Vine copula based modeling

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Abstract

With the availability of massive multivariate data comes a need to
develop flexible multivariate distribution classes. The copula approach
allows to construct marginal models for each variable separately and
join them with a dependence structure characterized by a copula. The
class of multivariate copulas was limited for a long time to elliptical
(including the Gaussian and t-copula) and Archimedean families (such
as Clayton and Gumbel copulas). Both classes are rather restrictive
with regard to symmetry and tail dependence properties. The class
of vine copulas overcomes these limitations by building a multivariate
model using only bivariate building blocks. This gives rise to highly
flexible models that still allow for computationally tractable estimation
and model selection procedures. These features made vine copula
models quite popular among applied researchers in numerous areas of
science. This paper reviews the basic ideas underlying these models,
presents estimation and model selection approaches, and discusses
current developments and future directions.

Contents

1. Introduction to copulas

For the analysis of large multivariate data sets, flexible multivariate statistical models are required that can adequately describe also the multivariate tail behavior. Standard distributions, such as the multivariate normal or Student t distribution, are too inflexible in their marginal and joint behavior. They often require that all univariate and multivariate marginal distributions are of the same type and only allow for highly symmetric dependence structures. These characteristics are rarely satisfied in applications. The copula approach allows to separate the univariate margins from the dependence structure. In particular a d-dimensional *copula C* is a multivariate distribution function on the d-dimensional hypercube $[0,1]^d$ with uniformly distributed marginals. For an absolutely continuous copula, the corresponding *copula density* can be obtained by partial differentiation, i.e. $c(u_1, ..., u_d) := \frac{\partial^d}{\partial u_1...\partial u_d} C(u_1, ..., u_d)$ for all $\boldsymbol{u}$ in $[0,1]^d$. Sklar (1959) proved the following fundamental representation theorem.

Theorem 1 (Sklar's Theorem). *Let $\boldsymbol{X}$ be a d-dimensional continuous random vector with joint distribution function F, marginal distribution functions F_j, and marginal density functions f_j for $j = 1, \ldots, d$. Then the joint distribution function can be expressed as*

$$F(x_1, ..., x_d) = C(F_1(x_1), ..., F_d(x_d)) \qquad\qquad 1.$$

with associated density $f(x_1, ..., x_d) = c(F_1(x_1), ..., F_d(x_d))f_1(x_1) \cdots f_d(x_d)$ for some d-dimensional copula C with copula density c.

For absolutely continuous distributions the copula C is unique. Equation 1 also holds for discrete random variables, however the probability mass function is different than the density above. For simplicity, we will work in the continuous case in what follows. Using this theorem, flexible multivariate distributions can be constructed from d-dimensional copulas. By inversion of Equation 1 we can use any d-dimensional distribution function to obtain the corresponding copula. Examples are the Gaussian and the Student t copula. Using these copula families together with arbitrary margins results in multivariate distributions which are much more flexible than the multivariate distribution classes used in the inversion. Archimedean copulas are another class of parametric copulas that are built directly using generator functions. The Gumbel, Clayton and Frank copula families are prime examples.

Two-parameter copulas such as the BB class allow for different, non-zero upper and lower tail behavior and are discussed in Section 5.2 of Joe (1997). A nice elementary introduction to copulas is given in Genest & Favre (2007) and more theoretical treatments are the books by Nelsen (2007) and Joe (1997).

From Theorem 1 for $d = 2$, we can immediately derive expressions for the conditional density and distribution functions, which are needed later. In particular the conditional density $f_{1|2}$ and distribution function $F_{1|2}$ can be expressed as

$$f_{1|2}(x_1|x_2) = c_{12}(F_1(x_1), F_2(x_2))f_2(x_2) \qquad\qquad 2.$$

$$F_{1|2}(x_1|x_2) = \frac{\partial}{\partial F_2(x_2)}C_{12}(F_1(x_1), F_2(x_2)) = \frac{\partial}{\partial v}C_{12}(F_1(x_1), v)|_{v=F_2(x_2)}. \qquad 3.$$

Since vine copulas are built out of bivariate copulas we now discuss properties of bivariate copulas. To investigate the dependence properties we consider several dependence measures. Since the Pearson correlation $\rho(X_1, X_2) = \text{Cor}(X_1, X_2)$ is not invariant with respect to monotone transformations of the margins, it is more useful to consider invariant dependence measures such as Kendall's τ and Spearman's ρ. In particular, Spearman's rank correlation is defined as the Pearson correlation of the random variables $F_1(X_1)$ and $F_2(X_2)$, i.e., $\rho_s(X_1, X_2) = \text{Cor}(F_1(X_1), F_2(X_2))$. Another popular measure invariant to marginal transformations is Kendall's τ, defined as

$$\tau(X_1, X_2) = P((X_{11} - X_{21})(X_{12} - X_{22}) > 0) - P((X_{11} - X_{21})(X_{12} - X_{22}) < 0),$$

where (X_{11}, X_{12}) and (X_{21}, X_{22}) are independent and identically distributed copies of (X_1, X_2). Since $\tau(X_1, X_2)$ and $\rho_s(X_1, X_2)$ are invariant with regard to margins they depend only on the underlying copula. More specifically it holds

$$\tau(X_1, X_2) = 4 \int_0^1 \int_0^1 C(u_1, u_2)dC(u_1, u_2) - 1$$

$$\rho_s(X_1, X_2) = 12 \int_0^1 \int_0^1 u_1 u_2 dC(u_1, u_2) - 3.$$

In contrast to these central measures of dependence, tail dependence coefficients are used to characterize dependence among extreme events. We consider the probability of the joint occurrence of extremely small or large values and define the upper and lower tail dependence coefficient as

$$\lambda^{upper} = \lim_{t\to1^-} P(X_2 > F_2^{-1}(t)|X_1 > F_1^{-1}(t)) = \lim_{t\to1^-} \frac{1 - 2t + C(t,t)}{1-t}$$

$$\lambda^{lower} = \lim_{t\to0^+} P(X_2 \le F_2^{-1}(t)|X_1 \le F_1^{-1}(t)) = \lim_{t\to0^+} \frac{C(t,t)}{t}.$$

The Gaussian and Frank copulas do not exhibit tail dependence, i.e., $\lambda^{upper} = \lambda^{lower} = 0$. The Student t copula has symmetric tail dependence, i.e., $\lambda^{upper} = \lambda^{lower}$. The Clayton and Gumbel copula have only lower or upper tail dependence, respectively. To allow for a visual comparison between different bivariate copula families, marginally normalized contour plots are helpful. For this we consider 3 different scales: the original scale (X_1, X_2), the copula scale $(U_1, U_2) = (F_1(X_1), F_2(X_2))$ and the marginally normalized scale (z-scale) $(Z_1, Z_2) = (\Phi^{-1}(U_1), \Phi^{-1}(U_2))$. Here Φ denotes the standard normal distribution function. Comparison of contours on the copula scale for different families is difficult, since copula
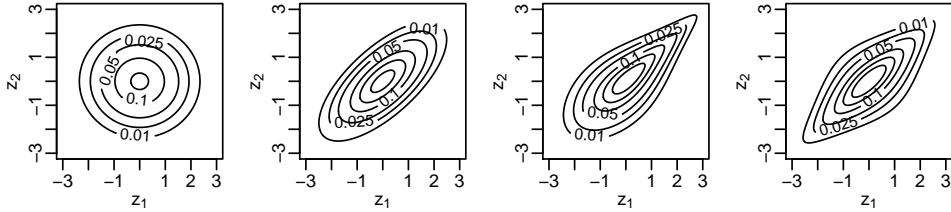
Examples of normalized contour plots. From left to right: Independence, Gaussian, Gumbel, Student copulas.

densities are in general unbounded at the corners of $[0, 1]^2$. This is not the case if one works on the z-scale. Here (Z_1, Z_2) has $N(0, 1)$ margins and thus any non-elliptical contour shape indicates a deviation from a Gaussian dependence. An example is given in Figure 1. The perfect circle in the leftmost panel corresponds to independence; the elliptical shape in the next panel to a Gaussian copula. Deviations from Gaussian dependence can be seen in the two right panels. The first, a Gumbel copula, shows a spike in the upper-right tail which is an indication of upper tail dependence. The rightmost panel is a t-copula, which has tail-dependence in both the upper and lower tails. To allow for further flexibility of bivariate parametric copulas their survival and reflection versions can be considered. For example, the survival version of a bivariate copula density c is given by $\bar{c}(u_1, u_2) = c(1 - u_1, 1 - u_2)$. These can be visualized through rotations of the normalized contours (Czado 2019, Section 3.6).

We now turn to estimation in the parametric setting. In a copula based model specified by Equation 1 we have to estimate both the marginal and copula parameters. Joint maximum likelihood estimation can be used, if the number of parameters is not too large. It is more common to use a two step approach, however. In a first step, the marginal parameters are estimated based on the *iid* observations $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{id})$ for $i = 1, \ldots, n$. This can be done separately for each of the d margins. In a second step, *pseudo copula data* is formed by setting

$$\boldsymbol{u}_i = (u_{i1}, \ldots, u_{id}) = (\hat{F}_1(x_{i1}), \ldots, \hat{F}_d(x_{id})), \qquad i = 1, ..., n. \qquad 4.$$

from which the copula parameters are estimated. If parametric marginal models are used, we speak of an inference for margins (IFM) approach (Joe 2005). If the empirical distribution function is used for the margins, we have a semiparametric approach (Genest et al. 1995). Genest et al. (2011) have further proposed to estimate copula parameters by the inversion of empirical Kendall's τ estimates, when there is a one-to-one relationship between τ and the copula parameter. However this approach is less efficient.

To help the reader to follow all reviewed concepts, we use the Abalone data set taken from the UCI database (`http://archive.ics.uci.edu/ml/datasets/Abalone`). Abalones are marine snails whose shells have a spiral structure. The data set contains measurements on diameter, height, several types of weight (whole, shucked, viscera and shell), and the number of rings. In our illustrations we restrict to female abalone shells. The upper right triangle of Figure 2 shows scatter plots of psuedo-copula data along with their empirical Kendall's τ for the weight variables shuck, vis and shell. The empirical Kendall's τ between shuck and vis, shuck and shell, and vis and shuck is .73, .65 and .69, respectively. Using
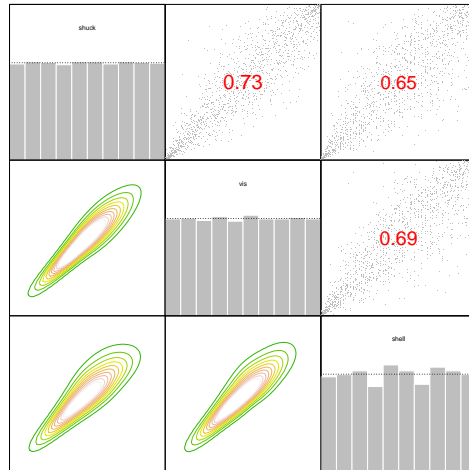
Figure 2

Dependence exploration for the weight variables shuck, vis and shell (diagonal: Histograms of the pseudo copula data using empirical margins; upper triangle: pairwise scatter plots of the pseudo copula data; lower triangle: pairwise normalized contour plots on the z-scale).

Table 1   Parametric copula estimation for the variable pair shuck and shell.

family	log-likelihood	AIC	BIC
Gaussian	802.79	-1603.58	-1598.40
Student t	825.01	-1646.02	-1635.68
Clayton	894.73	-1787.46	-1782.29
Gumbel	660.07	-1318.14	-1312.96
Survival Clayton	464.26	-926.52	-921.35
Survival Gumbel	914.87	-1827.74	-1822.57

empirical margins shows (diagonal of Figure 2) that the pseudo data (u-scale) is approximate uniform. Normalized pairwise contour plots (z-scale) are shown in the lower triangular panels of Figure 2. The panels indicate that dependence is asymmetric, with stronger dependence in the lower left tail. Since the normalized pairwise contours are not elliptical, a Gaussian copula is not appropriate. We start by searching for an appropriate parametric copula model for the variable pair shuck and shell. We allow for the Gaussian, Student t, (survival) Clayton and (survival) Gumbel copula. Corresponding log-likelihood, AIC and BIC values based on the pseudo copula data are given in Table 1, which shows that a survival Gumbel model is the best among the studied models.

In the case where copula models do not fit the data, we can also use a nonparametric approach. Transformation kernel estimators were shown to perform best in Nagler et al. (2017) and are implemented in the `kdecopula` and `rvinecopulib` R packages (Nagler 2018, Nagler & Vatter 2020a). Finally we note that copula estimation based on pseudo copula data requires approximately *iid* data. This is usually not the case for multivariate time series data or in the presence of covariates. Here we advise to first remove the time series

or regression structure for each margin by fitting appropriate univariate time series or regression models, respectively. For time series, the resulting standardized residuals can then be used to form the pseudo copula data. In regression models, the fitted conditional response distribution should be used for the transformation to pseudo observations.

2. Pair copula decompositions and constructions in three dimensions

While the catalogue of bivariate parametric copula families is large, this is not the case for $d > 2$. The motivation for vine copula models was to find a way to construct multivariate copulas using only bivariate copulas as building blocks. The appropriate tool to obtain such a construction is conditioning. Joe (1996) gave the first *pair copula construction* in terms of distribution functions, while Bedford & Cooke (2001) and Bedford & Cooke (2002) independently developed constructions in terms of densities. They also provided a framework to identify all possible constructions. We first illustrate this construction for $d = 3$ by starting with the recursive factorization

$$f(x_1, x_2, x_3) = f_{3|12}(x_3|x_1, x_2) f_{2|1}(x_2|x_1) f_1(x_1)$$
5.

and treat each part separately. Here $F_{j|D}$ and $f_{j|D}$ denote the conditional distribution or density function of X_j given $\boldsymbol{X}_D$, respectively. To determine $f_{3|12}(x_3|x_1, x_2)$ we consider the bivariate conditional density $f_{13|2}(x_1, x_3|x_2)$. The copula density $c_{13;2}(\cdot, \cdot; x_2)$ denotes the copula density associated with the conditional distribution of (X_1, X_3) given $X_2 = x_2$. Using Theorem 1 for $f_{13|2}(x_1, x_3|x_2)$ gives

$$f_{13|2}(x_1, x_3|x_2) = c_{13;2}(F_{1|2}(x_1|x_2), F_{3|2}(x_3|x_2); x_2) f_{1|2}(x_1|x_2) f_{3|2}(x_3|x_2).$$
6.

Now $f_{3|12}(x_3|x_1, x_2)$ is the conditional density of X_3 given $X_1 = x_1, X_2 = x_2$ which can be determined using Equation 2 applied to Equation 6, yielding

$$f_{3|12}(x_3|x_1, x_2) = c_{13;2}(F_{1|2}(x_1|x_2), F_{3|2}(x_3|x_2); x_2) f_{3|2}(x_3|x_2).$$
7.

Finally, direct application of Equation 3 gives

$$f_{2|1}(x_2|x_1) = c_{12}(F_1(x_1), F_2(x_2)) f_2(x_2)$$
8.

$$f_{3|2}(x_3|x_2) = c_{23}(F_2(x_2), F_3(x_3)) f_3(x_3).$$
9.

Inserting Equations 7–9 into Equation 5 yields a *pair copula decomposition* of an arbitrary three dimensional density $f(x_1, x_2, x_3)$ as

$$f(x_1, x_2, x_3) = c_{13;2}(F_{1|2}(x_1|x_2), F_{3|2}(x_3|x_2); x_2) \times c_{23}(F_2(x_2), F_3(x_3))$$
$$\times c_{12}(F_1(x_1), F_2(x_2)) f_3(x_3) f_2(x_2) f_1(x_1).$$
10.

We see that the joint density can be expressed in terms of bivariate copula densities, marginal densities, and conditional distribution functions. However, this decomposition is not unique:

$$f(x_1, x_2, x_3) = c_{23;1}(F_{2|1}(x_2|x_1), F_{3|1}(x_3|x_1); x_1) \times c_{13}(F_1(x_1), F_3(x_3))$$
$$\times c_{12}(F_1(x_1), F_2(x_2)) f_3(x_3) f_2(x_2) f_1(x_1)$$
11.

$$f(x_1, x_2, x_3) = c_{12;3}(F_{1|3}(x_1|x_3), F_{2|1}(x_2|x_1); x_3) \times c_{13}(F_1(x_1), F_3(x_3))$$
$$\times c_{23}(F_2(x_2), F_3(x_3)) f_3(x_3) f_2(x_2) f_1(x_1)$$
12.

are two different decompositions using a reordering of the variables in Equation 5.

All decompositions of the density have a conditional copula term of the form $c_{ij;k}(\cdot, \cdot; x_k)$, called *pair copula*. To facilitate estimation we normally neglect the dependence on the specific conditioning value x_k. This is called the simplifying assumption. For a three-dimensional density with copula parameter vector $\boldsymbol{\theta} = (\boldsymbol{\theta}_{12}, \boldsymbol{\theta}_{23}, \boldsymbol{\theta}_{12;3})$, we then get the following simplified pair copula construction:

$$f(x_1, x_2, x_3; \boldsymbol{\theta}) = c_{13;2}(F_{1|2}(x_1|x_2), F_{3|2}(x_3|x_2); \boldsymbol{\theta}_{13;2}) \times c_{23}(F_2(x_2), F_3(x_3); \boldsymbol{\theta}_{23})$$
$$\times \ c_{12}(F_1(x_1), F_2(x_2), \boldsymbol{\theta}_{12}) f_3(x_3) f_2(x_2) f_1(x_1),$$

13.

where $c_{13;2}(\cdot, \cdot; \boldsymbol{\theta}_{13;2})$, $c_{12}(\cdot, \cdot; \boldsymbol{\theta}_{12})$ and $c_{23}(\cdot, \cdot; \boldsymbol{\theta}_{23})$ are arbitrary parametric bivariate copula densities. The dependence on marginal parameters has been suppressed to ease notation. This is no longer a decomposition but a construction, where the dependence on x_2 in $c_{13;2}(F_{1|2}(x_1|x_2), F_{3|2}(x_3|x_2); \boldsymbol{\theta}_{13;2})$ is solely captured by the arguments. If the margins in Equation 13 are uniform, we have a three-dimensional parametric copula density.

For the estimation of the parameter $\boldsymbol{\theta}$ based on an i.i.d. sample $\boldsymbol{x}_k = (x_{k1}, x_{k2}, x_{k3}), k = 1, \ldots, n$, we follow the two-step approach discussed in Section 1. We create the associated pseudo data $\boldsymbol{u}_{k,j}, k = 1, \ldots, n, j = 1, \ldots 3$ as in Equation 4. This allows us to write the joint (pseudo-)likelihood for the trivariate copula density associated with Equation 13 as

$$\ell(\boldsymbol{\theta}; \boldsymbol{u}) = \prod_{k=1}^{n} c_{13;2}(C_{1|2}(u_{k,1}|u_{k,2}; \boldsymbol{\theta}_{12}), C_{3|2}(u_{k,1}|u_{k,2}; \boldsymbol{\theta}_{23}); \boldsymbol{\theta}_{13;2})$$
$$\times \ c_{23}(u_{k,2}, u_{k,3}; \boldsymbol{\theta}_{23}) c_{12}(u_{k,1}, u_{k,2}; \boldsymbol{\theta}_{12}).$$

14.

Maximizing Equation 14 gives the joint maximum likelihood estimator $\widehat{\boldsymbol{\theta}}$. However there is an alternative sequential estimation method, which remains computationally tractable in high dimensions. First, we find parameter estimates $\widehat{\boldsymbol{\theta}}_{12}$ and $\widehat{\boldsymbol{\theta}}_{23}$ by maximizing

$$\prod_{k=1}^{n} c_{12}(u_{k,1}, u_{k,2}; \boldsymbol{\theta}_{12}) \quad \text{and} \quad \prod_{k=1}^{n} c_{23}(u_{k,2}, u_{k,3}; \boldsymbol{\theta}_{23})$$

over $\boldsymbol{\theta}_{12}$ and $\boldsymbol{\theta}_{23}$, respectively. Second we define the pseudo observations

$$u_{k,1|2,\widehat{\boldsymbol{\theta}}_{12}} = C_{1|2}(u_{k,1}|u_{k,2}; \widehat{\boldsymbol{\theta}}_{12}) \quad \text{and} \quad u_{k,3|2,\hat{\boldsymbol{\theta}}_{23}} = C_{3|2}(u_{k,3}|u_{k,2}; \hat{\boldsymbol{\theta}}_{23}),$$

15.

for $k = 1, ..., n$. Under the simplifying assumption these provide an approximate i.i.d sample from the pair copula $C_{13;2}$. Further the marginal distribution associated with the pseudo observations Equation 15 is approximately uniform, since the transformation in Equation 15 is a probability integral transform with estimated parameter values. Therefore we use them to estimate the parameter(s) of the pair copula $c_{13;2}$ by maximizing

$$\prod_{k=1}^{n} c_{13;2}(u_{k,1|2,\widehat{\boldsymbol{\theta}}_{12}}, u_{k,3|2,\widehat{\boldsymbol{\theta}}_{23}}; \boldsymbol{\theta}_{13;2})$$

over $\boldsymbol{\theta}_{13;2}$. This splits the estimation $\boldsymbol{\theta}$ into three simpler problems. The sequential estimate can also be used as a starting value for the joint maximum likelihood estimation. A similar sequential approach can also be followed when estimating pair copulas nonparametrically.

We now estimate all three possible pair copula constructions for the weight variables shuck, vis and shell in the abalone data set. With the aid of normalized contour plots we

Table 2 Sequential parameter estimates, selected copula families, and implied dependence measures for the weight variables shuck (1), vis (2) and shell (3).

$c_{23} - c_{12} - c_{13;2}$	term	family	parameter(s)	Kendall's τ	λ^{upper}	λ^{lower}
	c_{23}	survival Gumbel	3.21	0.69	0.00	0.76
	c_{12}	survival Gumbel	3.65	0.73	0.00	0.79
	$c_{13;2}$	survival Gumbel	1.23	0.19	0.00	0.24
$c_{13} - c_{12} - c_{23;1}$	term	family	parameter(s)	Kendall's τ	λ^{upper}	λ^{lower}
	c_{13}	survival Gumbel	2.93	0.66	0.00	0.73
	c_{12}	survival Gumbel	3.65	0.73	0.00	0.79
	$c_{23;1}$	survival Gumbel	1.43	0.30	0.00	0.38
$c_{23} - c_{13} - c_{12;3}$	term	family	parameter(s)	Kendall's τ	λ^{upper}	λ^{lower}
	c_{23}	survival Gumbel	3.21	0.69	0.00	0.76
	c_{13}	survival Gumbel	2.93	0.66	0.00	0.73
	$c_{12;3}$	Student t	(0.62, 12.06)	0.43	0.11	0.11

Table 3 Fit statistics for three possible pair copula constructions for the weight variables shuck (1), vis (2) and shell (3).

model	log-likelihood	num. par.	AIC	BIC
$c_{23} - c_{12} - c_{13;2}$	2253.91	3	-4501.82	-4486.29
$c_{13} - c_{12} - c_{23;1}$	2247.47	3	-4488.95	-4473.42
$c_{13} - c_{23} - c_{12;3}$	2253.25	4	-4498.50	-4477.80

select appropriate pair copula families for the three possible constructions and the sequential parameter estimation results are contained in Table 2. We see that in all three models dependence is strong in the unconditional copulas, but weaker in the conditional copula. We should note that the latter estimates are only valid if the model assumptions are satisfied. In Table 3, fit statistics of the three models are compared, showing a superior performance of the pair copula construction $c_{23} - c_{12} - c_{13;2}$. This illustrates that it matters which pair copula construction is fitted to the data.

In more than three dimensions, it will be helpful to represent the density factorization as a graph called *vine tree structure*. Figure 3 shows the graphical representations of the three factorization given in Equations 10–12 (from left to right). Panel (a) consists of two levels. In the first level, the nodes labelled 1, 2, and 3 represent the random variables X_1, X_2, and X_3, respectively. They are connected by two edges, $1 - 2$ and $2 - 3$, correspond to the pair copula terms involving c_{12} and c_{23} in Equation 10. The graph in the second level is formed by turning the edges above into nodes and connecting them by an edge. This edge represents the pair copula term involving the conditional density $c_{13;2}(\cdot, \cdot; x_2)$, where the conditioning variable 2 is identified as the common element of the nodes $1, 2$ and $2, 3$. Hence, each edge in the vine graph is associated with a copula density. The factorization of the joint density corresponding to a given vine graph is then simply the product of marginal densities and all copula densities associated with the edges of the vine tree structure. The graphs in panels (b) and (c) correspond to the factorizations in Equations 11–12 in a similar manner.
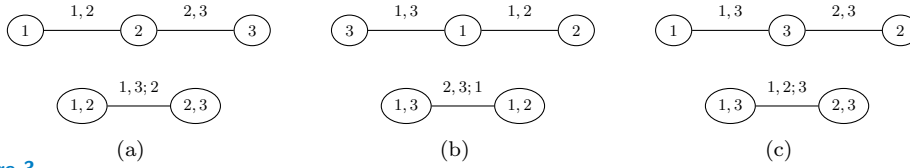
Graphical representation of the three pair copula constructions (a) $c_{23} - c_{12} - c_{13;2}$, (b) $c_{13} - c_{12} - c_{23;1}$, and (c) $c_{13} - c_{23} - c_{12;3}$.

3. Regular vine copulas and distributions

As we have seen in the previous section, there are three pair copula constructions available for $d = 3$. Similar arguments can be used to derive factorizations of the joint density $f(x_1, \ldots, x_d)$ for general d, but additional complications arise. For example, for $d = 4$ we can derive the two factorizations

$$
\begin{aligned}
f(x_1, &x_2, x_3, x_4) \\
&= c_{14;23}(F_{1|23}(x_1|x_2, x_3), F_{4|23}(x_4|x_2, x_3); x_2, x_3) \\
&\quad \times c_{13;2}(F_{1|2}(x_1|x_2), F_{3|2}(x_3|x_2); x_2) \times c_{24;3}(F_{2|3}(x_2|x_3), F_{4|3}(x_4|x_3); x_3) \\
&\quad \times c_{34}(F_3(x_3), F_4(x_4)) \times c_{23}(F_2(x_2), F_3(x_3)) \times c_{12}(F_1(x_1), F_2(x_2)) \\
&\quad \times f_4(x_4) f_3(x_3) f_2(x_2) f_1(x_1).
\end{aligned}
\qquad 16.
$$

and

$$
\begin{aligned}
f(x_1, &x_2, x_3, x_4) \\
&= c_{34;12}(F_{3|12}(x_3|x_1, x_2), F_{4|12}(x_4|x_1, x_2); x_1, x_2) \\
&\quad \times c_{23;1}(F_{2|1}(x_2|x_1), F_{3|1}(x_3|x_1); x_1) \times c_{24;1}(F_{2|1}(x_2|x_1), F_{4|3}(x_4|x_1); x_1) \\
&\quad \times c_{14}(F_1(x_1), F_4(x_4)) \times c_{13}(F_1(x_1), F_3(x_3)) \times c_{12}(F_1(x_1), F_2(x_2)) \\
&\quad \times f_4(x_4) f_3(x_3) f_2(x_2) f_1(x_1).
\end{aligned}
\qquad 17.
$$

The factorizations are represented as regular vine tree structures in Figure 4, where panel (a) correspond to Equation 16 and panel (b) to Equation 17. In panel (a), each graph level consists of a path. In contrast, in panel (b) each graph level consists of a star (where one node is connected to all the others).

By permuting the variable indices, the two types of vine structures generate 12 factorizations each for a total of 24 (compared to only three possible factorizations for $d = 3$). When $d \geq 5$, the sub-graphs are no longer restricted to be paths or stars and the number of possible decompositions increases superexponentially in d (Morales-Nápoles 2011). Furthermore, it becomes increasingly difficult to verify whether a factorization like 16–17 actually represents a valid density. To characterize and organize all valid factorizations, Bedford & Cooke (2001) and Bedford & Cooke (2002) developed a convenient graphical tool called *regular vine* tree structure. A regular vine consists of linked trees, where the edges in one tree become the nodes of the next.

More formally, recall that a tree is a connected acyclic graph $T = (N, E)$ with node set N and edge set E. The set of graphs $\mathcal{V} = (T_1, \ldots, T_{d-1})$ is a regular vine tree sequence on d elements if:

(1) T_1 is a tree with node set $N_1 = \{1, \ldots, d\}$ and edge set E_1.
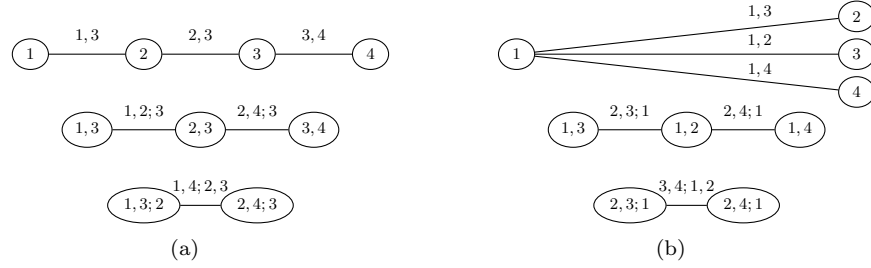
Figure 4

The two types of regular vine structures in four dimensions.

(2) For $j \geq 2$, T_j is a tree with node set $N_j = E_{j-1}$ and edge set E_j.

(3) For $j = 2, \ldots, d-1$ and $\{a, b\} \in E_j$ it must hold that $|a \cap b| = 1$ (proximity condition).

The proximity condition states that an edge between nodes in tree T_j is only possible, if the corresponding edges in T_{j-1} share a common node.

The R-vine tree structure corresponding to Equation 10 has nodes $N_1 = \{1, 2, 3\}$ and edges $E_1 = \{\{1, 2\}, \{2, 3\}\}$ in tree T_1 and nodes $N_2 = \{\{1, 2\}, \{2, 3\}\}$ and edges $E_2 = \{\{1, 2\}, \{2, 3\}\}$ in tree T_2. Since this set notation quickly becomes unwieldy, a simpler notation is needed. For any edge $e \in E_i$ define the complete union

$$A_e = \Big\{ j \in N_1 | \exists\, e_1 \in E_1, \ldots, e_{i-1} \in E_{i-1} \text{ such that } j \in e_1 \in \ldots \in e_{i-1} \in e \Big\}.$$

The conditioning set D_e of an edge $e = \{a, b\}$ is defined as $D_e := A_a \cap A_b$ and the conditioned sets $\mathcal{C}_{e,a}$ and $\mathcal{C}_{e,b}$ are given by

$$\mathcal{C}_{e,a} = A_a \setminus D_e \text{ and } \mathcal{C}_{e,b} = A_b \setminus D_e.$$

Kurowicka & Cooke (2006) showed that $\mathcal{C}_{e,a}$ and $\mathcal{C}_{e,b}$ are singletons, so we often abbreviate the edge $e = (\mathcal{C}_{e,a}, \mathcal{C}_{e,b}; D_e)$ by $e = (a_e, b_e; D_e)$. For example the edge $e = \{a = \{1, 2\}, b = \{2, 3\}\}$ has $A_a = \{1, 2\}$ and $A_b = \{2, 3\}$ and therefore $D_e = \{2\}$. It follows that $\mathcal{C}_{e,a} = \{1\}$ and $\mathcal{C}_{e,b} = \{3\}$ resulting in $e = (1, 3; 2)$.

We have already seen two common special cases in Figure 4 for $d = 4$. In a canonical (C-) vine all trees are stars: in every tree there is a single node, called the *root*, that is connecting all the others. A specific C-vine can be identified by the order of root nodes. Another example of a C-vine is shown in the middle panels of Figure 5, where the root nodes are 1, (1, 4), (6, 4; 1), (6, 2; 4, 1), (5, 2; 6, 4, 1). Since all indices from previous root nodes are contained in the label of later root nodes, we can also specify this order by only referencing the index that enters in the next tree. For example, the root node sequence above can be written as $1, 4, 6, 2, 5, 3$. In a drawable (D-) vine tree structure all trees are paths. More formally, this means that all but two nodes have exactly two neighbors. The two nodes with only one neighbor are called leaves. For a D-vine tree sequence, the proximity condition implies that the specification of tree T_1 determines all other trees. To characterize a D-vine structure, we therefore only need to specify the path in the first tree, called the order of a D-vine. The right panels in Figure 5 show a D-vine with order $3 - 5 - 6 - 2 - 1 - 4$ (or, equivalently, $4 - 1 - 2 - 6 - 5 - 3$). The tree structure of a D-vine can be drawn in a way
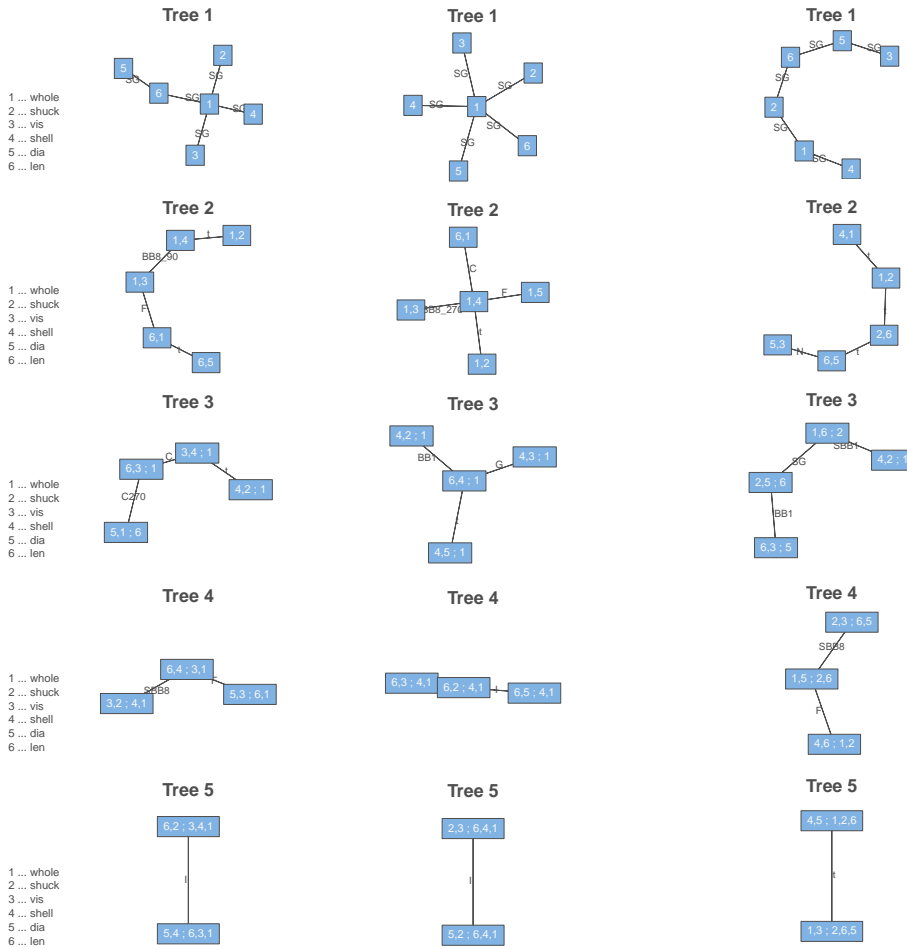
Figure 5

Vine tree structures for variables whole, shuck, vis, shell, dia and len from the female abalone data set (left: R-vine, middle: C-vine, right: D-vine).

that resembles a grape vine, which is why Bedford & Cooke (2001) called the linked tree sequence a vine.

After the building plan is defined, we can construct a regular vine distribution for a d-dimensional random vector $\boldsymbol{X} = (X_1, \ldots, X_d)$. This distribution is specified by the triplet $(\mathcal{F}, \mathcal{V}, \mathcal{B})$ with:

1. **Marginal distributions:** $\mathcal{F} = (F_1, \ldots, F_d)$ is a vector of continuous marginal distribution functions of the random variables $X_1, \ldots, X_d$.
2. **Regular vine tree sequence:** $\mathcal{V}$ is an R-vine tree sequence on d elements.
3. **Bivariate copulas:** The set $\mathcal{B} = \{C_e | e \in E_i; i = 1, \ldots, d-1\}$, where C_e is a bivariate copula with density. Here E_i is the edge set of tree T_i in the R-vine tree sequence $\mathcal{V}$.

4. **Relation between R-vine tree sequence and the set of bivariate copulas:**
   For each $e \in E_i$, $i = 1, \ldots, d-1$, $e = \{a, b\}$, $C_e(\cdot, \cdot)$ is the copula associated with the conditional distribution of $X_{\mathcal{C}_{e,a}}$ and $X_{\mathcal{C}_{e,b}}$ given $\boldsymbol{X}_{D_e}$.

The copula C_e corresponding to edge e is denoted by $C_{\mathcal{C}_{e,a}\mathcal{C}_{e,b};D_e}$ with corresponding density $c_{\mathcal{C}_{e,a}\mathcal{C}_{e,b};D_e}$. This copula is also called a pair copula. We already employed the simplifying assumption above: we assume that $C_e(\cdot, \cdot)$ does not depend on the specific value of $\boldsymbol{X}_{D_e}$. In non-simplified models, we would need a separate set $\mathcal{B}$ of bivariate copulas in (iii) for every possible value of the random vector $\boldsymbol{X}$. This means that for every edge e, the pair-copula C_e would depend on the value of $\boldsymbol{X}_{D_e}$. For simplicity, we only consider the simplified case. For the existence of such distributions Bedford & Cooke (2002) showed the following result.

Theorem 2 (Existence of a regular vine distribution). *Assume that $(\mathcal{F}, \mathcal{V}, \mathcal{B})$ satisfy the properties (1)-(3), then there is a valid d-dimensional distribution F with density*

$$f_{1,\ldots d}(x_1, \ldots x_d) = f_1(x_1) \times \cdots \times f_d(x_d) \tag{18}$$

$$\times \prod_{i=1}^{d-1} \prod_{e \in E_i} c_{\mathcal{C}_{e,a}\mathcal{C}_{e,b};D_e}(F_{\mathcal{C}_{e,a}|D_e}(x_{\mathcal{C}_{e,a}}|\boldsymbol{x}_{D_e}), F_{\mathcal{C}_{e,b}|D_e}(x_{\mathcal{C}_{e,b}}|\boldsymbol{x}_{D_e})),$$

such that for each $e \in E_i$, $i = 1, \ldots, d-1$, with $e = \{a, b\}$ we have for the distribution function of $X_{C_{e,a}}$ and $X_{\mathcal{C}_{e,b}}$ given $\boldsymbol{X}_{D_e}$

$$F_{\mathcal{C}_{e,a}\mathcal{C}_{e,b}|D_e}\left(x_{\mathcal{C}_{e,a}}, x_{\mathcal{C}_{e,b}}|\boldsymbol{x}_{D_e}\right) = C_e\left(F_{\mathcal{C}_{e,a}|D_e}(x_{\mathcal{C}_{e,a}}|\boldsymbol{x}_{D_e}), F_{\mathcal{C}_{e,b}|D_e}(x_{\mathcal{C}_{e,b}}|\boldsymbol{x}_{D_e})\right).$$

Further the one-dimensional margins of F are given by $F_i(x_i)$, $i = 1, \ldots, d$.

If all margins are standard uniform, we call the resulting distribution a regular vine copula. Let D be a set of indices from $\{1, ..., d\}$ not including i and j. The copula associated with the bivariate conditional distribution (X_i, X_j) given that $\boldsymbol{X}_D = \boldsymbol{x}_D$ is denoted by $C_{ij;D}(\cdot, \cdot)$. In contrast the conditional distribution function of (U_i, U_j) given $\boldsymbol{U}_D = \boldsymbol{u}_D$ is expressed as $C_{ij|D}(\cdot, \cdot|\boldsymbol{u}_D)$. This is in general not a copula.

Equation 18 involves conditional distribution functions as arguments of the pair copula densities. These can be determined recursively from conditional distributions associated with the pair copulas in the model. In particular, Joe (1996) showed the following result: Let X be a random variable and $\boldsymbol{Y}$ be a random vector with absolutely continuous joint distribution. Let Y_j a component of $\boldsymbol{Y}$ and denote the sub-vector of $\boldsymbol{Y}$ with Y_j removed by $\boldsymbol{Y}_{-j}$. In this case the conditional distribution of X given $\boldsymbol{Y} = \boldsymbol{y}$ satisfies the following recursion

$$F_{X|\boldsymbol{Y}}(\cdot|\boldsymbol{y}) = \frac{\partial C_{X,Y_j;\boldsymbol{Y}_{-j}}(F_{X|\boldsymbol{Y}_j}(x|\boldsymbol{y}_{-j}), F_{Y_j|\boldsymbol{Y}_j}(y|\boldsymbol{y}_{-j}))}{\partial F_{Y_j|\boldsymbol{Y}_{-j}}(y_j|\boldsymbol{y}_{-j})}, \tag{19}$$

where $C_{X,Y_j;\boldsymbol{Y}_{-j}}(\cdot, \cdot)$ is the copula corresponding to (X, Y_j) given $\boldsymbol{Y}_{-j}$.

For C- and D-vine tree sequences we call the associated regular vine distributions C- and D-vine distributions, respectively. Omitting arguments, their densities are given by

$$f_{1,\ldots,d}(x_1, \ldots, x_d) = \left[\prod_{j=1}^{d-1}\prod_{i=1}^{d-j} c_{j,j+i;1,\cdots,j-1}\right] \times \left[\prod_{k=1}^{d} f_k(x_k)\right],$$

$$f_{1,\ldots,d}(x_1, \ldots, x_d) = \left[\prod_{j=1}^{d-1}\prod_{i=1}^{d-j} c_{i,(i+j);(i+1)\ldots,(i+j-1)}\right] \cdot \left[\prod_{k=1}^{d} f_k(x_k)\right]$$

Using the first column of Figure 5 we can express the associated R-vine distribution as

$$f_{1,\ldots,6}^{rv} = c_{12}c_{13}c_{14}c_{16}c_{56}c_{15;6}c_{36;1}c_{34;1}c_{24;1}c_{23;14}c_{46;13}c_{35;16}$$
$$c_{45;136}c_{26;134}c_{24;1346}f_1f_2f_3f_4f_5f_6.$$

and the C- and D-vine tree structure corresponding to the middle and right column of Figure 5 respectively by

$$f_{1,\ldots,6}^{cv} = c_{12}c_{13}c_{14}c_{15}c_{16}c_{24;1}c_{34;1}c_{45;1}c_{46;1}c_{26;14}c_{36;14}c_{56;14}$$
$$c_{23;146}c_{25;146}c_{35;1246}f_1f_2f_3f_4f_5f_6. \qquad 20.$$
$$f_{1,\ldots,6}^{dv} = c_{41}c_{12}c_{26}c_{56}c_{35}c_{24;1}c_{16;2}c_{25;6}c_{36;5}c_{23;65}c_{15;26}c_{46;12}$$
$$c_{45;126}c_{13;256}c_{34;1256}f_1f_2f_3f_4f_5f_6. \qquad 21.$$

If all or some of the variables are discrete, similar vine-based factorizations of the joint probability density/mass function can be derived. We refer to Panagiotelis et al. (2012), Stöber (2013), and Stöber et al. (2015) for more details.

4. Estimation and selection of vine copula models under the simplifying assumption

As mentioned in the previous section, a stepwise approach to estimation is more tractable in higher dimensions. Here, we first estimate the marginal distribution functions and use them to create pseudo copula data. This copula data is then used to estimate an appropriate vine copula. For this vine copula model we have to solve three problems of increasing complexity:

(1) Given the vine tree sequence and pair copula families, estimate the copula parameters.
(2) Given the vine tree sequence and a catalogue of pair copula families, select the best family and estimate the corresponding parameters for each edge in the vine.
(3) Select the vine tree structure and the pair copula families and estimate the corresponding parameters for each edge.

We can solve Problem (1) using the sequential estimation approach discussed in Section 2. For this we extend the construction of the pseudo data from tree T_2 given in Equation 15 to trees T_3 to T_{d-1} using estimated conditional copula distribution functions. This approach is very fast since it allows to estimate the parameters of each pair copula term separately, starting from tree T_1 until T_{d-1}. The asymptotic properties of such parameter estimators, including standard errors, are studied in Haff et al. (2013), Stöber & Schepsmeier (2013) and Schepsmeier & Stöber (2014). For Problem (2), we can also proceed sequentially and consider each pair copula separately. We fit the parameters for each family in the catalogue and choose the one which minimizes the AIC or BIC criteria.

Problem (3) is the most challenging, since the number of vine tree structures grows as $d! \times 2^{(d-2)(d-3)/2-1}$ (Morales-Nápoles 2011). For example the number of regular vine tree structures for $d = 10$ is approximately 5×10^{14}. Even if one wants to restrict to C- and D-vines, there are almost 2 million structures to be investigated. In Dissmann et al. (2013), a greedy selection algorithm has been developed based on the idea to fit the strongest dependencies first. This is natural since estimation errors are propagated in the sequential estimation approach and we may hope to find sparse models. To measure the

Table 4 Sequential parameter estimates, selected copula families, and implied dependence measures for six variables of the female abalone data set.

tree	edge[a]	family	parameter(s)	Kendall's τ	λ^{upper}	λ^{lower}
1	6,5	survival Gumbel	6.39	0.84	0.00	0.89
1	6,1	survival Gumbel	5.20	0.81	0.00	0.86
1	1,3	survival Gumbel	4.92	0.80	0.00	0.85
1	1,4	survival Gumbel	4.82	0.79	0.00	0.85
1	1,2	survival Gumbel	5.64	0.82	0.00	0.87
2	5,1;6	Student t	(0.39, 6.24)	0.25	0.11	0.11
2	6,3;1	Frank	0.53	0.06	0.00	0.00
2	3,4;1	BB8 90°	(-1.37, -0.97)	-0.15	0.00	0.00
2	4,2;1	Student t	(-0.65, 5.46)	-0.45	0.00	0.00
3	5,3;6,1	Clayton 270°	-0.10	-0.05	0.00	0.00
3	6,4;3,1	Clayton	0.09	0.05	0.00	0.00
3	3,2;4,1	Student t	(-0.41, 4.93)	-0.27	0.01	0.01
4	5,4;6,3,1	Frank	1.47	0.16	0.00	0.00
4	6,2;3,4,1	survival BB8	(1.61, 0.85)	0.15	0.00	0.00
5	5,2;6,3,4,1	Independence	–	0.00	0.00	0.00

[a]variables: whole (1), shuck (2), vis (3), shell (4), dia (5), len (6).

strength of dependence, the empirical Kendall's τ is used. The Dissmann algorithm selects tree T_1 by using a maximal spanning tree algorithm with the absolute value of empirical Kendall's τ between any pair of variables as weights. Once tree T_1 is determined, all pair copula families and parameters are selected and estimated using the approaches outlined in Problems (1) and (2). For tree T_2 all possible edges allowed by the proximity condition are considered. This identifies pairs of variables in the pseudo data as defined in Equation 15. The absolute empirical Kendall's τ for these pairs is used as a weight for selecting the maximal spanning tree for T_2. We can again selected pair copula families and estimate parameters as in Problem (2). We continue that way until all trees, pair copula families, and parameters are selected and estimated. This approach can be adapted for C- and D-vine structures. For a C-vine, we choose the root node to the one maximizing the sum of absolute empirical Kendall's τ as illustrated in Czado et al. (2012). For D-vines, we search for the path that maximizes the sum of absolute empirical Kendall's τ. The above procedures also work with nonparametric pair-copulas, (see, Nagler et al. 2017, for a survey and comparison of available methods) and censored data (Barthel et al. 2018, 2017).

We illustrate the modeling process using the variables whole, shuck, vis, shell, dia and len of the abalone data set. In a preliminary step, nonparametric estimates of the marginal distribution functions are used to create pseudo copula data. Then we apply Dissmann's algorithm to fit R-, C- and D-vine copula models to the pseudo data. The fitted vine tree structures are shown in Figure 5. Table 4 contains the selected pair copula families and estimated parameters for the R-vine copula model. As expected, the fitted dependence strength decreases as we move from T_1 to T_5. As a benchmark, we also fit a Gaussian vine copula model. This is equivalent to a Gaussian copula, but more general than a multivariate Gaussian model, since we allow for non-Gaussian marginal distributions. Table 5 compares the different vine copula models and shows that the R-vine copula model provides the best fit. In particular a Gaussian copula model is clearly insufficient.

Table 5   Fit statistics for several vine copula models for variables whole, shuck, vis, shell, dia and len from the female abalone data set.

copula model	log-likelihood	num. par.	AIC	BIC
R-vine copula	9097.57	17	-18161.14	-18073.17
Gaussian vine copula	8257.21	14	-16486.43	-16413.98
C-vine copula	9097.85	17	-18159.70	-18066.56
D-vine copula	9073.32	22	-18102.65	-17988.80

5. Computational aspects

The flexibility of R-vine copula models comes with computational challenges. First, the number of pair-copulas grows quadratically in the dimension, which necessitates efficient algorithm for inference and simulation. Second, such algorithms must deal with the huge number of possible vine tree structures. Most of these issues have been addressed by the research community in the last years, but the algorithms are difficult to implement for non-experts. Hence, the availability of user-friendly software libraries was key to the popularity of vine copula models. These libraries include: the R packages `VineCopula` (Nagler et al. 2020b), `rvinecopulib` (Nagler & Vatter 2020a); the MATLAB toolboxes `VineCopulaMatlab` (Kurz 2015) and `MATvines` (Coblenz 2020); the C++ library `vinecopulib` (Nagler & Vatter 2020c); and Python libraries `pyvinecopulib` (Vatter et al. 2020) and `pyvines` (Yuan & Hu 2019). This relieves applied researchers from algorithmic difficulties, but they still need to translate the model into a form the software can work with.

Morales-Nápoles (2011) developed a compact representation of the vine tree structure in the form of a triangular matrix. This representation was later used by Dissmann et al. (2013) to encode entire vine copula models. For example, the tree sequence in the left column of Figure 5 can be translated into the array

$$
M = \begin{pmatrix}
6 & 1 & 1 & 1 & 1 & 1 \\
1 & 3 & 4 & 2 & 2 & \\
3 & 4 & 2 & 4 & & \\
4 & 2 & 3 & & & \\
2 & 6 & & & & \\
5 & & & & &
\end{pmatrix}
$$

The label of j-th edge in tree t is given by $(m_{j,d-j+1}, m_{t,j}; m_{t-1,j}, \ldots, m_{1,j})$. Less formally:

- start with the counter-diagonal element of column j (first conditioned variable),
- jump up to the element in row t of column j (second conditioned variable),
- gather all entries further up than row t in column j (conditioning set).

For example, the first column encodes the edges $(5, 2; 4, 3, 1, 6)$, $(5, 4; 3, 1, 6)$, $(5, 3; 1, 6)$, $(5, 1; 6)$, and $(5, 6)$. Dissmann et al. (2013) derived conditions that ensure the array corresponds to a valid R-vine tree sequence.

For parametric vine copula models, the pair-copula families and parameters can be stored in similar arrays. For example, if $\theta_{t,j}$ is the parameter of the j-th edge in the t-th

tree, we can store the model parameters in the array

$$\Theta = \begin{pmatrix} \theta_{1,1} & \theta_{1,2} & \theta_{1,3} & \theta_{1,4} & \theta_{1,5} \\ \theta_{2,1} & \theta_{2,2} & \theta_{2,3} & \theta_{2,4} \\ \theta_{3,1} & \theta_{3,2} & \theta_{3,3} \\ \theta_{4,1} & \theta_{4,2} \\ \theta_{5,1} \end{pmatrix}$$

In software libraries, the arrays are usually written as square matrices, where empty entries in the matrix are filled with zeros by convention. For our example this would mean to use a 6×6 matrix for both M and Θ. The orientation of the matrices above is arbitrary and different software libraries adopt different conventions. The upper-left triangular form above is used by the `vinecopulib` library and its interfaces. In this format, the (t, j)-entry of the matrices is the pivotal element for the j-th edge of tree t, which is intuitive and simplifies indexing in algorithms. In several other libraries, the rows of the matrix are reversed, making it lower-left triangular. The software accompanying the book of Joe (2014) reverses the column order, making it upper-right triangular.

Vine copula models are often used for simulation, which is achieved through the *Rosenblatt transform* (Rosenblatt 1952) and its inverse. The Rosenblatt transform turns a random vector $\boldsymbol{U} = (U_1, \ldots, U_d)$ with copula C into another vector $\boldsymbol{V} = (V_1, \ldots, V_d) = R(\boldsymbol{U})$ containing independent uniform variables. It is given by

$$V_j = C_{j|j-1,\ldots,1}(U_j|U_{j-1}, \ldots, U_1), \quad j = 1, \ldots, d.$$

where $C_{j|D}$ is the conditional distribution of U_j given $\boldsymbol{U}_D$. The corresponding inverse operation $\boldsymbol{U} = R^{-1}(\boldsymbol{V})$ turns independent uniform variables $\boldsymbol{V}$ into a vector $\boldsymbol{U}$ with copula C. It is given by,

$$U_j = C_{j|j-1,\ldots,1}^{-1}(V_j|V_{j-1}, \ldots, V_1), \quad j = 1, \ldots, d,$$

In vine copula models, the conditional distributions and inverses appearing in the transformations can be computed efficiently using recursion over conditional distributions associated to the pair copulas in the model; see Equation 19 and Chapter 6 in Czado (2019). The same technique can be used to simulate conditionally from a vine copula model, provided the required conditional distributions can be expressed by pair copula terms without the need for integration (see, for example, Aas et al. 2021, Section 4.2). A specialized implementation for D- and C-vines is given in the `CDVineCopulaConditional` library (Bevacqua 2017).

6. Current and future research directions

In what follows, we summarize the literature of four particularly active areas of research and point to future directions, mainly focusing on methodological developments. Further topics and applications of vine copulas were reviewed recently by Czado (2019, Chapter 11) and Aas (2016); see also `vine-copula.org` for a broad collection of papers, talks and videos.

6.1. Statistical learning

In recent years, vine copula models have been used increasingly in statistical learning problems. One of the main tasks in statistical learning is regression. In the context of vine copulas, regression problems are solved by building conditional response distributions. This allows to extract, among others, conditional means and conditional quantiles.

A first question is how to best set up the vine structure in such a context. One approach builds a vine distribution for the covariates alone and adds the response in a way that the resulting conditional distribution is available in closed form, i.e., without the need for integration over the vine copula density (Chang & Joe 2019, Chang et al. 2019, Cooke et al. 2019). These approaches focus on the vine structure of the covariates first, which may be unnatural in the regression context. An alternative is to start with the response as the first vine node and then add in such a way that the conditional distribution remains available in closed form. The selection procedure stops if the conditional (penalized) log-likelihood is no longer increasing. This idea was first developed for D-vine models by Kraus & Czado (2017a) and later extended to certain R-vine structures by Zhu et al. (2021). Tepegjozova et al. (2021) considered both D- and C-vines, but generalized the procedure to look two steps ahead before adding a new variable. While the D- and C-vine methods are feasible in large dimensions, the search for R-vines is restricted to smaller dimensions because of the huge number of possibilities. How to select the covariates in high-dimensional R-vine copula regression models therefore remains an open problem.

In the context of quantile regression, we need to adequately model tail dependence. The classical approach is the linear quantile regression model of Koenker & Bassett (1978). Bernard & Czado (2015) showed that for univariate Gaussian margins, the Gaussian copula is the only one complying with linear regression quantiles. Thus linear quantile regression is of little use for data with tail dependence. A further problem is that linear quantile lines usually cross for different levels if the true multivariate distribution is not Gaussian. Noh et al. (2015) formulated a copula-based quantile regression approach, which was later extended to censored response variables (De Backer et al. 2017) and other regression problems (Nagler & Vatter 2020b). In these papers, the conditional response distribution is not necessarily available in closed form, but is found through copula-based estimating equations. In contrast, Kraus & Czado (2017a) proposed a D-vine model where the conditional quantile function can be computed by inverting the conditional response distribution function, which is available in closed form. Extensions including ordinal discrete variables and nonparametric pair copulas were considered in Schallhorn et al. (2017) and Tepegjozova et al. (2021).

Another important task of statistical learning is clustering. For model based clustering finite mixtures of distributions are often assumed. Here, the random vector $\boldsymbol{X} = (X_1, \ldots, X_d)$ has a density given by

$$f(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{j=1}^{k} \pi_j f_j(\boldsymbol{x}; \boldsymbol{\theta}_j), \qquad\qquad 22.$$

where $\pi_j \geq 0$, $\sum_{j=1}^{k} \pi_j = 1$ and $f_j(\cdot; \boldsymbol{\theta}_j)$ is the density of the j-th cluster with parameters $\boldsymbol{\theta}_j$. The task is to estimate the unknown mixing probabilities $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_k)$, the unknown parameter vector $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_k)$ as well as the number of clusters k. Given a fitted mixture model, observations are assigned to the cluster with the highest conditional probability given the data. Estimation in finite mixture models is facilitated with

the EM algorithm of Dempster et al. (1977). Mixtures of normals are the most prominent models (Fraley & Raftery 2002), but require cluster distributions to have elliptical shape. To achieve non-elliptical cluster shapes Diday (2002) utilized copulas and adapted the EM algorithm. A restrictive d-dimensional Clayton copula was used by Cuvelier & Noirhomme-Fraiture (2005). Vrac et al. (2005) use the expectation/conditional maximization (ECM) algorithm of Meng & Rubin (1993) together with the Frank copula to jointly cluster bivariate atmospheric profiles.

There has been some work connecting finite mixture models to vine copulas. Markov tree models are equivalent to vine copulas truncated after the first tree (see, e.g., Brechmann et al. 2012) and have been considered by Kirshner (2008) and Silva & Gramacy (2009). Kim et al. (2013) consider parametric D-vine copulas with a single pair copula family and estimate parameters jointly in the M-step, which is only tractable for small d. Roy & Parui (2014) use mixtures of D-vine distributions for the analysis of observed principal components, where the node order is determined by the magnitude of the eigenvalues. In contrast, Sun et al. (2017) consider C-vine copulas as mixture components and sequential estimation for the mixture components. In the M-step, the stepwise selection and estimation approach for C-vines outlined in Section 4 is used. However, their method neglects the fact that the choice of the C-vine copula families and parameters might depend on the weights resulting from the E-step. Sahin & Czado (2021) extend these methods and allow to select and estimate different R-vine distributions for each cluster based on the ECM algorithm. All methods above implicitly assume that all variables in the data set are relevant for the clustering. In high dimensions, this may not be the case and improvements can be expected when restricting to only relevant variables. How to select this set of variables is an open problem, however.

The mixture model Equation 22 can also be used for classification problems. Here, we assign observations to the class with the highest posterior probability. Classification algorithms based on this rule are called as *Bayes classifiers*. Copula-based Bayes classifiers were already considered by Elidan (2012) using Bayesian networks and Salinas-Gutiérrez et al. (2017) using chain graph models. Chen (2016), Carrera et al. (2016), and Carrera et al. (2019) employed parametric vine copulas for the mixture components. Nagler & Czado (2016) used nonparametric pair copulas and Schellhase & Spanhel (2018) allowed for nonsimplified vines with a penalized spline approach. Tekumalla et al. (2017) used D-vine models but, in contrast to the previous methods, allowed for multiple classes and discrete variables through a computationally challenging Bayesian approach. Most works show good performance compared to other competitors, but do not address important methodological issues. In particular, variable selection and hyperparameter tuning in vine copula based classifiers remains an open problem.

6.2. Structure selection and high-dimensional models

In Section 3, we saw that there are many possible regular vine structures. In principle, classical likelihood-based criteria (like AIC or BIC) can be used to determine the best structure. Because the number of possible vines grows superexponentially (see Section 4), such procedures become infeasible already in moderate dimensions, however. This explosion and the complex algebraic structure of vine tree sequences makes their selection an extremely challenging problem.

Dissmann's heuristic mentioned in Section 4 greedily maximizes the dependence in each

tree based on the absolute value of Kendall's τ. Variants replacing Kendall's τ with AIC, BIC, or p-values of Goodness-of-Fit tests were investigated in Czado et al. (2013), variants with nonparametric pair-copulas by Nagler et al. (2017), and a variant taking the simplifying assumption into account by Kraus & Czado (2017b). The empirical studies in these papers indicate small improvements in performance, but these gains appear negligible in view of the the added computational demand. Non-heuristic methods based on MCMC (Gruber & Czado 2015, 2018) and neural networks (Sun et al. 2019) lead to more notable improvements but take orders of magnitude longer to compute and are therefore only feasible in rather small dimension. In view of the above, Dissmann's heuristic remains the gold standard, even a decade after it was initially developed in his thesis. A promising path for improvement is to find ways to efficiently explore the space of vine structures. A first step along these lines based on the concept of *common sampling orders* was taken by Cooke et al. (2015) and Zhu et al. (2020). Another approach by Chang et al. (2019) limits the greediness of the algorithm by looking ahead a fixed number of trees using Monte Carlo Tree Search. Despite improving significantly over the benchmark on various data sets, there appears to remain a lot of room for improvement — especially in higher dimensions.

In high-dimensional models, further challenges for model selection arise. The number of model parameters grows quadratically in the dimension, which calls for *sparse* vine copula models. A vine copula model is sparse when many pair-copulas correspond to (conditional) independence. A natural sub-class are *truncated* vine copulas, i.e., models where all pair-copulas after a certain tree are set to independence. The question then becomes how to select the right truncation level and several solutions have been proposed (Kurowicka 2011, Brechmann et al. 2012, Brechmann & Joe 2015, Joe 2018). An alternative model class are *thresholded* vine copulas, where all pairs with sufficiently weak dependence are set to independence. Traditionally, the thresholding is done by an independence test based on Kendall's τ (e.g., Dissmann et al. 2013) as implemented in the `VineCopula` package. A modified BIC criterion specifically tailored to high-dimensional vines was proposed by Nagler et al. (2019) and is suitable to select both truncation level and thresholding level. This method is implemented in the `vinecopulib` library. A separate line of research (Müller & Czado 2018, 2019a,b) exploits connections between vine copulas and Gaussian DAGs to find sparsity patterns. A completely different approach is to use dimension reduction techniques before employing a copula model as in Tagasovska et al. (2019).

In high-dimensional linear models, it is well known that theoretical guarantees for estimation and inference break when the number of parameters is large compared to the number of samples. There is no reason to believe that vine copula models are exempt from this phenomenon, but it is unclear where the breakpoint lies. The only known theoretical results in this regime were given in the model selection context by Nagler et al. (2019), but they rely on an unverified assumption of consistent parameter estimates. Thus, asymptotic results for inference in high-dimensional vine copula models are in dire need.

6.3. The simplifying assumption

As mentioned in Sections 2 and 3, vine copula models are usually built under the simplifying assumption. The assumption is much weaker than conditional independence. Conditional dependence of any strength and form is allowed, but only if it does not change with the conditioning value. It is worth emphasizing that the simplifying assumption is only required for explicit pair-wise dependencies in the model, i.e., those corresponding to an edge

in the vine. All other pair-wise dependencies can (and often will) be non-simplified. An obvious question, first raised by Hobæk Haff et al. (2010), is how constraining the simplifying assumption is. Some popular multivariate parametric copulas, most notably elliptical copulas and the Clayton copula, are known to satisfy the simplifying assumption (Stöber et al. 2013) – in a very strong sense: due to their closedness in conditioning and marginalization, they are simplified for every possible R-vine structure. Hobæk Haff et al. (2010) provided numerical examples suggesting that a simplified parametric model can be a very good approximation even if the true model is not simplified.

To check whether the simplifying assumption holds for a particular data set, several statistical tests have been developed. Most of them focus on a simpler setting, where there is only one bivariate copula and one or more covariates (e.g., Acar et al. 2013, Gijbels et al. 2017, Derumigny & Fermanian 2017). The problem is more difficult in the context of vine copulas, because the assumption needs to be tested for every pair-copula. A procedure tailored to parametric vine copulas was developed by Kurz & Spanhel (2018) and implemented in the `pacotest` R package (Kurz 2017). The authors perform an empirical study suggesting that the assumption cannot be rejected in several financial data sets, but is rejected already in the second tree for some others. Even if the assumption is violated, Portier & Segers (2018) showed that a simplified empirical copula can be estimated non-parametrically at $\sqrt{n}$-rate, as suggested by simulations in the context of simplified vines by Haff & Segers (2015). In a similar vein, Nagler & Czado (2016) proved that simplified vine copula densities can be estimated at a rate equivalent to a two-dimensional problem. Their simulations suggest that, in a nonparametric setting, the simplifying assumption can be beneficial even if it is severely violated.

It is also possible to build non-simplified models. Acar et al. (2012) developed a kernel method for three-dimensional semiparametric vines. A fully parametric model, where the conditional dependence is modeled similar to a GLM was proposed by Han et al. (2017). A semiparametric model allowing for more general, additive relationships was developed by Vatter & Nagler (2018) and is implemented in the `gamCopula` R package (Vatter & Nagler 2017). A fully nonparametric method based on splines and dimension reduction of the covariate space was proposed by Schellhase & Spanhel (2018) and is available through the `pencopulaCond` R package (Schellhase 2017).

The fact that vine copula models contain multiple interrelated pair-copulas complicates interpretation of the simplifying assumption. Killiches et al. (2017) used visualizations of three-dimensional density contours to provide some geometrical intuition. However, Spanhel et al. (2019) showed in several toy examples that the simplifying can have several unintuitive implications. First, using the true pair-copulas in the first tree is often suboptimal. Second, spurious dependence can appear in higher tree levels, which makes interpretation of those pair copulas difficult. Mroz et al. (2021) further proved that any copula can be approximated arbitrarily well by a simplified vine copula in the supremum metric, but not for more intuitive notions of distance (like KL divergence or total variation metric) and the distance can be quite large. This alone should not discourage researchers from employing a simplified model. The exact validity of a model's assumptions is not the primary determinant of its usefulness, but some care is in order when interpreting the results.

6.4. Time series models

Time series models based on vine copulas have become quite popular, especially in financial econometrics. In the context of a multivariate time series $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_T \in \mathbb{R}^d$, there are two types of dependence: serial dependence (dependence across different points in time) and cross-sectional dependence (dependence in the vector $\boldsymbol{X}_t$ at a given point in time).

The majority of works separate the two types of dependence. Classical time-series models (such as ARMA/GARCH models) are used to filter the univariate serial dependence in each margin and a vine copula model is employed for the cross-sectional dependence across residuals. A first instance of such a model with ARMA-GARCH filters was already given in the seminal paper by Aas et al. (2009) and in higher dimensions by Brechmann & Czado (2013). Later Min & Czado (2014) additionally allowed for nonparametric estimation of the marginal residual distribution and provided asymptotic results for the copula parameter estimates. Other marginal filters can be used as well, for example in the presence of non-stationary trends (e.g., Jäger et al. 2019).

In most early works, the cross-sectional dependence was assumed to be fixed. Chollete et al. (2009) relaxed this assumption by allowing the parameters of a C-vine copula to switch between two regimes depending on a latent Markov process. This model was generalized by Stöber & Czado (2014) and Fink et al. (2017) to multiple regimes, each corresponding to a different R-vine copula. Other works modelled the change of dependence on a finer scale by explicitly specifying the dynamics of copula parameters. In So & Yeung (2014), each parameter follows observation-driven dynamics similar to the DCC-GARCH model (Engle 2002). Another line of research considers model-driven dynamics, where copula parameters are modelled as latent AR(1) processes. Almeida et al. (2016) and Goel & Mehra (2019) developed frequentist estimation procedures for C- and D-vine models. Kreuzer & Czado (2019) and Kreuzer & Czado (2021) proposed Bayesian approaches for general R-vine models and parsimonious factor copulas expressed as C-vines. A different approach was taken by Vatter & Nagler (2018) and Acar et al. (2019), where the model parameters are modeled as smooth functions of time and estimated by spline and kernel techniques, respectively.

The separation of serial and cross-sectional dependence is convenient because it allows to rely on well-established models for univariate series. But serial dependence can be characterized by a copula, too, and conceptually there is no reason to treat the serial part differently from the cross-sectional one. Around the same time, three papers independently proposed vine copula models that capture both types of dependence simultaneously: the COPAR model of Brechmann & Czado (2015), the D-vine model of Smith (2015), and the M-vine model of Beare & Seo (2015). The three models differ in the vine structure, but their motivation is the same. The idea is to choose a structure that ensures stationarity of the model by imposing a simple restriction on the pair-copulas: if we shift all indices of an edge in time, the associated pair-copula must remain the same. This idea was formalized by Beare & Seo (2015) and called *translation invariance*. Nagler et al. (2020a) gave a complete characterization of the class of vine structures that ensure stationarity under translation invariance. Surprisingly, the COPAR model does not fall under this category and, hence, may not be stationary. Nagler et al. (2020a) also derived asymptotic properties of parameter estimates and simulation-based predictions from such models. They also pointed to an open problem regarding to the mixing properties of the resulting time series. Another interesting venue for future research is to adapt these models for non-stationary and long-memory time series.

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