

The full partition of \mathbb{I} obtained after the split is denoted $\mathcal{L}_{x,D} = \mathcal{L} \setminus \{\ell\} \cup L(\ell, x, D)$. When $D = \{1, ..., d\}$, we might omit it in the subscripts.

Remark 3.9 (Degrees of freedom). In a simple split on a set of dimension D, the weighting of the new leaves is a quadratic program with $2^{|D|}$ parameters responding to |D| + 1 linear constraints. Hence, there exists a tradeoff between complexity and expressivity of the model in the dimension |D| of the breakpoints. We will exploit this characteristic of the recursive procedure for sparsity purposes later on.

Remark 3.10. Note that the copula constraints will not allow for estimation with only one-dimensional splits ($|\mathbf{D}| = 1$), as in [42], since there would be no degrees of freedom in the weights. This represents a huge problem as multivariate splits often imply bigger computational burden. Furthermore, the constraint themselves are *not* localized, but on the global scale, hence including them forbids a parallel implementation. We will see later that this issue can be avoided by delaying the constraint problem to a later stage of the optimisation process.

Note that, neglecting the constraints, knowing D, we are going to choose the splitting point $x_{\ell,D}^*$ as:

$$\boldsymbol{x}_{\ell,\boldsymbol{D}}^{*} = \operatorname*{arg\,min}_{\boldsymbol{x}\in\ell} - \sum_{k\in L(\ell,\boldsymbol{x},\boldsymbol{D})} \frac{\mathrm{f}_{k}^{2}}{\lambda(k)}$$
(3.6)

In the next subsection, before giving a complete description of the fitting algorithm, we will talk about the localized dimension reduction procedures that are possible with these simple splits, and describe how we construct the splitting dimensions D.

3.3 Optimal splitting dimensions D^*

Suppose that we found x_{ℓ}^* to split a leaf ℓ in all the dimensions $\{1, ..., d\}$. Before effectively splitting the leaf, we will check if, by chance, some dimensions are uniform enough to avoid being splitted further. We will choose the splitting dimensions D based on a statistical test whose hypothesis writes:

Hypothesis 3.11 (Sparsity hypothesis \mathcal{H}_j). Denoting $U \sim C$, define for a given dimension $j \in \{1, ..., d\}$ the sparsity hypothesis as:

$$\mathcal{H}_{i}: (U_{i} \perp U_{-i}) \mid U \in \ell \text{ and } U_{i} \mid U \in \ell \sim \mathcal{U}(\ell_{i})$$

When \mathcal{H}_j is accepted in a leaf ℓ , we will reduce the dimension of the breakpoint x_{ℓ}^* in this leaf and in all child leaves accordingly, by removing j from the set of splitting dimensions D^* .

To check this hypothesis using the integrated square error, as analysed by [5], suppose without loss of generality that ℓ is rescaled to \mathbb{I} , containing *n* observations of the random vector $U \sim F$, for *F* the restriction of *C* to ℓ , rescaled to \mathbb{I} (note that *F* is not a copula). This allows to remove the conditioning in the hypothesis. Then, define the test statistic as follows.

Definition 3.12 (Test statistic). Denote by $f_{\mathbf{f},\mathcal{L}}^{(n)}$ the piecewise constant density that will be estimated on data $U \sim F$, using the surrogate loss in (3.6), solution of the unconstraint quadratic program from Lemma 3.3, and by $e_{j,n}(x) = \mathbb{E}\left(f_{\mathbf{f},\mathcal{L}}^{(n)}(x)|\mathcal{H}_j\right)$ the expectation of this estimate under \mathcal{H}_j . The test statistic is given by:

$$\mathcal{I}_{j} = \|e_{j,n} - f_{\mathbf{f},\mathcal{L}}^{(n)}\|_{2}^{2}$$

where \mathcal{L} , $e_{j,n}$ and $f_{\mathbf{f},\mathcal{L}}^{(n)}$ are stochastic objects, depending on the independent and identically distributed (i.i.d.) random vectors $U_1, ..., U_n$.

Remark 3.13. This test statistic does not test hypothesis \mathcal{H}_j per se, but rather tests \mathcal{H}_j under the hypothesis of piecewise constant density. This is a weaker assertion but it is enough to decide if local dimension reduction is possible or not given the current estimation stage and the data. More classical tests for independence and/or uniformity can be founded in [20, 53, 54, 11, 49, 24].

The statistic \mathcal{I}_j has the nice property that it is constructed as a square distance, and hence is always non-negative and is 0 only under \mathcal{H}_j . On the other hand, it requires that we compute the full patchwork distribution in the two cases (under \mathcal{H}_j or not), which can be costly. Instead, we can only compute *the next split*, which will reduce the computation and simplify the statistic. The drawback is that the test is weakened. The next property gives an empirical form of this statistic, using this simplification.

Property 3.14 (Empirical form of the statistic). On a sample of data $(u_{i,j})_{n \times d}$, we can approximate the statistic \mathcal{I}_j by:

$$\widehat{\mathcal{I}}_{j} = \sum_{k \in \mathcal{L}_{x^{*}, \{1, \dots, d\} \setminus \{j\}}} \left(\frac{\mathbf{f}_{k}^{2}}{\lambda(k)} + \sum_{\substack{\ell \in \mathcal{L}_{x^{*}, \{1, \dots, d\}}\\\ell \subset k}} \left(\frac{\mathbf{f}_{\ell}^{2}}{\lambda(\ell)} - 2\frac{\mathbf{f}_{k}\mathbf{f}_{\ell}}{\lambda(k)} \right) \right)$$
(3.7)

Proof. Remark that the estimator will cut on the same breakpoints on dimensions other than j whether or not we work under \mathcal{H}_j . This gives the definition of the partitions, and hence the expression for $e_{j,n}$ and $f_{\mathbf{f},\mathcal{L}}^{(n)}$, allowing to derive the expression of $\hat{\mathcal{I}}_j$.

The law of the statistic (3.7) under \mathcal{H}_j cannot be computed explicitely. We use a Monte-Carlo simulation to compute the p-value of the test. To that purpose, simulate n uniform random variables to replace $\boldsymbol{u}_{.,j}$, and recompute the statistic (3.7), N times. Indeed, note that under the null, the values of $\boldsymbol{u}_{.,-j}$ can be held fixed.

The full localized dimension reduction procedure is formalised in Algorithm 3.1.

Algorithm 3.1: Localised dimension reduction
Data: $N \in \mathbb{N}$, a leaf ℓ , observations $u_1,, u_n \in \ell$, and a threshold probability α
Result: The splitting dimensions D^*
1 Obtain \boldsymbol{x}_{ℓ}^* and $\mathcal{L}_{\boldsymbol{x}_{\ell}^*,\{1,\ldots,d\}}$ by greedily minimizing the loss in (3.6) on ℓ .
2 foreach $j \in 1,, d$ do
3 Denote by s the statistic $\hat{\mathcal{I}}_j$ given by (3.7).
4 foreach $i \in 1,, N$ do
5 Simulate n uniform random variables on ℓ_j and replace the <i>j</i> th coordinate
of the data by this simulation;
6 Denote s_i the value of the statistic from (3.7) on this new dataset;
7 end
8 Set $p_j = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{s < s_i}$
9 end
10 return $D^* = \{j \in 1,, d : p_j > 1 - \alpha\}$

We will now formalise in the next subsection the complete estimation procedure.

3.4 Full estimation procedure

Suppose that we start from the independence copula, which writes $C_{\{1\},\{0\}}$ in our framework. Then, if the sample of observations belonging to the sole leaf is too far from independence, i.e if \mathcal{H}_j does not hold for all j, we construct the first breakpoint by greedily minimising the loss (3.6) over the splitting point \boldsymbol{x} . Rescaling the new leaves to \mathbb{I} allows to start over and split again, until a proper stopping condition is reached: either there is no points anymore in the leaf or the leaf passes the uniformity tests. A third stopping condition is that the loss is no more reduced by splitting.

To fasten the computation, we decided to ignore the copula constraints while splitting, and enforce them at the end on the constructed partition to correct the empirical weights. Later properties of convergence back up this decision, and this futhermore allows to parallelize the splitting process. Experiments showed that the algorithm that enforces the constraints at each split is much slower (since for the optimisation of the breakpoint, sub-optimisation corresponding to the quadratic program of Property 3.6 must be run for each evaluation) and does not provide much better results.

More formally, Algorithm 3.2 below states the complete estimation procedure.

Algorithm 3.2: CORT estimation

Data: Observed ranks $u_1, ..., u_n \in \mathbb{I}$ **Result:** Parameters p and \mathcal{L} of the estimated piecewise linear copula 1 Initialize the tree by $\mathcal{L} = \{\mathbb{I}\}$ and $p_{\mathcal{L}} = \{1\}$. while there exist leaves $\ell \in \mathcal{L}$ that are still splittable do $\mathbf{2}$ 3 for each $\ell \in \mathcal{L}$ that is splittable do Run Algorithm 3.1 in ℓ to find D^* . 4 if $D^* \neq \emptyset$ then 5 Find x^*_{ℓ,D^*} minimizing the surrogate loss (3.6). 6 Set $\mathcal{L} = \mathcal{L}_{x^*_{\ell, D^*}, D^*}$. 7 \mathbf{end} 8 end 9 10 end 11 Compute $p_{\mathcal{L}}^* = P_{\mathcal{L},\mathcal{C}_L}(\mathbf{f}_{\mathcal{L}})$ from Property 3.6. 12 return $(p_{\mathcal{L}}^*, \mathcal{L})$.

The resulting estimator of the copula density, denoted by $c_{p_{\mathcal{L}}^*,\mathcal{L}}^{(n)}$, is called CORT for Copula Recursive Tree. The current implementation of this algorithm is available on CRAN, as an R package¹. Note that the conditions for a leaf to be splittable can vary: by default, we consider that a leaf becomes non-splittable when it contains less than two observations.

Remark 3.15. Before step 11 of Algorithm 3.2, the builded model is simply the density estimate $f_{\mathbf{f}_{\mathcal{L}},\mathcal{L}}^{(n)}$. This additional outcome of the fitting procedure will be used in the next sections to perform fitting analysis.

Remark 3.16. If we restrict the breakpoint possibility to all points with coordinates in $\left(\frac{i}{m+1}\right)_{i \in \{1,...,m\}}$ where *m* divides the number of observations *n*, this gives us only m^d candidates. This corresponds to a form of checkerboard copula, see [10] for more details. Since the ISE loss we use is tractable enough, the breakpoint can be chosen by directly minimizing the criterion over the continuous space \mathbb{I} if the dimension of the problem is not too big.

After talking about consistency of this estimation procedure, we will turn ourselves in Section 4 to some possibles extensions, notably through bagging principles.

3.5 Consistency

We will show the consistency of the CORT estimator (in the L_2 almost-sure sense). Recall from [42, Theorem 1] the following result about the *unconstraint* estimator.

¹See https://cran.r-project.org/web/packages/CORT/index.html

Property 3.17 (Consistency of $f_{\mathbf{f}_{\mathcal{L}},\mathcal{L}}^{(n)}$). Assuming the maximum diameter of leaves goes to 0 as n goes to ∞ , we have:

$$\mathbb{P}\left(\lim_{n \mapsto +\infty} \|f_{\mathbf{f}_{\mathcal{L}},\mathcal{L}}^{(n)} - c\|_{2}^{2} = 0\right) = 1$$

A detailed proof, based on a generalisation by Vapnik-Chervonenkis [50] of the Glivenko-Cantelli Theorem, can be found in [42]. Denote now by $q_{\mathcal{L}}$ the volumes given by the true copula on the leaves:

$$\forall \ell \in \mathcal{L}, \ q_{\ell} = \int_{\ell} c(\boldsymbol{u}) d\boldsymbol{u}.$$

Then, one can easily check that $q_{\mathcal{L}} \in C_{\mathcal{L}}$, and Property 3.17 leads to the following useful corollary:

Corollary 3.18. $d_{\mathcal{L}}(\mathbf{f}_{\mathcal{L}}, \boldsymbol{q}_{\mathcal{L}})^2 \rightarrow 0, \ a.s.$

Indeed, replacing c by a piecewise constant density with partition \mathcal{L} and weights $q_{\mathcal{L}}$ does not change the value of $\|f_{\mathbf{f}_{\mathcal{L}},\mathcal{L}}^{(n)} - c\|_2^2$ and hence $\|f_{\mathbf{f}_{\mathcal{L}},\mathcal{L}}^{(n)} - c\|_2^2 = d_{\mathcal{L}}(\mathbf{f}_{\mathcal{L}}, \mathbf{q}_{\mathcal{L}})^2$.

Definition 3.19 (Integrated constraint influence). Define the integrated constraint influence as the following squared norm:

$$\|c_{\boldsymbol{p}_{\mathcal{L}}^{*},\mathcal{L}}^{(n)} - f_{\mathbf{f}_{\mathcal{L}},\mathcal{L}}^{(n)}\|_{2}^{2} = d_{\mathcal{L}}(\boldsymbol{p}_{\mathcal{L}}^{*},\mathbf{f}_{\mathcal{L}})^{2}$$
(3.8)

In the simulation studies in Section 5, this quantity will be monitored via burn-in techniques, to see how it behaves as n grows. Property 3.20 below gives the corresponding theoretical result.

Property 3.20 (Asymptotical effect of constraints). As $n \mapsto \infty$, the integrated constraint influence goes to 0.

Proof. Recall from 3.6 that $p_{\mathcal{L}}^*$ is the orthogonal projection of $\mathbf{f}_{\mathcal{L}}$ into $\mathcal{C}_{\mathcal{L}}$. Since $q_{\mathcal{L}} \in \mathcal{C}_{\mathcal{L}}$, we have that $d_{\mathcal{L}}(\mathbf{f}_{\mathcal{L}}, p_{\mathcal{L}}^*)^2 \leq d_{\mathcal{L}}(f_{\mathcal{L}}, q_{\mathcal{L}})^2$, which concludes the argument by Corollary 3.18.

The consistency of the estimator is now easy to obtain.

Property 3.21 (Consistency). For c the density of the true copula, assuming the diameter of the leaves goes to 0 as n goes to ∞ , the estimator $c_{\mathbf{p}_{\mathcal{L}}^*,\mathcal{L}}^{(n)}$ is consistent, i.e.

$$\mathbb{P}\left(\lim_{n \mapsto +\infty} \|c_{\boldsymbol{p}_{\mathcal{L}}^{*},\mathcal{L}}^{(n)} - c\|_{2}^{2} = 0\right) = 1$$

Proof. Remark that $\|c_{p_{\mathcal{L}}^*,\mathcal{L}}^{(n)} - c\|_2^2 = d_{\mathcal{L}}(p_{\mathcal{L}}^*, q_{\mathcal{L}})^2$. Then, $p_{\mathcal{L}}^*$ being the orthogonal projection of $\mathbf{f}_{\mathcal{L}}$ into $\mathcal{C}_{\mathcal{L}}$ and $q_{\mathcal{L}}$ being in $\mathcal{C}_{\mathcal{L}}$, we have $d_{\mathcal{L}}(p_{\mathcal{L}}^*, q_{\mathcal{L}})^2 \leq d_{\mathcal{L}}(\mathbf{f}_{\mathcal{L}}, q_{\mathcal{L}})^2$ and we conclude by Corollary 3.18.

In the next section, we consider bagging methods to increase the performance of the model.

4 Bagging of density estimators

Two estimates \hat{g}_1 and \hat{g}_2 of a function g can be bagged into an estimate $\frac{\hat{g}_1+\hat{g}_2}{2}$, candidate for the estimation of g if the estimates are close to be uncorrelated. This principle gave rise to the bagging algorithm in regression, developed by Breiman in [6]. In density estimation, bagging can also be exploited: if the estimator has a high variance and a small biais, then bagging it might yield a better result, regarding the biais/variance trade-off.

Recall that, while bootstrapping over n observations, the chance that an observation does not appear in the bootstrap sample is given by $\left(1 - \frac{1}{n}\right)^n \rightarrow \frac{1}{e}$. Hence, asymptotically 36.8 percent of the dataset will end up *out-of-bag*. These samples can be used to check for accuracy of the model, and sometimes to set hyper-parameters when some are needed. Following the work of [6] in regression models, [43] formalized the cross-validation and bagging process for density estimation. Note that usually, the *leave-one-out* method is used in kernel density estimation to select hyperparameters (mainly the bandwidth), see e.g [32], but the more involved *out-of-bag* procedure we propose is inspired by [52].

In the following, we denote by \hat{C} the empirical copula of the whole dataset \boldsymbol{u} , a $n \times d$ matrix.

Definition 4.1 (CORT Forest). Define $\boldsymbol{u}^{(1)}, ..., \boldsymbol{u}^{(N)}$ as N bootstrap resamples of the same size n, and $\hat{c}^{(1)}, ..., \hat{c}^{(N)}$ (resp $\hat{C}^{(1)}, ..., \hat{C}^{(N)}$) the densities (resp. d.f.) of the CORT estimators on these resamples fitted by Algorithm 3.2. Define the CORT forest with weights $\boldsymbol{\omega} = (\omega_1, ..., \omega_N)$ as the mixture distribution with density :

$$\hat{c}_{\boldsymbol{\omega}}(\boldsymbol{v}) = \sum_{j=1}^{N} \omega_j \hat{c}^{(j)}(\boldsymbol{v}) \; \forall \boldsymbol{v} \in \mathbb{I}.$$

For each observation u_i in the original training set, we recall the out-of-bag density and distribution function estimates as:

$$\hat{c}^{oob}_{\boldsymbol{\omega}}(\boldsymbol{u}_i) = \frac{\sum_{j=1}^N \omega_j \hat{c}^{(j)}(\boldsymbol{u}_i) \mathbf{1}_{\boldsymbol{u}_i \notin \boldsymbol{u}^{(j)}}}{\sum_{j=1}^N \omega_j \mathbf{1}_{\boldsymbol{u}_i \notin \boldsymbol{u}^{(j)}}}$$

We define \hat{C}_{ω} and \hat{C}_{ω}^{oob} accordingly. Note that \hat{c}_{ω}^{oob} is not a proper density as it may fail to sum to 1 and it is only defined on the observation points. Because trees were fitted independently to each other, this is however, on observation points, a good approximation of the forest density itself. From \hat{c}_{ω}^{oob} , based on [32], [52] defines out-of-bag version of common fitting statistics as follows.

Definition 4.2 (Out-of-bag statistics). Define respectively the out-of-bag empirical integrated square error, the out-of-bag Kullback-Leibler divergence and two out-of-bag Cramer-von-Mises distances associated to the forest as:

$$\begin{split} \hat{J}(\hat{c}_{\boldsymbol{\omega}}) &= \|\hat{c}_{\boldsymbol{\omega}}\|_2^2 - \frac{2}{n} \sum_{i=1}^n \hat{c}_{\boldsymbol{\omega}}^{oob}(\boldsymbol{u}_i) \\ \hat{K}(\hat{c}_{\boldsymbol{\omega}}) &= -\frac{1}{n} \sum_{i=1}^n \ln\left(\hat{c}_{\boldsymbol{\omega}}^{oob}(\boldsymbol{u}_i)\right) \\ \hat{M}(\hat{C}_{\boldsymbol{\omega}}) &= \frac{1}{n} \sum_{i=1}^n \left(\hat{C}_{\boldsymbol{\omega}}^{oob}(\boldsymbol{u}_i) - \hat{C}(\boldsymbol{u}_i)\right)^2 \\ \hat{N}(\hat{C}_{\boldsymbol{\omega}}) &= \frac{1}{n} \sum_{i=1}^n \hat{C}_{\boldsymbol{\omega}}(u_i)^2 - 2\hat{C}_{\boldsymbol{\omega}}^{oob}(\boldsymbol{u}_i)\hat{C}(\boldsymbol{u}_i). \end{split}$$

Note that $\hat{K}(\hat{c}_{\boldsymbol{\omega}})$ is obtained as an empirical version of $\int \ln\left(\frac{c(\boldsymbol{u})}{\hat{c}_{\boldsymbol{\omega}}^{oob}(\boldsymbol{u})}\right) dC(\boldsymbol{u})$. $\hat{M}(\hat{c}_{\boldsymbol{\omega}})$ estimates the Cramer-Von-Mises distance between the out-of-bag d.f. of the forest and the empirical copula. On the other hand, $\hat{N}(\hat{c}_{\boldsymbol{\omega}})$ keeps the true norm of the model, in the same spirit as $\hat{J}(\hat{c}_{\boldsymbol{\omega}})$, see [32, 52] for more details about these cross-validation tools.

We call *Optimal* the forest with the weights minimising $\hat{J}(\hat{c}_{\omega})$. We use an optimisation program to find weights given the resampling and the trees:

$$\boldsymbol{\omega}^* = \underset{\boldsymbol{\omega}}{\operatorname{arg\,min}} \ \hat{J}(\hat{c}_{\boldsymbol{\omega}}).$$

Note that this method makes out-of-bag observations contribute to the final estimation through weights.

The forest estimation and the corresponding analysis are studied in the next section. Note that the constructions of this section are the same if you use another base estimator than the CORT estimator: in the next section, we will use these tools to compare bagging of the CORT estimator with bagging of other copula estimators.

5 Investigation of performance

In this section, we will investigate the performance of the proposed estimation procedure on several simulated datasets². We will compare our results with several other models:

- Deheuvel's empirical copula, hereafter denoted by "Empirical".
- The empirical beta copula[44], hereafter denoted "Beta".
- A Checkerboard copula[10] with m = 10, denoted by "Cb(m=10)".
- Another less-precise Checkerboard copula with m = 5, denoted by "Cb(m=5)".

Recall from [10] that a checkerboard copula with a parameter m is a piecewise linear copula with a partition \mathcal{L} composed of a regular grid of hypercubes with side length m^{-1} . See the reference for details about the empirical beta copula. They are all non-parametric or semi-parametric models, with a straightforward estimation procedure³.

We will compare results of differents models in term of dependence measures, Kendall tau and Spearman rho first. Then, we will look at predictive performance metrics defined in the previous section, \hat{J} , \hat{K} , \hat{M} and \hat{N} , computed via a weighted bagging of each model.

Last but not least, to observe the predictive performance of the CORT forest, we designed a cross-validation procedure: on 20 resamples of each dataset, we compute the Cramer-Von-Mises and ISE errors on test samples, given respectively by:

$$\hat{P}(\hat{D}) = \sum_{i \in T} \left(\hat{D}(u_i) - \hat{C}(u_i) \right)^2$$
$$\hat{Q}(\hat{d}) = \|\hat{d}\|_2^2 - \frac{2}{|T|} \sum_{i \in T} \hat{d}(u_i),$$

where T is the test dataset used to obtain \hat{D} , a given copula estimator with density \hat{d} . Note that \hat{P} is focused on the distribution function and \hat{Q} on the density. We now present results for the first dataset.

 $^{^{2}}$ To ensure reproducibility, we provide all the datasets in the R package *cort*, with the code and parameters needed to resimulate them.

 $^{^{3}}$ The two checkerboard copulas are provided by the R package *CORT*, and the empirical beta copula, as well as the empirical copula, are from the R package *copula*.

Dataset 5.1 (Piecewise linear copula). This dataset is a simple test: we simulate random samples from a density *inside* the piecewise copula class, and test wheter or not the estimator can recover it. For that, we will use a 2-dimensional sample with 500 observations, uniform on \mathbb{I} , and apply the following function:

$$h_1(\boldsymbol{u}) = \left(u_1, \frac{u_2 + \mathbb{1}_{u_1 \leqslant \frac{1}{4} + 2\mathbb{1}_{u_1 \leqslant \frac{1}{2} + \mathbb{1}_{\frac{3}{4} \leqslant u_1}}}{4} \right).$$



Figure 5.1: Plot of Dataset 5.1

This dataset has the particularity of belonging to the piecewise linear copula class. Figure 5.2 (a) shows a simulation from the fitted CORT estimator on Dataset 5.1.



(a) In black, lower left, the input data. In red, upper-right, a simulation from the estimated tree.

(b) On the left, \hat{K} and \hat{J} in function of the number of trees. On the right, the Integrated Constraint Influence and square norm of each tree against the weight of the tree in the forest.

Figure 5.2: (Dataset 5.1) (a) The CORT estimator (b) Statistics of the forest.

We observe on Figure 5.2 (a) that the algorithm splitted the space as requested. The few simulated points *outside* the four main boxes are there because the algorithm did not split *exactly* on $(\frac{1}{4}, \frac{3}{4}), (\frac{1}{2}, \frac{1}{2})$ and $(\frac{3}{4}, \frac{1}{4})$, and the constraints forced him to put some weight on some leaves that do not contain points. Bagging the CORT algorithm on this dataset, we obtain statistics given by Figure 5.2 (b). We observe that the out-of-bag statistics are decreasing in the number of trees fitted, although the weighting of the forest did select less than 10 trees over 500. Altogether, the algorithm sucedded into finding the right breakpoints. A comparaison of the fit in term of dependence measure to other models is available in Table 5.1.

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort	Bagged Cort
Kendall Tau						
$ au_{1,2}$	-0.534	-0.515	-0.465	-0.527	-0.525	-0.393
Spearman Rho						
$\rho_{1,2}$	-0.773	-0.757	-0.697	-0.766	-0.762	-0.604

Table 5.1: Obtained dependence measures of several models on Dataset 5.1

On Table 5.1, we display pairwise dependence measures (Kendall τ and Spearman ρ) of the obtained fits. To read these measures, consider the first column, corresponding to the empirical copula, as the goal for other models. We observe that all models perform correctly regarding dependence measures on this dataset, although the Cherckerboard with m = 5 (which has a pretty rough partition, not including the $\frac{1}{4}$ multiples) has a Spearman ρ a little too high. Furthermore, bagging the cort model gives the worst results.

Performing a standard weighted bagging procedure, we obtain fit statistics $\hat{K}, \hat{J}, \hat{M}$ and \hat{N} , displayed in Table 5.2. The experiment fits every model 500 times on resamples of the dataset and then weights the resulting models to minimise \hat{J} .

Table 5.2: Results of the bagging of each model on Dataset 5.1

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort
$\hat{J}(\hat{c}_{\omega})$	0.002	-3.16	-2.37	-2.98	-4.81
$\hat{K}(\hat{c}_{\omega})$	Inf	-1.06	-0.743	-1.18	-0.837
$\hat{M}(\hat{c}_{\boldsymbol{\omega}})$	8.72 e- 06	4.13e-05	0.000281	1.58e-05	0.000633
$\hat{N}(\hat{c}_{\boldsymbol{\omega}})$	-0.0277	-0.0277	-0.0275	-0.0277	-0.0262

Note that the Kullback-Leibler out-of-bag divergence \hat{K} is infinite for the empirical copula, since is does not assign weights to points it did not see. We observe in baging results that the predictive performance of the checkerboards is quite poor, that the forest based on empirical Beta copulas is a lot better and that the CORT forest generalised even better regarding the density-based measures \hat{J} and \hat{K} . Note that the bagging of empirical beta copula is a very powerfull model.

Figure 5.3 gives a boxplot of \hat{P} Cramer-Von-Mises errors. Remember that for this experiment, we compute each model on 20 resamples of the dataset: we obtain 20 \hat{P} values per model.



Figure 5.3: (Dataset 5.1) Boxplots of resulting errors for 20 resamples for each model

On Figure 5.3, remember that smaller values of \hat{P} (d.f. based) and \hat{Q} (density based) means a better model. We observe that, although the bagging procedure is not worth it, the CORT estimator is very good on this example, both for density and d.f. estimation. Unfortunately, it is not always the case, as shown by the following example on Dataset 5.2.

Dataset 5.2 (Another piecewise linear copula). As for Dataset 5.1, we simulate from a density inside the piecewise linear copula class, by applying the function:

$$h_2(\boldsymbol{u}) = \left(u_1, \frac{u_2}{2} + \frac{1}{2}\mathbb{1}_{u_1 \notin [\frac{1}{3}, \frac{2}{3})}\right)$$

to a 200×2 uniform sample, and taking ranks.



Figure 5.4: Plot of Dataset 5.2

This second dataset is also in the piecewise linear class, but it splits the space in a ternary way, which the recursive splitting procedure of the CORT estimator cannot reproduce. In Figure 5.5 (a), you can observe simulation from the CORT copula and the CORT forest fitted on Dataset 5.2.



(a) In black, lower left, the input data. In red, upper-right, a simulation from the estimated tree.

(b) In black, lower left, the input data. In red, upper-right, a simulation from the estimated forest.

Figure 5.5: (Dataset 5.2) (a) The estimated tree (b) The estimated forest.

Remember that the algorithm splits recursively on only one breakpoint. If the data is splitted in a ternary way, as in Dataset 5.2, it will not succeed. Looking at details from the fitting procedure, we see that the constraints forced the algorithm to return exactly the independence copula (by setting weights of each leaf equal to its volume). Indeed, while splitting, two splits in adjacent leaves are *not* synchronised: since the optimisation routines are independent from each other, it is unlikely that they return the same breakpoint value for a given dimension, meaning that weights will not be transferable between the two zones: in our case, the constraints forced the weights back to independence. We see that the forest tried to correct this behavior, but the result is quite bad. Tables 5.3, 5.4 and Figure 5.6 contains the same results as for the previous dataset.

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort	Bagged Cort
Kendall 7	Fau					
$ au_{1,2}$	0.006	0.005	0.004	0.014	0	-0.010
Spearman Rho						
$ ho_{1,2}$	0.010	0.011	0.009	0.021	0	-0.014

Table 5.3: Obtained dependence measures of several models on Dataset 5.2

The dependence measures are here structurally 0: variations from Table 5.3 are therefore irrelevant. Table 5.4 and Figure 5.6 shows the same results as for the previous model.

Table 5.4: Results of the bagging of each model on Dataset 5.2

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort
$\hat{J}(\hat{c}_{\boldsymbol{\omega}})$	0.00501	-1.48	-1.39	-1.21	-2.55
$\hat{K}(\hat{c}_{\boldsymbol{\omega}})$	Inf	-0.346	-0.271	-0.426	-0.311
$\hat{M}(\hat{c}_{\boldsymbol{\omega}})$	3.03e-05	5.16e-05	0.00016	7.38e-05	0.000907
$\hat{N}(\hat{c}_{\boldsymbol{\omega}})$	-0.134	-0.134	-0.134	-0.134	-0.134



Figure 5.6: (Dataset 5.2) Boxplots of resulting errors for 20 resamples for each model

Note that the out-of-bag ISE did not decrease during the fit of the forest, so that more complexity was added without any gain. We also observe that many trees in the forest have zero weights, they do not fit the data enough. Finally, Table 5.4 shows that the predictive performance of the CORT algorithm is quite bad, and the boxplot of \hat{P} error confirms this analysis: in this case, the empirical beta copula performs a lot better.

We now turn ourselves to the third dataset.

Dataset 5.3 (Modified Clayton). This dataset is a simulation of 200 points from a 3-dimensional Clayton copula [26] with $\theta = 7$ (hence highly dependent), for the first, third and fourth marginals. The second marginal is added as independent uniform draws. Lastly, the third marginal is flipped, inducing a negative dependence structure.



Figure 5.7: Plot of Dataset 5.3

Dataset 5.3 is based on the Clayton copula, a commonly used dependence structure

in many fields of applications. The estimator developped in Algorithm 3.2 has several options: the most important one is the inclusion, or not, of the localized dimension reduction through Algorithm 3.1. Since here we have a completely independent dimension, this option is worth it: it reduces by a factor of 2 the number of leaves, and hence the complexity of the model, by setting the same second edge [0, 1] to each leaf. Figure 5.8 gives a representation of the tree and the statistics of the forest.



(a) In black, lower left, the input data. In red, upper-right, a simulation from the estimated tree.

(b) On the left, \hat{K} and \hat{J} in function of the number of trees. On the right, the Integrated Constraint Influence and square norm of each tree against the weight of the tree in the forest.

Figure 5.8: (Dataset 5.3) (a) Representation from the tree (b) Forest Statistics.

On the left of Figure 5.8 (b), the convex, decreasing shape of the Kullback-Leibler divergence with respect to the number of trees shows that the generalisation error of the forest decreases with the number of trees. The decreasing trend of the constraint influence and the square norm of trees with respect to the assigned weights by the forest, on the right of Figure 5.8 (b) shows how the weighting procedure selected trees. Table 5.5 shows dependence measures obtained from the different models.

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort	Bagged Cort
Kendall T	laus					
$ au_{1,2}$	-0.003	0.010	0.006	-0.014	0.000	-0.020
$ au_{1,3}$	-0.796	-0.750	-0.673	-0.799	-0.780	-0.493
$ au_{1,4}$	0.779	0.732	0.659	0.779	0.707	0.474
$ au_{2,3}$	0.015	0.010	0.011	0.029	0.000	0.031
$ au_{2,4}$	-0.024	-0.009	-0.010	-0.038	0.000	-0.045
$ au_{3,4}$	-0.775	-0.728	-0.654	-0.773	-0.695	-0.566
Spearman	n Rhos					
$ ho_{1,2}$	-0.005	0.013	0.010	-0.023	0.000	-0.029
$ ho_{1,3}$	-0.934	-0.915	-0.868	-0.936	-0.926	-0.648
$ ho_{1,4}$	0.924	0.903	0.857	0.925	0.872	0.626
$ ho_{2,3}$	0.023	0.014	0.016	0.045	0.000	0.047
$ ho_{2,4}$	-0.035	-0.016	-0.016	-0.057	0.000	-0.068
$\rho_{3,4}$	-0.922	-0.901	-0.853	-0.922	-0.862	-0.735

Table 5.5: Obtained dependence measures of several models on Dataset 5.3

Table 5.6: Results of the bagging of each model on Dataset 5.3

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort
$\hat{J}(\hat{c}_{\omega})$	0.00501	-9.27	-7.69	120	-54.6
$\hat{K}(\hat{c}_{\omega})$	Inf	Inf	Inf	-0.582	-1.97
$\hat{M}(\hat{c}_{\boldsymbol{\omega}})$	2.84e-05	$\mathbf{2.51e}\text{-}05$	5.25e-05	3.38e-05	9.41e-05
$\hat{N}(\hat{c}_{\boldsymbol{\omega}})$	-0.000666	-0.000669	-0.000641	-0.000657	-0.000639

The comparaison of Table 5.5 shows that, even if the CORT algorithm performs correctly, the forest tends to be biaised in the dependence measures, toward more independence. On the other hand, the predictive performance of the model from Table 5.6 is really high on the density-based estimates $(\hat{J} \text{ and } \hat{K})$, and is less good on the distribution function based versions $(\hat{M} \text{ and } \hat{N})$. The boxplot of \hat{P} and \hat{Q} in Figure 5.9 confirms this analysis: recall that \hat{P} is a distribution-based statistic, while \hat{Q} is density-based.



Figure 5.9: (Dataset 5.3) Boxplots of resulting errors for 20 resamples for each model

To understand more precisely what happened with the dependence measures, we ran a burn-in experiment on Dataset 5.3: we fit trees on subsamples of increasing size. We can then observe the burn in Kendall taus and Spearmann rhos, represented on Figure 5.10



Figure 5.10: (Dataset 5.3) Burn in of dependence measures: on the top row, Kendall's tau; on the bottom row, Spearman's rho; on the left column, empirical values from subsamples of increasing sizes; on the right column, values obtained by the fitted CORT esitmators on the same subsamples. The size of the subsamples is in abscissa. Each line type correspond to a couple of variables.

We see that the fitted values, on the right of Figure 5.10, are convergent but biaised compared to the empirical observed values of the dependence measures directly computed on resamples of the dataset, on the left. We also observe the high variance of the estimator, which is one of the good reason to use a bagging procedure.

The last dataset was produced based on a function h_3 defined by :

$$h_3(\boldsymbol{u}) = \left(u_1, \sin(2\pi u_1) - \frac{u_2}{\pi}, \left(1 + \frac{u_3}{\pi^2}\right) \left(\frac{u_3}{2}\mathbb{1}_{\frac{1}{4} \ge u_1} - \sin(\pi^{x_1})\mathbb{1}_{\frac{1}{4} < u_1}\right)\right).$$

Dataset 5.4 (Simulated functional). We choosed to produce a voluntarily hard to estimate dependence structure, by applying the above function h_3 to uniformly drawn 3-dimensional random vectors. The dataset is the ranks of $(h_3(\boldsymbol{u}_i)))_{i\in 1,...,500}$.



Figure 5.11: Plot of Dataset 5.4

Figure 5.12 shows the CORT estimator and the bagging statistics on this dataset.



(a) In black, lower left, the input data. In red, upper-right, a simulation from the estimated tree.



(b) On the left, \vec{K} and \vec{J} in function of the number of trees. On the right, the Integrated Constraint Influence and square norm of each tree against the weight of the tree in the forest.

Figure 5.12: (Dataset 5.3) (a) Representation from the tree (b) Forest Statistics.

Although the estimation on the second and third marginals is not very good, the statistics of the forests are good, showing that the etimator get better and better while adding trees. Indeed, on Figure 5.12 (b), left, we observe decreasing out-of-bag errors, but we also observe on Figure 5.12 (b), right, a very skewed and fat-tailed density for the constraint influence, meaning that certain trees did not produce very good partitions.

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort	Bagged Cort
Kendall '	Taus					
$ au_{1,2}$	-0.495	-0.491	-0.471	-0.500	-0.458	-0.451
$ au_{1,3}$	0.089	0.042	-0.002	0.084	0.171	0.048
$ au_{2,3}$	0.005	0.015	0.004	0.007	-0.109	0.013
Spearma	n Rhos					
$ ho_{1,2}$	-0.743	-0.737	-0.715	-0.747	-0.713	-0.674
$ ho_{1,3}$	-0.156	-0.154	-0.146	-0.159	0.246	0.060
$ ho_{2,3}$	-0.019	0.012	-0.001	-0.010	-0.177	0.020

Table 5.7: Obtained dependence measures of several models on Dataset 5.4

Table 5.7 shows that the bivariate projections were not all treated as well as others by the CORT algorithm: the values of $\tau_{1,2}$ and $\rho_{1,2}$ are suprisingly quite good compared to $\tau_{1,3}, \tau_{2,3}, \rho_{1,3}, \rho_{2,3}$, for the CORT stimator. Hopefully, the bagging corrects this biais quite correctly.

Table 5.8: Results of the bagging of each model on Dataset 5.4

	Empirical	Cb(m=10)	Cb(m=5)	Beta	Cort
$\hat{J}(\hat{c}_{\omega})$	0.002	-15.7	-7.22	-23	-23.3
$\hat{K}(\hat{c}_{\omega})$	Inf	-2.52	-1.79	-3.12	-1.72
$\hat{M}(\hat{c}_{\boldsymbol{\omega}})$	1.69e-05	0.000172	0.000736	4.76e-05	0.00233
$\hat{N}(\hat{c}_{\boldsymbol{\omega}})$	-0.0201	-0.0199	-0.0194	-0.0201	-0.0177

Finally, the predictive performance from Table 5.8 is still two-sided : the density-based results are quite good, but the distribution-function based one are not very good. The boxplot of Figure 5.13 confirms this analysis.



Figure 5.13: (Dataset 5.4) Boxplots of resulting errors for 20 resamples for each model

6 Conclusion

From a simple density estimation procedure designed by [42], we constructed a piecewise constant, tree-shaped, recursive copula density estimator. We computed several closed-form expressions for this estimator, and we gave an asymptotical result.

If, intuitively, constraining the space of potential weighting solutions will help the convergence of optimisation routines, the copula constraints forced us to split the space in more than one dimension, making the resulting estimation procedure complex with the increasing dimension. The localised dimension reduction procedure helps reducing the complexity.

The CORT estimator has good generalisation performance and is straightforward to use since it does not have restrictive hypothesis on the true dependence structure. Although the implementation we provide is very fast, a balance between computation time and precision is available in the number of trees you use in the bagging procedure. However, more work needs to be done to correct defaults of the splitting procedure, which is not able to understand certain kinds of dependence structures.

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