

Application of vine copulas to dependence analysis of water quality data

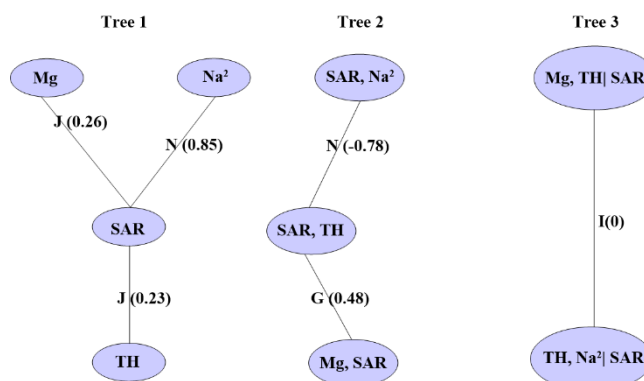
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GRAPHICAL ABSTRACT



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ABSTRACT

In this study, using vine copulas and tree sequences, dependence analysis of groundwater quality variables (Total hardness (TH), Sodium adsorption ratio (SAR), Sodium percentage (Na %) and magnesium (Mg)) was performed. For this purpose, the tree sequence of vine copulas including regular vine (R-vine), independent version of R-vine, also Gaussian version of R-vine, Gaussian independent version of R-vine, canonical vine (C-vine), independent version of C-vine, drawable vine (D-vine) and independent D-vine were evaluated independently in pairwise variables analysis. The study results of dependence structures and tree sequences of Vine copulas showed that among the studied copulas, the performance of the independent C-vine was 3.8 % better than R-vine and 0.25 % (insignificant and negligible) better than D-vine. The tree sequences provided by independent C-vine preserve correlation of pairwise variables until the last tree. In the last tree of independent C-vine, edge correlation of Mg, Na % | TH, and SAR reaches zero. Due to the proper performance of D-vine in dependence analysis of the studied variables, this copula is introduced as the selected copula.

1. Introduction

Copula functions were introduced by Sklar in 1959. Copula function is able to show correlation analysis between random variables that is used as an efficient and practical method for dependency modeling (Joe 1997; Nelsen 2006; Ramezani et al. 2019; Salvadori et al. 2007; Serinaldi et al. 2009). The application of copula functions in hydrology has increased rapidly in recent years. For more dimensions, to reduce complexity of calculations, vine copulas were introduced and presented. There are 240 different structures for a five-dimensional structure (Aas et al. 2009). To help organize them, Bedford and Cooke (2001a & b) developed a graphical model called the regular vine. Regular class of copulas is very broad. This class all possible pair-copula structures. Having the same dependence in all series is one of the main points of frequency analysis studies in univariate or traditional multivariate mode. For example, 3D copula means the dependence of the first pair variable and the third variable, and the joint cumulative distribution function (CDF) of the first pair variable, which is not actually possible. As the dimensions increase, the accuracy of these methods decreases sharply. This limitation does not exist in vine copulas, which

include all dependencies, and larger dimensions can be easily modeled (Czado et al. 2019). To better understand the structure of multidimensional copulas, one must first understand its multivariate density function. Grimaldi and Serinaldi (2006a & b) constructed a complete or asymmetric 3-D distribution of flood variables using Archimedean mixed functions and performed extensive simulations to highlight differences with the well-known Archimedean symmetric correlations. Serinaldi et al. (2009) to analysis the drought characteristics used the copula functions. Hui-Mean et al. (2019) for investigation the correlation between drought characteristics in Malaysia used trivariate copula functions. The results of this research showed copula functions are suitable tools for analysis the multivariate hydrological simulation. Xu et al. (2020) proposed a framework with multinomial analysis based on R-vine for multidimensional uncertainty analysis and confirmed its performance. Li et al. (2021) used vine copula-based parametric sensitivity analysis for multidimensional dependencies. The results indicated that the vine copula is a powerful tool for modeling variable dependencies.

Since analysis of dependence structure with more than 2 dimensions as well as its modeling is complex, vine copulas will be very

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useful. Analysis of dependence structure of pairwise variables is one of the first steps for copula-based modeling. Therefore, the aim of the present study is to analyze dependence structure of pairwise qualitative variables in the study area. In this study, we have tried to investigate dependence of pairwise variables by investigating tree sequence of Vine copulas. Therefore, in this study, tree sequence of different vine copulas including C-vine, D-vine and R-vine copulas is investigated. In this study, using the copula approach and its rotational state, the dependence analysis of water qualitative data has been investigated.

2. Materials and methods

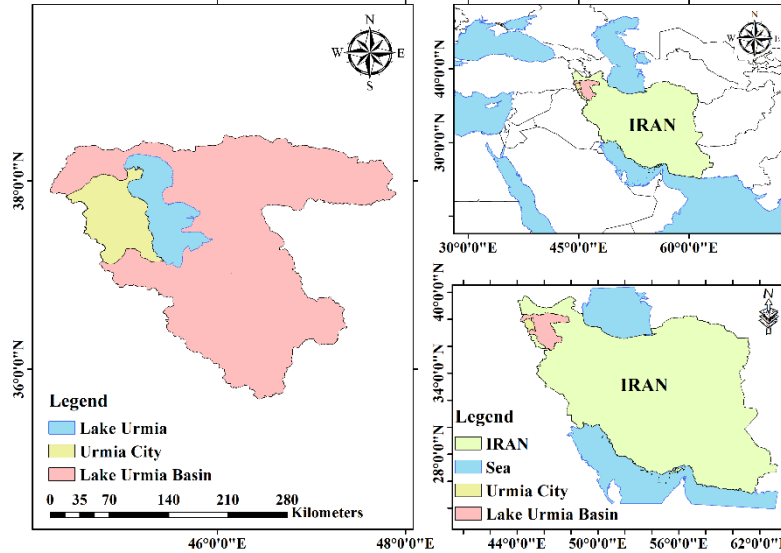


Fig. 1. Location map of Urmia city in Iran and Lake Urmia Basin.

In this study, Kendall's Tau method was used due to its common use in the studies of copula functions. This method has high accuracy in correlation analysis and is more accurate than other methods (Dastourani and Nazeri Tahroudi. 2022; Khashei-Siuki et al. 2021; Khozayemnezhad and Nazeri-Tahroudi. 2020; Nazeri Tahroudi et al. 2021&2022a; Tabatabaei et al. 2022).

2.1. Correlation analysis

In this study, Kendall's tau (τ) was used to evaluation the correlation analysis that for two random variables X_1 and X_2 is defined as:

$$\tau(X_1, X_2) = \frac{P((X_{11} - X_{21})(X_{12} - X_{22}) > 0) - P((X_{11} - X_{21})(X_{12} - X_{22}) < 0)}{1} \quad (1)$$

In above equation P is the probability occurring of (.) and $(X_{11} - X_{12})$ and $(X_{21} - X_{22})$ are independent (Hollander et al. 2014). In another form, based on Kurowicka and Cooke (2006) τ will be as:

$$\hat{\tau}_n := \frac{N_c - N_d}{\sqrt{N_c + N_d + N_1} \sqrt{N_c + N_d + N_2}} \quad (2)$$

where, N_d and N_c are the number of discordant pairs and the number of concordant pairs respectively. N_1 and N_2 are the number of extra x_1 pairs and extra x_2 pairs of random sample $\{x_{11}, x_{12}, \dots, x_{1n}\}$ respectively from the joint distribution of (X_1, X_2) . Finally the Kendall's τ is as follow (Genest and Favre. 2007; Nazeri-Tahroudi et al. 2022):

$$\hat{\tau}_n := \frac{N_c - N_d}{\binom{n}{2}} \quad (3)$$

2.2. Using the vine copulas to multivariate analysis

The same independence structure is requires to the analysis of multidimensional series in past researches. With increasing the dimensions reach to 4 and also more, the accuracy and efficiency of the ordinary copula methods is reduced (Nazeri Tahroudi et al. 2022b). For this reason, the vine copula was introduced. A vine copula is made of 2-variable copula in the form of tree sequence. Canonical vine (C-Vine), Regular vine (R-Vine) and also Drawable vine (D-Vine) are three popular types of vines that can be selected. One of the most important capabilities of the vine Copula family is multi-dimensional modeling. Number of D-, C-, and R-vine tree structures for $d = 3$ to 9 are reported

In this study, the structure of vine copulas and its parameters have been investigated using 4 time series of groundwater quality data in Urmia city, West Azerbaijan Province located in northwestern Iran. The studied values are total hardness (TH), sodium adsorption ratio (SAR), magnesium (Mg) and percentage of sodium (Na%) on a monthly scale. Fig 1 shows the location of the Urmia city in the north west of Iran. The investigated parameters were selected according to their importance in the discussion of drinking water.

as Table 1 (Czado, 2019). An example of D-vine (Fig 2-b) and C-vine (Fig. 2-a) were presented in figure 2 in five dimensions. Both of D- and C-vine copulas have $d-1$ tree sequence. In the T_2 tree of Fig. 2 (left), $e = 2, 5, 1$ is edge, 1, 5 and 1, 2 call the node and root, respectively.

Table 1. Number tree structure of C-vine, D-vine, and R-vine for different values of d .

d	Number of vine structures (C and D)	Number vine structures (R)
$d=3$	3	3
$d=4$	12	24
$d=5$	60	480
$d=6$	360	23040
$d=7$	2520	2580480
$d=8$	20160	660602880
$d=9$	181440	380507258880

2.3. Vine Copula, Type C

The dependence on a special variable in a C-vine tree (the first node's root) for each pair is modeled by bivariate copulas. In each tree, one root of node is selected and all pair dependencies are modeled according to this node (Fig 2-a). According to Czado (2019), multivariate density is as follow:

$$f(x) = \prod_{k=1}^d f_k(x_k) \times \prod_{i=1}^{d-1} \prod_{j=i+1}^d c_{i,j|i(i-1)}(F(x_i | x_1, \dots, x_{i-1}), F(x_{i+j} | x_1, \dots, x_{i-1}) | \theta_{i,j|i(i-1)}) \quad (4)$$

where, $c_{i,j|i(i-1)}$ is the density of the bivariate copula and had the

$\theta_{i,j|i(i-1)}$ parameters ($i_k; i_m$ means: i_k, \dots, i_m) and

$f_k, k = 1, \dots, d$ is the marginal density. The C-vine's log-likelihood function with the θ_{CV} parameter is as follows:

$$l_{CV}(\theta_{CV} | u) = \sum_{k=1}^d \sum_{i=1}^{d-1} \sum_{j=i+1}^d \log [c_{i,j|i(i-1)}(F_{i|i(i-1)}(u_i), F_{i+j|i(i-1)}(u_{i+j}) | \theta_{i,j|i(i-1)})] \quad (5)$$

where, $F_{j|i(i-1)} = F(u_{k,j} | u_{k,i_1}, \dots, u_{k,i_m})$ and the marginal distributions are also uniform.

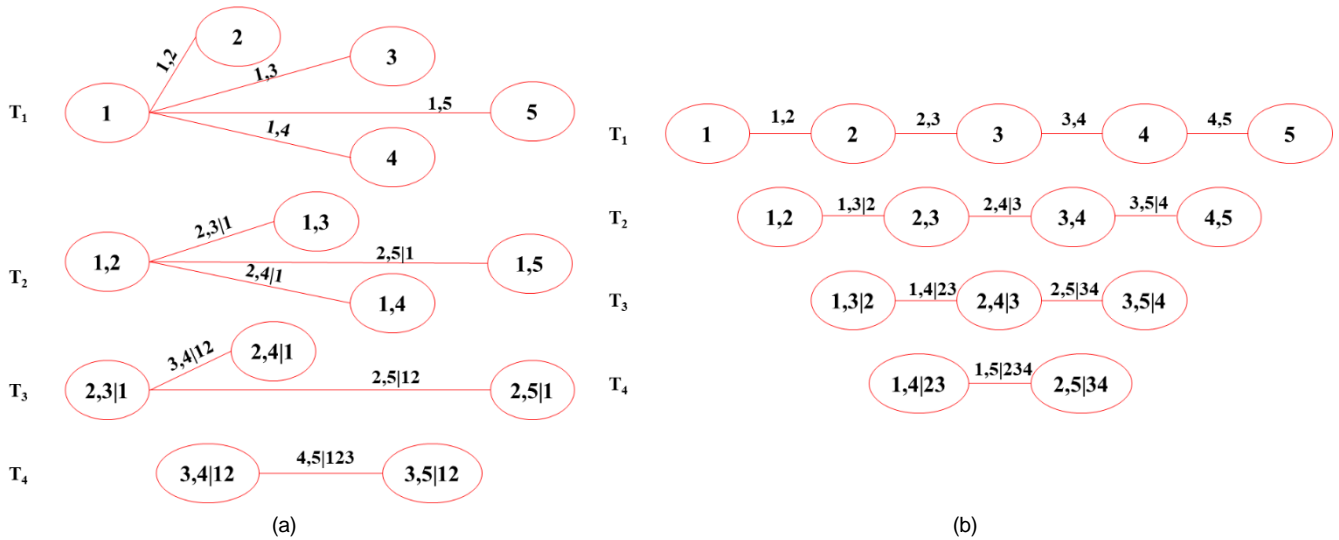


Fig. 2. Example of 5 dimension copula (a: C-vine b: D-vine) (Nazeri Tahroudi et al. 2022c).

2.4. Vine Copula, Type D

The D-vine offers a different way of choosing the order of tree structures (Fig. 2-b). At the first tree, all pair variables are modeled. Then, T_2 , pair (1,3|2), in the T_3 pair (2,4|3) and in T_4 pair (1,5|234) were modeled. The density of a D-vine is (Aas and Berg. 2009):

$$f(x) = \prod_{k=1}^d f_k(x_k) \times \prod_{i=1}^{d-1} \prod_{j=i+1}^d c_{j,i+1(j+1)(j+i-1)}(F(x_j | x_{j+1}, \dots, x_{j+i-1}), F(x_{j+i} | x_{j+1}, \dots, x_{j+i-1}) | \theta_{j,i+1(j+1)(j+i-1)})$$

For the vector v with m dimension, the conditional distribution functions $F(x|v)$, define as:

$$h(x | v, \theta) := F(x | v) = \frac{\partial C_{cvj|v_{-j}}(F(x | v_{-j}), (F(v_j | v_{-j}) | \theta))}{\partial F(v_j | v_{-j})} \quad (7)$$

where, v_j is an arbitrary component of v . v_{-j} represents the $(m-1)$

dimension vector with the exception of v_j . $C_{cvj|v_{-j}}$ is a bivariate copula distribution function with parameter θ in the m tree. In a D-vine, the log-likelihood with the θ_{DV} parameter is:

$$l_{DV}(\theta_{DV} | v) = \sum_{k=1}^N \sum_{i=1}^{d-1} \sum_{j=i+1}^d \log[c_{j,i+1(j+1)(j+i-1)}(F_{j,i+1(j+1)(j+i-1)}(x_j | x_{j+1}, \dots, x_{j+i-1}), F_{j,i+1(j+1)(j+i-1)}(x_{j+i} | x_{j+1}, \dots, x_{j+i-1}) | \theta_{j,i+1(j+1)(j+i-1)})] \quad (8)$$

2.5. Vine Copula, Type R

The R-vine or Regular vine is more flexible than the C-vine and D-vine. The structure of the R-vine is very discrete compared to the C and D types (Nazeri Tahroudi et al. 2022c). These functions include many structures and are so diverse that the user has more choice. The tree structure of R-vine copula in 5 dimension is plotted in Fig. 3. According to Dibmann et al. (2013):

$$f(x) = \prod_{k=1}^d f_k(x_k) \times \prod_{i=1}^{d-1} \prod_{e \in E_i} c_{C_{e,a}, C_{e,b}|D_e}(F_{C_{e,a}|D_e}(x_{C_{e,a}} | x_{D_e}), F_{C_{e,b}|D_e}(x_{C_{e,b}} | x_{D_e})) \quad (9)$$

where, x_{D_e} is equal to D_e , $e = a, b$ and $x_{D_e} = x_i | i \in D_e$. The log-likelihood function of the R-vine copula is as follows with parameter θ_{RV} and E_1, E_2, \dots, E_{d-1} :

$$l_{RV}(\theta_{RV} | v) = \sum_{k=1}^N \sum_{i=1}^{d-1} \sum_{e \in E_i} \log[c_{j(e),k(e)|D(e)}(F(u_{i,j(e)} | u_{i,D(e)}) | \theta_{j(e),k(e)|D(e)})] \quad (10)$$

where, $u_i = (u_{i,1}, \dots, u_{i,d})' \in [0,1]^d$, $i = 1, \dots, N$. $c_{j(e),k(e)|D(e)}$ equal to bivariate copula density with edge e and parameter $\theta_{j(e),k(e)|D(e)}$. Due to the fact that each copula function covers a certain range of dependence, in this study, the rotational state of copula functions was used to fully cover tail dependence.

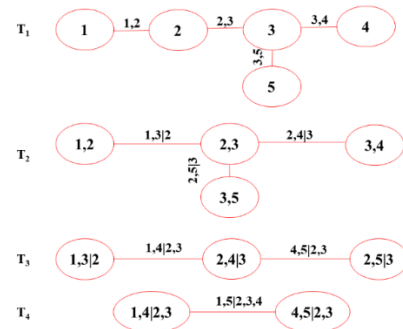


Fig. 3. R-vine copula in 5 dimension (Czado. 2019).

3. Results and discussion

The studied variables including TH, SAR, Na % and Mg are presented in Fig. 4 as described. As shown, the changes in the studied values is 200-1200 mg/L of calcium carbonate, 1-8, 1-50 %, and 1-15 mg/L, respectively. The scatter plot in both measured and normalized and standardized states was shown in Figs. 5 and 6. Using these plots, correlation between the studied parameters can be observed. As shown in Fig. 5, scattering and correlation of Na % and SAR are better than other variables. As shown in Fig. 5, correlation between TH and Mg is also in the second place. Fig. 6 shows the changes of all the studied variables can be seen between zero and one. Also, according to this figure, scattering of the studied variables can be dimensionless. The correlation between the studied variables is clearly visible. Na % and SAR have the highest correlation.

To investigate correlation between the variables, the Kendall's tau was used. For this, normalized and standardized data were used. The study results of Kendall's tau were presented in Fig. 7. The upper triangular elements show the Kendall's tau in this Fig., the main diameter elements show the data histogram. The lower triangular elements of Fig. 7 show the data scatter plot along with the normalized and standardized contour lines. Based on Fig. 7, the highest correlation is between SAR and NA % (0.98). The correlation between TH-Mg pairwise variables is also in the second place (0.72). The lowest correlation belongs to TH-Na % pairwise variables (0.10).

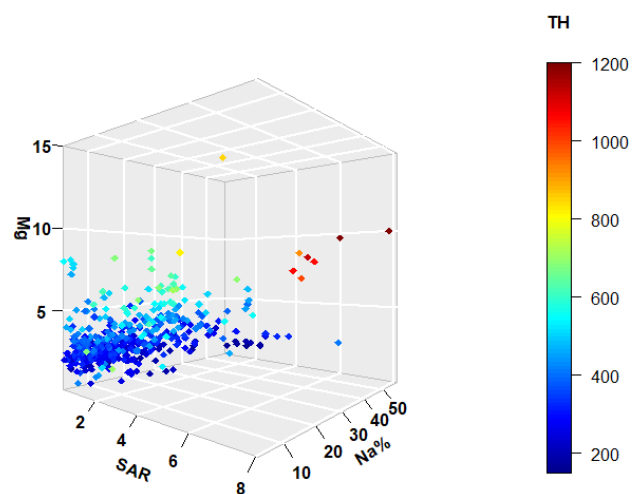


Fig. 4. Studied quality data in Urmia city.

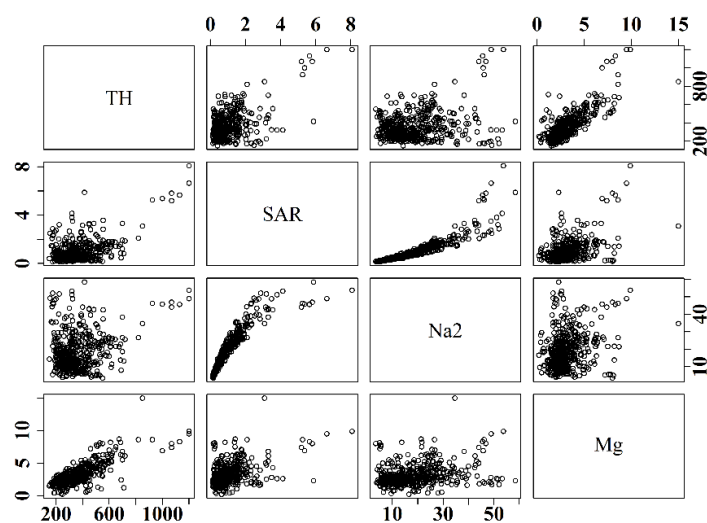


Fig. 5. Scatter plot of studied quality data in original scale.

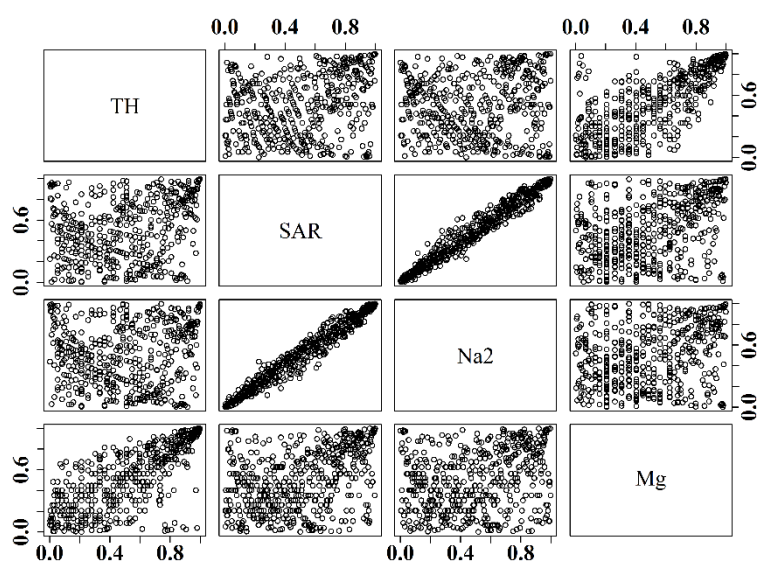


Fig. 6. Scatter plot of studied quality data in copula scale.

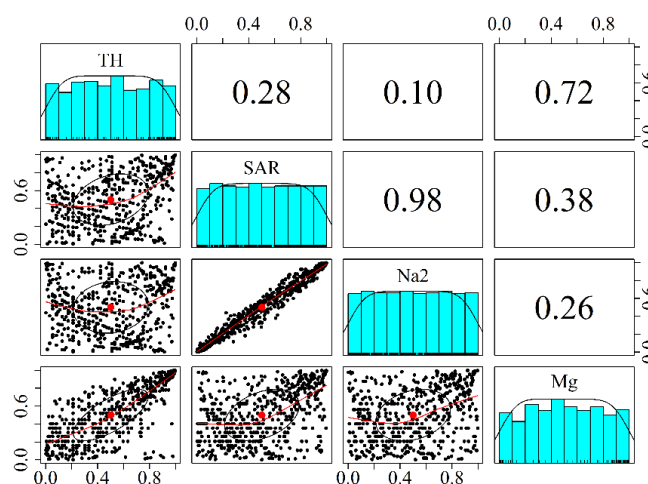


Fig. 7. Histogram, correlation and empirical contour lines of studied data in copula scale.

3.1. Evaluation of vine copula

The values of Kendall's tau in evaluating correlation between pairwise variables SAR-Na%, Mg-TH, Mg-SAR, SAR-TH, Mg-Na % and Na % -TH are equal to 0.98, 0.72, 0.38, 0.28, 0.26 and 0.10, respectively. After investigating correlation between pairwise variables, different copula functions were evaluated based on Akaike information criterion (AIC), Bayesian information criterion (BIC) and Log Likelihood criteria. C-, D- and R-vine copulas were used to make multivariate distributions.

R-vine copula tree sequence was investigated using the studied qualitative variables. The results of tree sequence of R-vine copulas were investigated in four states: R-vine, independent R-vine, Gaussian R-vine and Gaussian independent R-vine. The study results of all four states were presented in Tables 2 to 5. Finally, the top tree sequence is selected based on mentioned criteria. In these tables, the expression 270 means a 270-degree rotation of the copula function regarding the complete coverage of the tail dependence.

Table 2. Results of fitting the R-vine copula.

Tree	Edge	Copula	Kendall τ
T ₁	SAR, Na %	Gaussian	0.85
	Mg, TH	Joe	0.51
	Mg, SAR	Joe	0.26
T ₂	Mg, Na% SAR	Gumbel 270	-0.44
	SAR, TH Mg	Joe 270	-0.05
T ₃	TH, Na% Mg, SAR	Frank	-0.69

LogLik: 1495, AIC: -2979, BIC: -2953

Table 3. Results of fitting the independent R-vine copula.

Tree	Edge	Copula	Kendall τ
T ₁	SAR, Na%	Gaussian	0.85
	Mg, TH	Joe	0.51
	Mg, SAR	Joe	0.26
T ₂	Mg, Na% SAR	Gumbel 270	-0.44
	SAR, TH Mg	independence	0.00
T ₃	TH, Na% Mg, SAR	Gaussian	-0.67

LogLik: 1507, AIC: -3004, BIC: -2983

Table 4. Results of fitting the Gaussian R-vine copula.

Tree	Edge	Copula	Kendall τ
T ₁	SAR, Na%	Gaussian	0.85
	Mg, TH	Gaussian	0.50
	Mg, SAR	Gaussian	0.24
T ₂	Mg, Na% SAR	Gaussian	-0.42
	SAR, TH Mg	Gaussian	0.04
T ₃	TH, Na% Mg, SAR	Gaussian	-0.68

LogLik: 1425, AIC: -2838, BIC: -2812

According to the results presented in Tables 2 to 5, it can be seen that the lowest value of Akaike information criterion (AIC) and Bayesian information criterion (BIC) and the highest value of Log Likelihood criteria (LogLik) is related to independent R-vine copula (Table 3). For independent R-vine copula, AIC, BIC and LogLik are -3004, -2983 and 1507, respectively. Among 4 R-vine copulas studied, independent copula has the best performance in the studied qualitative variables. The values of Kendall's tau are preserved in tree sequence of this

copula at all edges. In the last tree at the edge of TH, Na% | Ma, SAR correlation is -0.67. The accuracy and performance of independent R-vine copula to the last tree showed an acceptable correlation. Gaussian and Joe copulas were selected for the first tree, Gumbel 270 ° and independent copulas were selected for the second tree, and Gaussian copulas were selected for the third tree in the selected tree sequence. After investigating tree sequence of R-vine copulas, tree sequence of C-vine copula was investigated. The study results of C-vine copula tree sequence in two independent C-vine and C-vine states were presented in Tables 6 and 7.

Table 5. Results of fitting the Gaussian independent R-vine copula.

Tree	Edge	Copula	Kendall τ
T ₁	SAR, Na%	Gaussian	0.85
	Mg, TH	Gaussian	0.50
	Mg, SAR	Gaussian	0.24
T ₂	Mg, Na% SAR	Gaussian	-0.42
	SAR, TH Mg	independence	0.00
T ₃	TH, Na% Mg, SAR	Gaussian	-0.68

LogLik: 1422, AIC: -2834, BIC: -2813

Table 6. Results of fitting the C-vine copula.

Tree	Edge	Copula	Kendall τ
T ₁	SAR, Na%	Gaussian	0.85
	SAR, TH	Joe	0.23
	Mg, SAR	Joe	0.26
T ₂	TH, Na% SAR	Gaussian	-0.78
	Mg, TH SAR	Gumbel	0.48
T ₃	Mg, Na% TH, SAR	Joe 270	-0.01

LogLik: 1554, AIC: -3096, BIC: -3071

Table 7. Results of fitting the independent C-vine copula.

Tree	Edge	Copula	Kendall τ
T ₁	SAR, Na%	Gaussian	0.85
	SAR, TH	Joe	0.23
	Mg, SAR	Joe	0.26
T ₂	TH, Na% SAR	Gaussian	-0.78
	Mg, TH SAR	Gumbel	0.48
T ₃	Mg, Na% TH, SAR	Independence	0.00

LogLik: 1554, AIC: -3097, BIC: -3076

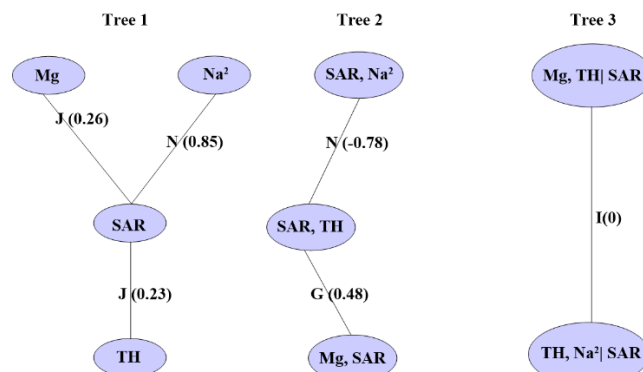
According to the results presented in Tables 6 and 7 for independent C-vine and C-vine copulas, respectively, it can be seen that Log Likelihood are the same in both Tables. However, due to the lowest values of AIC and BIC, independent C-vine copula performs better than C-vine. The correlation to the third tree is well preserved, but in both copulas, correlation is zero in the third tree. According to BIC, AIC and Log Likelihood, compared to C- and R-vine, C-vine has better performance, but due to flexibility of R-vine copulas, tree sequence of this copula preserved correlation until the last tree. For better comparison, D-vine copula tree sequence was also investigated.

The study results of D-vine copula tree sequence in two states of independent D-vine and D-vine copulas are presented in Table 8.

Table 8. Results of fitting the D-vine and the independent D-vine copula.

Tree	Edge	Copula	Kendall τ
T ₁	Na%, Mg	Joe	0.17
	SAR, Na%	Gaussian	0.85
	TH, SAR	Joe	0.23
T ₂	SAR, Mg Na %	Gumbel	0.48
	TH, Na % SAR	Gaussian	-0.78
T ₃	TH, Mg SAR, Na %	Frank	0.23

LogLik: 1550, AIC: -3088, BIC: -3063

**Fig. 8.** Independent C-vine tree sequence in 4D analysis of the studied qualitative variables.

As shown in Fig. 8, in the first tree, the qualitative variable SAR is selected as the center and the other variables are related to the internal copulas. In the second tree, SAR-TH pairwise variable is located in the center of the tree sequence due to the higher correlation than the other pairwise variables. The study results of the C-vine structure showed the acceptable correlation in the first tree between pairwise variables. In the last tree, the correlation of the edges is reduced. This increases the model uncertainty in higher trees. So that in the third tree, correlation between the edges reaches zero. However, based on the values of Log Likelihood, AIC and BIC, independent C-vine copula showed a better fit than other vine copulas. In general, increasing correlation in tree sequence as well as reducing AIC and BIC and increasing Log Likelihood increases reliability of the model. Hence, D-vine copula tree sequence can replace independent C-vine copula. The results indicate flexibility and capability of vine copulas in analyzing dependence structure with more than two dimensions, which has been emphasized in various studies, including Czado (2019), Khashei-Siuki et al. (2021), and Nazeri Tahroudi et al. (2022a). In more than two dimensions, due to complexity of the models, analysis of dependence structure of the variables requires high accuracy, which can be done well using vine copulas.

4. Conclusions

In this study, dependence structure analysis of qualitative variables TH, SAR, Na % and Mg was investigated using vine copulas. This study was conducted aimed to investigate tree sequences of vine copulas in dependence structure analysis of the studied qualitative variables. After confirming correlation using Kendall's tau, 4-dimensional vine copulas and their tree sequences were investigated according to BIC, AIC, and Log Likelihood criteria. The correlation results of the studied qualitative pairwise variables showed that correlation between normalized and standardized values is acceptable. Tree sequences of vine copulas with different R-vine copulas were investigated. Among tree sequences of R-vine copula, independent R-vine copula gave better results based on evaluation criteria. By analyzing dependence structure and tree sequences of C- and D-vine copulas, it was found that among the 4 D-vine, independent D-vine, C-vine and independent C-vine copulas, independent C-vine copula had better performance. The results showed that D-vine copula performed 3.5 % better than R-vine copula according to Log Likelihood. Similarly, according to Log Likelihood, the percentage improvement in the performance of independent C-vine copula compared to D-vine copula is about 0.25 %, which is insignificant and can be ignored. In general, the results indicated that among vine copulas including C-, R- and D-vines, Gaussian R-vine and their independent version, independent C-vine copula has better performance than other copulas according to Log Likelihood, AIC and BIC. After independent C-vine copula, D-vine and independent R-vine copulas have the best performance for investigating and analyzing dependence of the studied qualitative variables. However, due to zero

The same tree sequence of both independent D-vine and D-vine copulas was obtained. The correlation presented in this sequence at the first edge and Na%, Mg edge is less than the other edges. Correlation is preserved at almost all edges and trees. According to the results provided by Log Likelihood, AIC and BIC, the best performance is related to independent C-vine copula. In fact, among the studied copulas, C-vine copula has the best performance and the best fit with the studied quality variables. R-vine copula has more flexibility than C-vine and D-vine copulas. For this reason, Kendall's tau at different edges of R-vine tree sequence were better than C- and D-vine copulas. The superior copula tree sequence is presented in Fig. 8.

correlation in the last tree of independent C-vine copula, it is better to replace independent C-vine copula with D-vine copula. In D-vine copula, correlation is preserved until the last tree. Due to the fact that there is no limitation for copula-based models regarding the increase in dimension, therefore, by adding climatic parameters, their impact can be easily considered. Also, due to the fact that the proposed approach is based on the marginal distribution of data, there are no geographical and climatic restrictions in this regard.

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