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Copulas approach for modeling the stochastic dependence of three physico-chemical components of groundwater in the province of Sissili (Burkina Faso)

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Abstract. This study aims to model the stochastic dependence between potassium (K^+), iron (Fe^{2+}), and ammonium (NH_4^+) concentrations in groundwater from the Sissili province in Burkina Faso. To achieve this, we rely on the Student, Frank, and Hüsler–Reiss copulas to capture the full range of hydro-geochemical dependence structures. This statistical approach provides a reliable, flexible, and robust tool for analyzing environmental characteristics while supporting the sustainable management of water resources.

Cette étude a pour objectif de modéliser la dépendance stochastique entre les concentrations de potassium (K^+), de fer (Fe^{2+}) et d'ammonium (NH_4^+) dans les eaux souterraines de la province du Sissili au Burkina Faso. Pour ce faire, nous avons recours aux copules de Student, de Frank et de Hüsler-Reiss, afin de capturer l'ensemble des formes de dépendances hydro-géochimiques.. Cette approche statistique constitue un outil fiable, flexible et robuste, permettant à la

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Key words: copulas; stochastic dependence; groundwater; modeling.
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Résumé. Cette étude a pour objectif de modéliser la dépendance stochastique entre les concentrations de potassium (K^{+}), de fer (Fe^{2+}) et d'ammonium (NH_4^{+}) dans les eaux souterraines de la province du Sissili au Burkina Faso. Pour ce faire, nous avons recours aux copules de Student, de Frank et de Hüsler-Reiss, afin de capturer l'ensemble des formes de dépendances hydro-géochimiques.. Cette approche statistique constitue un outil fiable, flexible et robuste, permettant à la fois d'analyser les caractéristiques de l'environnement et de soutenir une gestion durable des ressources en eau.

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1. Introduction

Groundwater is an essential resource for drinking water supply, irrigation and other uses in many regions of West Africa, particularly in Burkina Faso. The physico-chemical quality of these water resources is being extensively tested due to the increased anthropogenic pressures. In the province of Sissili, as elsewhere, monitoring of chemical components such as iron, potassium and ammonium reveals significant fluctuations, highlighting the need for statistical approaches able of capturing not only central trends, but also extreme relationships between variables. Classical methods based on simple correlations or linear models are often insufficient to model non-linear or asymmetric dependencies. It is in this context that copulas offer a powerful alternative, by allowing to model separately the margins and dependency structure between variables Sklar (1959),Gianfausto et al. (2007). A study by Bárdossy and Li (2006), have demonstrated the interest of copulas to model groundwater quality parameters in Germany, by showing that spatial dependencies are not necessarily Gaussian and that non-Gaussian copulas often offer a better fit than traditional models (variograms, classical correlations). Furthermore, Maity, (2022) offers an extensive theoretical review of the use of copulas in hydrology and hydroclimatology, including multivariate frequency analyses, extreme modeling, and multivariate stochastic simulation.

Despite these advances at the international level, few studies in Burkina Faso use copulas to model the stochastic dependence between several physico-chemical parameters of groundwater. The central issue is as follows: simultaneous large (extreme) fluctuations in iron, potassium and ammonium concentrations may indicate environmental disturbances or contamination, but they are poorly captured by conventional methods. Thus, two main difficulties arise: capturing dependencies in the distribution lines, which is crucial for environmental risk management and choosing the most suitable copula family to model central dependence and strong dependencies in extremes.

This study aims to apply copula approach to understand the stochastic dependence between three physico-chemical components (Iron, Potassium, Ammonium) in groundwater from the province of Sissili. We address the following specific objectives:

i) to characterize the marginal distributions of each variable (Iron, Potassium, Ammonium);
ii) to estimate the stochastic dependence between each of the variable pairs by fitting different families of copulas (notably Frank, Student-t and Hüsler-Reiss);
iii) to quantify extreme dependencies through tail dependency coefficients;
iv) to compare the performance of models according to criteria such as AIC or maximum likelihood;
v) to interpret these results in a local hydrogeochemical framework to propose implications for groundwater quality management in the region.

This document is organized as follows. Section 2 summarizes the tools necessary for the application to our data (water components). Section 3 presents the different results and discussion, while section 4 presents the conclusion of this study.

2. Materials and methods

2.1. Description of the study area

The province of Sissili, located in the central-western region of Burkina Faso, covers an area of approximately $7,147km^2$ (see figure [1]). It is bordered at the south by Ghana and has a dense hydrographic network, including the Sissili river, a tributary of the White Volta Basin. Climate is Sudano-sahelien type, characterized by a rainy season from May to October and a dry season from November to April. This seasonal rainfall strongly influences the availability of water resources, both at the surface and underground.

From a hydrogeological point of view, the Sissili is characterized mainly by a fractured crystalline basement, which is typical of the basement areas of West Africa. Groundwater is contained in discontinuous and shallow aquifers, often located in fracture zones. Access to water is mainly through boreholes equipped with human-powered or motorized pumps. Water plays a fundamental role in agricultural activities, livestock breeding and domestic supply. However, increasing pressure on the resource, the effects of climate change and anthropogenic activities (fertilizers, pesticides, poor sanitation) contribute to spatial and temporal variability of groundwater water quality .

In this context, the study of the dynamics, quality and interactions between the different components of water (physico-chemical and biological) is essential for sustainable management of water resources in the province of Sissili. Groundwater samples were taken from 60 drillings located in the province of Sissili. The concentrations of K^+, Fe^{2+} and NH_4^+ were measured in laboratories according to the standards of the World Health Organization.

2.2. statistical analysis

2.2.1. Estimation of the parameters of probability laws

The analysis of the stochastic dependence between several physico-chemical components of water (such as potassium, ammonium and total iron) is based on an accurate estimation of the marginal probability laws of each variable. This step is crucial before any joint modeling using copulas.

Thus, let $Z \rightsquigarrow N(\mu_z, \sigma_z)$ with σ_z unknown. The estimator of the average of Z calculated on a sample $(Z_1, \ldots, Z_n)$ is such that:

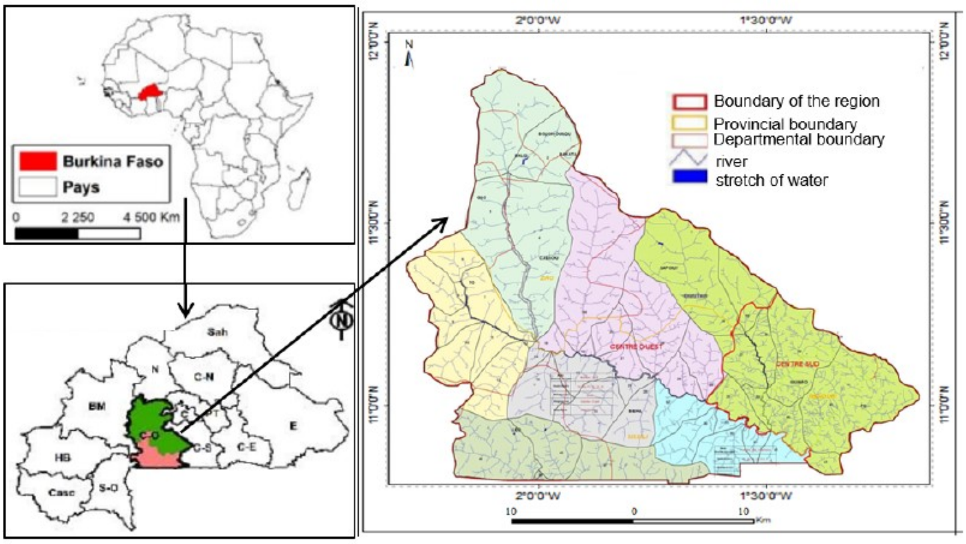


Fig. 1: Localization of the study zone of study

$$\overline{Z} = \frac{Z_1 + \cdots + Z_n}{n}$$

with, $\overline{Z} \rightsquigarrow N(\mu_z, \frac{\sigma_z}{\sqrt{n}})$. For a risk $\alpha = 5\%$, the normal distribution table gives the value $u_{\frac{\alpha}{2}} = 1,645$ such as:

$$P(\overline{Z} - u_{\frac{\alpha}{2}} \frac{\sigma_z}{\sqrt{n}} \leq \mu \leq \overline{Z} + u_{\frac{\alpha}{2}} \frac{\sigma_z}{\sqrt{n}}) = 1 - \alpha$$

For an unknown mu_z mean, the estimator of the variance $S_{n,z}2$ is such that

$$\frac{(n-1)}{\sigma^2} S_{n,z}^2 = \frac{\sum_{i=1}^{n} (Z_i - \overline{Z})^2}{\sigma^2} \rightsquigarrow \chi_n^2$$

For a confidence level of 95% the ability of $\chi 2$ at n degree of freedom gives z_1 and z_2 such that

$$P(z_1 \leq \frac{(n-1)}{\sigma^2} S_{n,z}^2 \leq z_2) = 1 - \alpha.$$

where, $[z_1, z_2]$ depend on the risks α_1 and α_2.

Name	Symbol / Formula	Interpretation
Pearson linear correlation	$\rho = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$	Measures the linear relationship between two quantitative variables. Sensitive to outliers. $\rho \in [-1, 1]$.
Spearman's rho	$\rho_s = 1 - \frac{6\sum_{i=1}^{n} d_i^2}{n(n^2-1)}$	Captures monotonic relationships (not necessarily linear). Based on ranks rather than actual values.
Kendall's tau	$\tau = \frac{C - D}{\frac{1}{2}n(n-1)}$	Based on concordant (C) and discordant (D) pairs. More robust to outliers than Spearman's rho.
Upper Tail Dependency	$\lambda_U = \lim_{u \to 1^-} \mathbb{P}\big(Y > F_Y^{-1}(u) \mid X > F_X^{-1}(u)\big)$	Measures the probability that both X and Y take large values simultaneously (dependence in the upper tail).
Lower Tail Dependency	$\lambda_L = \lim_{u \to 0^+} \mathbb{P}\big(Y \le F_Y^{-1}(u) \mid X \le F_X^{-1}(u)\big)$	Measures the probability of co-occurrence of low extreme values (dependence in the lower tail).

Table 1: Summary of correlation and tail dependency coefficients.

2.2.2. Dependency modeling tools between random variables

To model the coexistence of components in heterogeneous geological contexts such as those encountered in the province of Sissili in Burkina Faso, where recharge dynamics and anthropogenic activities influence groundwater quality, we used linear and non-linear correlations (see Table 1). These tools allow to better appreciate the dependency between these parameters.

2.3. Copulas approach for modeling water components

Multivariate copulas are essential for robust modeling of aquatic systems in the face of uncertainty and complexity of interactions between variables, combining statistical precision and relevant physical interpretation.

We present three copulas namely: the Hüsler–Reiss copula, the Student copula and the Frank copula (see Figure 2). Indeed, the Hüsler–Reiss copula is useful for modeling asymptotic dependence in tails (extremes): strong dependency in large values (upper tails). It was applied by Hüsler and Reiss(1989) in the context of bivariate extreme values. It's defined for two variables U and V uniform on $[0,\ 1]$ by:

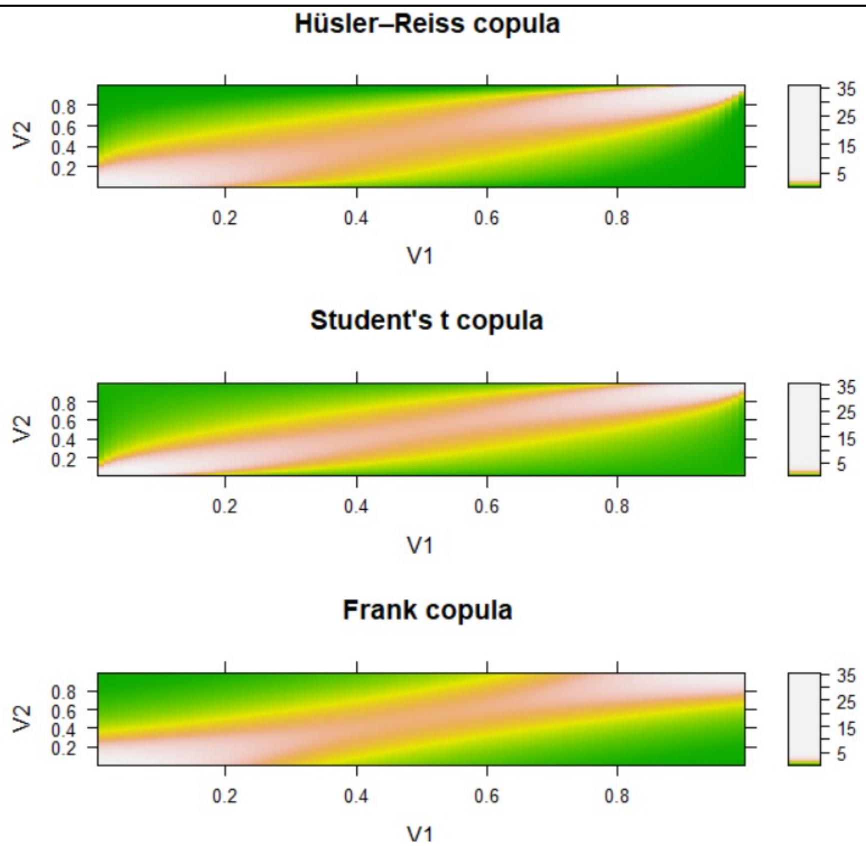


Fig. 2: Simulation of the densities of the three copulas

$$C_{\lambda}^{HR}(u,v) = \exp\left(-\left[\frac{1}{u}\Phi\left(\frac{\lambda}{2}+\frac{\log(v/u)}{\lambda}\right)+\frac{1}{v}\Phi\left(\frac{\lambda}{2}+\frac{\log(u/v)}{\lambda}\right)\right]\right)$$

where Φ is the distribution function of the standard normal and $\lambda > 0$ is a dependency parameter.

Student's copula (t-copule) is robust in the presence of noisy data or strong nonlinear dependencies. The t-copule is commonly used in studies of pollutants such as potassium and ammonium Demarta and McNeil (2005). It models the dependency in the two tails (lower and upper), i.e the probability that extreme values appear simultaneously. This copule is defined as follow:

$$C_{\nu,\Sigma}^{t}(u,v) = t_{\nu,\Sigma}(t_{\nu}^{-1}(u), t_{\nu}^{-1}(v))$$

Variable	Minimum	Maximum	Mean	Median	Standard deviation
Potassium	0.6	15.09	2.488	1.7	2.54
Iron	0	2.9	0.2244	0.02	0.51
Ammonium	0.01	2.21	0.083	0.02	0.2839

Table 2: Statistics of the variables

where t_ν^{-1} is the quantile function of Student's t law at nu degrees of freedom, and $t_{\nu,\Sigma}$ is the joint distribution function of the bivariate law.

The Frank copula belongs to the family of archimedean copulas and is effective for modeling moderate and continuous relationships between parameters (e.g.: potassium and sodium). It's often used in hydrology and geochemistry to model moderate and symetrical dependency, suitable for centered relations, without asymmetry (Nelsen (2006)).

$$C_\theta^{Frank}(u,v) = -\frac{1}{\theta}\log\left(1+\frac{(e^{-\theta u}-1)(e^{-\theta v}-1)}{e^{-\theta}-1}\right), \quad \theta \neq 0$$

For the rest, we use these three copulas to model the physico-chemical components of water.

3. Results and discussion

3.1. Descriptive analysis of the database

The database used for this analysis contains 73 observations and 15 random variables. The objective of our analysis is to model the distribution of the three variables. The statistic descriptives of the variables are summarized in table 2.
The variable potassium has a minimum value of 0.6 and a maximum value of 15.09. Its mean value is 2.488 and its median is 1.7. The median is different from the average, indicating that the distribution of potassium is not symmetrical. The iron has a minimum value of 0 and a maximum value of 2.9. Its mean is 0.2244 and its median is 0.02. According to the above, its distribution is not normal. The minimum value of ammonium is 0.01 with a maximum of 2.21. The average concentration of this variable is 0.0083. About 50% of the samples collected for this variable have a concentration less than or equal to 0.02 with a standard deviation of 0.2839. In light of this information, we can deduce that the distribution of this variable is not normal. In the following, we will perform the statistical tests to determine the distributions of these variables.

3.2. Marginal distributions of variables

Looking at the histograms obtained (see Figure 3), we can say that the three variables are not normally distributed. To confirm this information, we used statistical

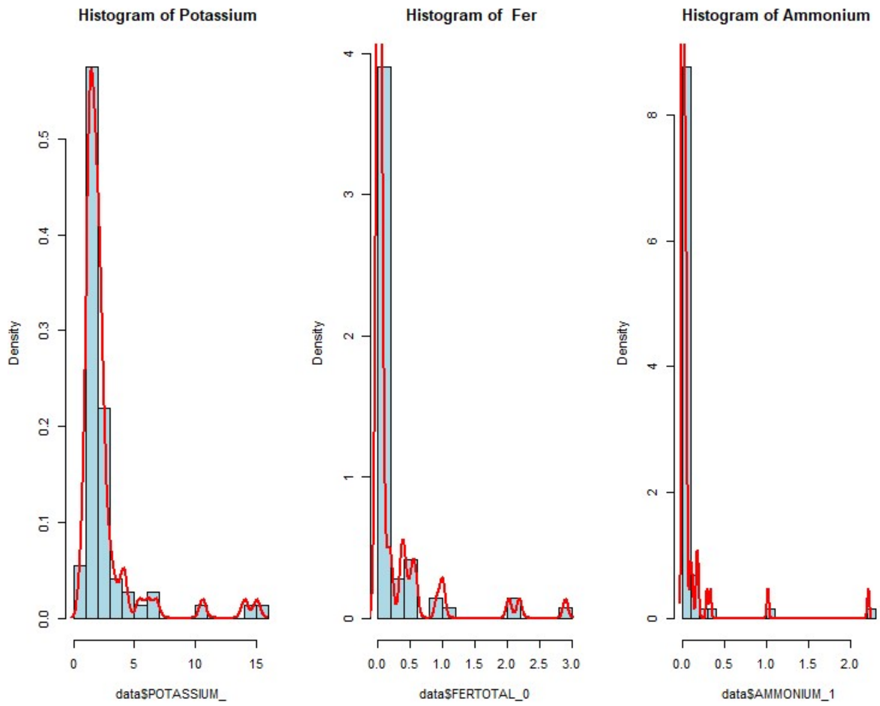


Fig. 3: Histogram of tree variables

tests such as the Shapiro-Wilk test, Kolmogorov-Smirnov test, and t-test (see Table 3).

The result of the Chi-square test show that for H_0 the random variable follows the chosen distribution, whereas for the alternate hypothesis H_1 the variable does not follow the chosen distribution. The table[3] summarizes the different tests. Thus, based on the P-value of the Shapiro test, it appears that the three variables do not follow a normal distribution. Furthermore, the P-value of the Kolmogorov–Smirnov test shows that the three variables do not follow neither a normal distribution, nor an exponential distribution. Finally, the P-value of the t-test indicates that the three variables do not follow the student distribution. In the rest of our analysis, we will study the dependence of these variables.

3.3. Study of the dependence between variables

The results of the linear dependence between these three variables indicate that the variable Fe^{2+} is strongly positively correlated with the variable NH_4^+ (see Table [4]). This high positive correlation suggests that the two elements are influenced by similar factors, such as intensive agricultural practices or geological conditions favoring their joint presence. On the other hand, an increase or a decrease in K^+ has no predictable effect on Fe^{2+}.

Test	Variable	Statistic value	P-value	df	Decision
Shapiro–Wilk test	K^+	0.529	6.144×10^{-14}	–	H_0 rejected
	Fe^{2+}	0.4642	7.09×10^{-15}	–	H_0 rejected
	NH_4^+	0.260	$< 2.2 \times 10^{-16}$	–	H_0 rejected
Kolmogorov–Smirnov test	K^+	0.3023	3.195×10^{-6}	–	H_0 rejected
	Fe^{2+}	0.3450	5.697×10^{-7}	–	H_0 rejected
	NH_4^+	0.3972	1.975×10^{-10}	–	H_0 rejected
Student t-test	K^+	8.3675	3.159×10^{-12}	72	H_0 rejected
	Fe^{2+}	3.7587	3.44×10^{-4}	72	H_0 rejected
	NH_4^+	2.5267	0.0137	72	H_0 rejected

Table 3: Summary of the different normality and mean comparison tests for the three physicochemical components.

	τ	ρ_s	ρ
K^+ vs Fe^{2+}	-0.137	-0.17	-0.092
NH_4^+ vs K^+	0.096	0.1199	-0.086
NH_4^+ vs Fe^{2+}	0.411	0.4815	0.73

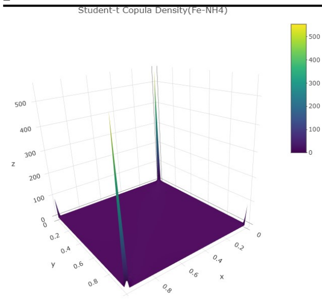
Table 4: Table summarizing the different linear and non-linear correlations

Similarly, NH_4^+ and K^+ do not appear to interact significantly. This could be attributed to distinct factors influencing their distribution in soils. The coefficients of positive ranks (NH_4^+ vs K^+) and (NH_4^+ vs Fe^{2+}) suggest a weak increasing relationship. But, the slightly negative Pearson correlations (NH_4^+ vs K^+) and (K^+ vs Fe^{2+}) indicate that the relationships between these components are not linear (see Table [4]). Hence the interest in using copules to better model these complex dependencies.

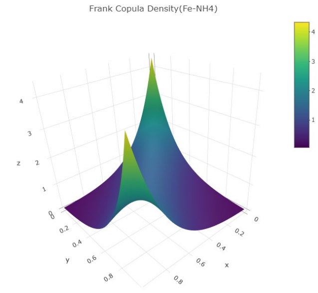
3.4. Analyzing the impact of extremes on copulas.

We used three families of copulas: Student, Frank and Hüsler–Reiss to model the dependence of the physical-scale parameters of water (K^+, Fe^{2+} and NH_4^+). The table [5] presents the upper tail dependency coefficients λ_U and lower λ_L estimated for these three families of copulas. In addition, these coefficients measure the probability that two variables simultaneously adopt extreme values (high or low). A high value of λ_U or λ_L shows a marked dependence in the tails of the distribution, while a zero value indicates extreme independence.

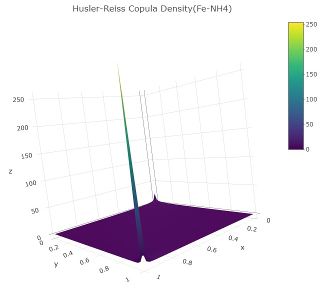
For the Student model, the lower and upper tail parameters show perfect symmetry, stipulating that this copula captures a balanced dependency between the extreme low and high values (see Figure 4 a),d) and g)). The pairs $(NH_4^+,\ K^+)$ and $(NH_4^+,\ Fe^{2+})$ have values 0.25 and 0.58, respectively, indicating a moderate dependency in the extremes. In contrast, the pair $(K^+,\ Fe^{2+})$ shows an index close to zero (5.9×10^{-22}), revealing near independence. So, the copula of Student turns out



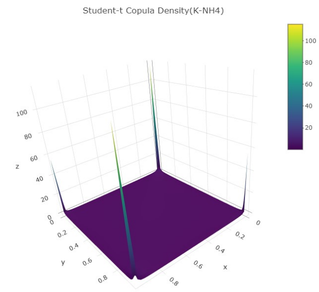
(a) Student-t Copula Density(Fe-NH4)



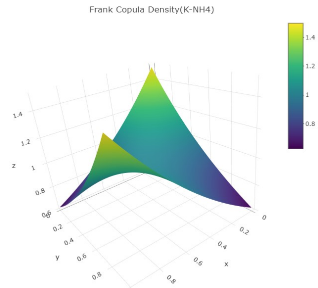
(b) Frank Copula Density(Fe-NH4)



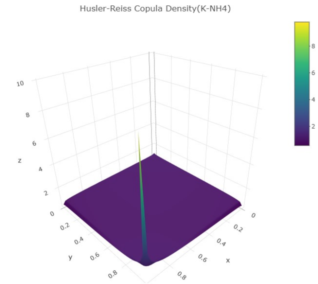
(c) Husler-Reiss Copula Density(Fe-NH4)



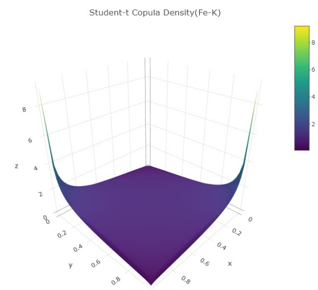
(d) Student-t Copula Density(K-NH4)



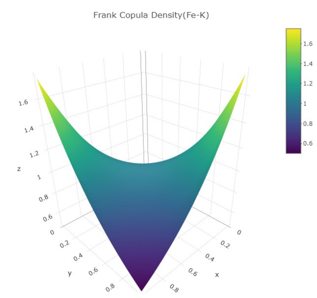
(e) Frank Copula Density(K-NH4)



(f) Husler-Reiss Copula Density(K-NH4)



(g) Student-t Copula Density(Fe-K)



(h) Frank Copula Density(Fe-K)

Fig. 4: Comparing the estimated densities of the three families of copulas and the various ion pairs.

to be appropriate to describe symmetrical extreme dependencies, notably between NH_4^+ and the other ions.
The Frank copula, on the other hand, models the central dependency. In our case, only the pair $(NH_4^+,\ K^+)$ has a value of $\lambda = 0.59$, reflecting a significant dependence in the central part of the distribution (see Figure 4 b),e) and h)). The

	Student			Franck			Hüsler-Reiss		
	λ_U	λ_L	AIC	λ_U	λ_L	AIC	λ_U	λ_L	AIC
K^+ vs Fe^{2+}	5.93 $\times 10^{-22}$	5.93 $\times 10^{-22}$	0.73	NA	NA	NA	-	-	-
NH_4^+ vs K^+	0.25	0.25	-3.23	0.59	0.59	NA	0.82	0	1.97
NH_4^+ vs Fe^{2+}	0.58	0.58	-46.99	NA	NA	NA	0.44	0	-29.9

Table 5: Tail dependency coefficients and AIC value for each pair of ions and each copula.

other pairs display unavailable values (NA), suggesting a statistically weak fit. So this copula is suitable for moderate dependencies without marked extremes, but does not capture rare or extreme phenomena properly.

The Hüsler–Reiss copula reveals a markedly asymmetric dependency, with a total absence of lower tail dependency ($\lambda_L = 0$) and a positive upper tail dependency ($\lambda_U > 0$) (see Figure 4 c) and f)). The pair $(NH_4^+, \ K^+)$ shows a strong upper dependence ($\lambda_U = 0.82$), while $(NH_4^+, \ Fe^{2+})$ shows a moderate dependence ($\lambda_U = 0.44$). These values indicate that when the concentrations of these ions are simultaneously high, their behavior is strongly correlated. So, the Hüsler–Reiss copula is particularly suitable for modeling higher extreme dependencies.

Given the different AIC values, we can conclude that the Student copula well models the extreme behavior of the three pairs of variables because it has the smallest value per pair.

4. Discussion

The application of copulas has proved to be particularly a relevant tool for the analysis of stochastic dependence between the physico-chemical parameters of groundwater in the province of Sissili (see Gianfausto et al. (2007), Sklar (1959)). See also a modern proof of Sklar's theorem in Lo (2018). Unlike classical methods based on linear correlation, copulas allow to model complex, non-linear and asymmetric relationships between variables. Therefore, this approach offers a more detailed understanding of the dependency structure between chemical components, particularly in situations where extreme values play a major role in groundwater dynamics.

The results obtained highlight the complementarity of the different families of copulas used. The Student copula, characterized by its ability to capture symetrical extreme dependencies, allowed to highlight the joint behaviors of ions in high or low concentration situations. This symetry indicates that extreme phenomena tend to occur simultaneously for certain ion pairs, thus reflecting common geochemical or hydrogeological processes. The Frank copula, more suitable for modeling central dependencies (see Nelsen (2006)) , highlighted moderate and regular correlations between variables. This type of dependency is typical of underlying relationships, often related to the general geological composition of the aquifer environment or to diffuse sources of natural origin. It suggests a continuous but balanced interaction between certain parameters, without the dominance of extreme events. Regarding the Hüsler-Reiss copula, it revealed the presence of asymmetric dependencies in the upper tails. This unilateral behavior often reflects the effect of localized processes such as soil leaching, occasional anthropogenic inputs or the presence of preferential infiltration zones.

From a physico-chemical point of view, the significant association between NH_4^+ and K^+ observed for high concentrations suggests the existence of similar sources or transport mechanisms. These two ions can be derived from the decomposition of organic matter, the use of nitrogen and potassium fertilizers, or even from leaching phenomena in areas with high agricultural activity. Their correlation in extreme values reflects a common dynamic related to human activities or ion exchanges within the soil and groundwater. In contrast, the low dependency between K^+ and Fe^{2+} indicates distinct origins or limited interactions between these elements. Iron, often resulting from the reductive dissolution of ferrous minerals or oxidation-reduction processes, seems to follow a different geochemical logic, less influenced by surface contributions or anthropogenic activities.

These results are of major practical interest. By identifying ion couples with high dependency, water resource managers can better target sensitive areas and anticipate pollution risks (see Maity, (2022)) . Moreover, the detailed knowledge of the dependency structure helps to improve predictive models of water quality, particularly in a context of climate change and increasing anthropogenic pressure.

5. Conclusion and perspectives

This study demonstrated that copulas constitute a powerful methodological framework for the multidimensional analysis of hydrogeochemical parameters. It appears that NH_4^+ and K^+ have a significant extreme dependency. This states that these ions have similar sources or transport mechanisms. In contrast, the low dependency between K^+ and Fe^{2+} indicates distinct origins or limited interactions between these elements. The current study can be extended to other regions and other combinations of variables to improve the management of sustainable water resources.

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