






Joint stochastic simulation of petrophysical properties with elastic attributes based on parametric copula models

Daniel Vázquez-Ramírez^{1*}, Van Huong Le², Martín A. Díaz-Viera³, Raúl del Valle-García⁴, Arturo Erdely⁵

Resumen

El método de co-simulación estocástica espacial, basado en cópulas, es un método general que permite simular variables con cualquier tipo de dependencia y funciones de distribución de probabilidad. Esta flexibilidad proviene del uso de un modelo de cópula para la representación de la función de distribución de probabilidad conjunta. El método se ha implementado principalmente a través de un enfoque no paramétrico utilizando cópulas de Bernstein y se ha aplicado con éxito para la simulación de propiedades petrofísicas usando atributos sísmicos elásticos como variables secundarias. En el presente trabajo este método se implementa mediante otros dos enfoques: paramétrico y semi-paramétrico. Específicamente, para el enfoque paramétrico se usa la familia de cópulas Arquimedeanas. Primero, el enfoque paramétrico se valida con un caso publicado y luego se realiza una comparación de los tres enfoques en términos de precisión y rendimiento. Los resultados mostraron que el enfoque paramétrico es el que peor reproduce las estadísticas de los datos y presenta mayor incertidumbre con un menor costo computacional, mientras que el enfoque no-paramétrico resultó el que mejor reproduce la dependencia de los datos a un alto costo computacional. El enfoque semi-paramétrico reduce un 10% el costo computacional respecto al no-paramétrico, pero se degrada significativamente su precisión.

Palabras Clave: co-simulación, cópulas, Bernstein, Arquimedeanas, propiedades petrofísicas, atributos sísmicos elásticos.

Abstract

The spatial stochastic co-simulation method based on copulas is a general method that allows simulating variables with any type of dependency and probability distribution functions. This flexibility comes from the use of a copula model for the representation of the joint probability distribution function. The method has been mainly implemented through a non-parametric approach using Bernstein copulas and has been successfully applied for the simulation of petrophysical properties using elastic seismic attributes as secondary variables. In the present work this method is implemented through two other approaches: parametric and semi-parametric. Specifically, for the parametric approach the family of Archimedean copulas is used. First, the parametric approach is validated against a published case, and then a comparison of the three approaches in terms of accuracy and performance is made. The results showed that the parametric approach is the one that reproduces the data statistics worse and presents greater uncertainty with a lower computational cost, while the non-parametric approach was the one that best reproduces the dependence of the data at a high computational cost. The semi-parametric approach reduces the computational cost by 10% compared to the non-parametric approach, but its accuracy is significantly degraded.

Keywords: co-simulation, copulas, Bernstein, Archimedean, petrophysical properties, elastic seismic attributes.

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* Corresponding author: Daniel Vázquez Ramírez

¹ Posgrado de Ciencias de la Tierra, Universidad Nacional Autónoma de México, Circuito de Posgrado S/N, Coyoacán Ciudad Universitaria, 04510 Ciudad de México, Mexico, daniel.geofisico89@comunidad.unam.mx ORCID: 0000-0002-6326-9141

² Department of Plant & Soil Sciences, University of Delaware, Newark, Delaware 19716, United States, levanhuong15011989@gmail.com ORCID: 0000-0002-3700-9987

³ Instituto Mexicano del Petróleo, Eje Central Lázaro Cárdenas No. 152, Col. San Bartolo Atepehuacan, México D.F. 07730, Mexico, mdiazv@imp.mx ORCID: 0000-0001-5811-6186

⁴ Independent consultant, Ciudad de México, México. raul.vontal@gmail.com ORCID: 0000-0001-8964-714X

⁵ Universidad Nacional Autónoma de México, FES Acatlán, Avenida Alcanfores y San Juan Totoltepec S/N, Santa Cruz Acatlán, 53150 Naucalpan de Juárez, Mexico, aerdely@acatlan.unam.mx ORCID: 0000-0003-1653-8342

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1. Introduction

One of the most common problems of reservoir geological-petrophysical modeling workflow (Cosentino, 2001) consists in predicting petrophysical properties considering the dependency relationships with the seismic attributes. For this purpose, different methods and approaches have been used, ranging from empirical relationships (Diaz-Viera *et al.*, 2006), regression methods, neural networks (Parra *et al.*, 2014), (Iturraran-Viveros & Parra, 2014) to spatial stochastic models. The latter being more flexible since they better reproduce the statistical and spatial behavior of petrophysical properties (Pyrzcz & Deutsch, 2014).

In the last decade, various spatial stochastic simulation methods, also known as geostatistical simulation methods, have been developed. Among the most used are: Monte Carlo simulation (Bosch *et al.*, 2007), (Oh & Kwon, 2001) and (Grana, 2014), sequential indicator simulation (Caers *et al.*, 2000), direct simulation (Azevedo & Soares, 2017) or sequential Gaussian simulation whose methods are widely developed in the works of (Chilès & Delfiner, 1999), (Dubrule *et al.*, 2003), (Bortoli *et al.*, 1993) and (Pyrzcz & Deutsch, 2014).

The disadvantage of most of these methods is that they assume that the data follow Gaussian distributions and that the dependency relationships between them are linear, which makes their application to real problems very limited. In the best case, it is forced to be applied by data transformation, which produces biased results when they are back transformed.

The copula-based spatial stochastic co-simulation method was proposed by (Diaz-Viera *et al.*, 2017) as an alternative to the aforementioned simulation methods. This method can be basically divided into two steps. Firstly, a dependence model between the primary and secondary variables is established by estimating and modeling the joint cumulative probability distribution function (CPDF) using a copula. The CPDF model is used in conjunction with a variogram (spatial correlation) model to simulate the primary variable using the second one as a conditioning variable. This last step can be done in a global optimization framework using one method, such as simulated annealing, but other methods, such as genetic algorithms, can also be applied.

Recently, the copula-based simulation method was successfully applied for the prediction of petrophysical properties using seismic attributes as a secondary variable in (Le, 2021), (Le *et al.*, 2020), (M. Díaz-Viera *et al.*, 2018), (Vázquez, 2018). But in these works, the method was implemented using a non-parametric approach with Bernstein copulas. The non-parametric approach has the disadvantage that it requires a high computational cost, especially when calculating the joint probability distribution function estimated with the Bernstein copula.

In this work it is proposed to use a parametric copula model, through the implementation of Archimedean copula family. This approach is expected to reduce the computational cost. The paper aim is to compare the parametric, semi-parametric and non-parametric approaches in terms of precision and performance. The comparative study is carried out through the application to two case studies in a marine reservoir in the Gulf of Mexico, where the total porosity and the density are simulated by means of the acoustic impedance and the P-wave velocity as secondary variables, respectively.

The paper has the following structure. First, the copula-based spatial stochastic co-simulation method is briefly described, distinguishing between non-parametric, semi-parametric and parametric approaches. In particular, the members of Archimedean copula family are defined. An outline of the method application workflow is provided. Subsequently, the validation of the method is carried out by applying it to a previously published case study and the three approaches are compared. Finally, the parametric approach is applied to a new case study and the conclusions are given. In appendices, the definition of copula and its basic properties, as well as the Bernstein copula simulation method description are shown.

2. Copula-based spatial stochastic co-simulation method

Copula-based spatial stochastic co-simulation had its origins in the works of (Diaz-Viera & Casar-González, 2005), (Erdeley *et al.*, 2012) and (Hernandez-Maldonado *et al.*, 2014). The method has the advantages of not requiring linear dependence or a specific type of distribution and has been successfully applied to simulate petrophysical properties using seismic attributes as a secondary variable. The method has been implemented mainly by a non-parametric approach using Bernstein copulas, where the copula is estimated using the empirical copula and the variables are interpolated using Bernstein polynomial function (Appendix 10.2).

However, there are two more approaches that have not been sufficiently explored and used in the dependency model estimation: semi-parametric and parametric approaches. The semi-parametric approach estimates margins non-parametrically using empirical distribution functions and parametric copula is estimated (Jaworski *et al.*, 2010) or the margins are estimated using parametric functions and the copula is estimated non-parametrically. The parametric approach uses different parametric distribution functions that are selected and best fit the petrophysical property or seismic attribute and then couple them within the parametric copula.

The difference between the non-parametric, parametric and semi-parametric approaches lies in the estimation procedure. In the non-parametric approach, the behavior of the joint sampling distribution function is adapted by means of a polynomial approximation, reducing the estimation variance.

In the parametric approach, the data samples are fitted to copula models and parametric probability distribution functions. While the semi-parametric approach is a combination of the two previous approaches, and therefore, there are two options: parametric copulas with non-parametric marginals, or non-parametric copulas with parametric marginals. Therefore, if the joint distribution function that allows relating two or more petrophysical properties and seismic attributes in terms of their dependence is generated, it is possible to obtain more consistent simulations with their data sample statistics without having to assume a specific distribution or dependency. In the following subsections the parametric joint distribution functions are analyzed, especially the Archimedean copula family.

2.1 Parametric copula approach

The parametric copulas are a classification of copula whose advantage is to use the parameters of the joint function to control the dependence. There are three great parametric copula families: elliptical, Archimedean and extreme values (Joe, 2014).

The elliptical copulas are recommended when the dependence model is derived from elliptical distributions and the symmetry should be elliptical respect to the diagonal (Shemyakin & Kniazev, 2017). Gaussian and t -copula are examples of elliptical copulas.

The extreme value copulas are based on random vectors distributed according to multivariate extreme value distributions. Galambos, Hüstle-Reis and Tawn are examples of extreme values copulas (Hofert *et al.*, 2019).

Archimedean copulas are the most used copulas because they are easier for implementation, they just need one parameter θ to control the dependence and the differentiation and integration to obtain the generator and inverse is simple (Shemyakin & Kniazev, 2017). Frank, Gumbel and Clayton are examples of Archimedean copulas.

2.1.1 Archimedean copulas

After describing the basic properties of copulas (Appendix 10.1), it is necessary to study a class of copulas that will be useful for the development of Copula-based spatial stochastic co-simulation: Archimedean copulas. These copulas are very useful alternatives because they are easy to build and there is a wide variety of families of copulas with interesting properties (Nelsen, 2006).

$$C(u,v)=\varphi^{[-1]}(\varphi(u)+\varphi(v)) \quad (\text{Eq. 1})$$

The (Eq. 1) is the Archimedean copula. The φ function is called copula generator. Consider that if $\varphi(0)=\infty$ then φ is strictly generator, in that case $\varphi^{[-1]}=\varphi^{-1}$ and $C(u,v)=\varphi^{[-1]}(\varphi(u)+\varphi(v))$ and is said to be strictly an Archimedean cop-

ula. Another important property is the Archimedean density copula (Eq. 2), this can be expressed through the generator and its derivatives as (Shemyakin & Kniazev, 2017):

$$c(u,v)=\frac{\delta^2 C(u,v)}{\delta u \delta v}=\frac{\varphi''(C(u,v))\varphi'(u)\varphi'(v)}{(\varphi'(C(u,v)))^3} \quad (\text{Eq. 2})$$

2.1.1.1 Clayton copula

This family of copulas has been used when the dependence of the tails is strong on the left and weak on the right. Generally, Clayton copula does not accept negative dependencies, the copula parameter θ is restricted into the region $(0,\infty)$, if the value of θ is zero, then the marginals become independent (Trivedi & Zimmer, 2007). Some members of Clayton copula can be implemented in models with negative dependencies; however, its use is not suggested under those conditions because the copula is not strict and it can violate the region restriction; reflecting the shape of the countermonotocity copula as the value of θ approaches -1, which itself is not an Archimedean copula. It cannot properly capture the negative dependency nor estimate the value of the parameter θ special conditions are needed to guarantee that the copula is strict (Cooray, 2018). The Clayton copula that can be evaluated in negative dependencies is defined as:

$$C_{\theta}(u,v)=\left\{ \left(u^{-\theta}+v^{-\theta}-1 \right)^{-\frac{1}{\theta}}, 0 \right\} \quad \theta \in [-1;0] \cup (0,\infty) \quad (\text{Eq. 3})$$

Whose generator is:

$$\varphi(t)=\frac{1}{\theta}t(t^{-\theta}-1) \quad (\text{Eq. 4})$$

2.1.1.2 Frank copula

This family of copulas is well known because it can be used in models with positive and negative dependencies between their marginals, it is a symmetric copula on both tails and includes both Frechet limits throughout the region $(-\infty,\infty)$. The disadvantage of Frank's copula is that the dependency tends to be weak in the tails and strong in the central part of the marginals; therefore, it is recommended to use this type of copula if the dependency model exhibits tails with low dependency (Trivedi & Zimmer, 2007). The Frank copula is defined as:

$$C_{\theta}(u,v)=\frac{1}{\theta} \ln \left(1 + \frac{(e^{-\theta u}-1)(e^{-\theta v}-1)}{e^{-\theta}-1} \right) \quad \theta \neq 0 \quad (\text{Eq. 5})$$

Whose generator is:

$$\varphi(t) = -\ln \frac{e^{-\theta t} - 1}{e^{-\theta} - 1} \quad (\text{Eq. 6})$$

2.1.1.3 Gumbel-Hougaard copula

This family of copulas, like Clayton's copula, does not allow negative dependencies. The parameter θ is restricted to the interval $[1, \infty)$, if the value is 1 the copula is considered independent, if the value of θ is ∞ it is a countermonotocity copula or upper Frechet limit. Gumbel copula exhibits strong dependence on the tails located on the right and weak on left tails, therefore, it is recommended when the highest values of the sample have strong dependence, while the low values have less dependency (Trivedi & Zimmer, 2007). The Gumbel-Hougaard copula is defined as:

$$C_{\theta}(u, v) = \exp \left(- \left(\left(-\ln(u)^{\theta} \right) + \left(-\ln(v)^{\theta} \right) \right)^{\frac{1}{\theta}} \right) \quad \theta \geq 1 \quad (\text{Eq. 7})$$

Whose generator is:

$$\varphi(t) = \left(-\ln(t) \right)^{\theta} \quad (\text{Eq. 8})$$

2.1.1.4 Joe copula

This copula family is based on Sibuya distribution LT (Joe, 2014). It only works with positive dependence and the goodness of fit is reasonably well when it is applied to small samples with moderate dependence (Hofert *et al.*, 2019). The Joe copula is:

$$C_{\theta}(u, v) = 1 - \left((1-u)^{\theta} + (1-v)^{\theta} - (1-u)(1-v)^{\theta} \right)^{\frac{1}{\theta}} \quad \theta \in [1 - \infty] \quad (\text{Eq. 9})$$

And the generator is:

$$\varphi(t) = -\ln \left(1 - (1-t)^{\theta} \right) \quad (\text{Eq. 10})$$

3. Method application workflow

The workflow follows the next steps:

1. Exploratory data analysis: this step studies the variable using statistical properties, histograms and scatter plot.
2. Variographic analysis: this step consists in estimating and modeling a spatial correlation function, as the variogram, from a random function sample (M. A. Díaz-Viera, 2002).
3. Marginal estimation and model fitting: for this step the variable is fitting using parametric probability functions, the best option is selected considering the

result of log-likelihood, Akaike information criteria (AIC) and Bayesian information criteria (BIC). In case of (AIC) and (BIC) criteria, the parametric function with the lowest value will be the best fit, while the log-likelihood with the highest criterion value is the best fit. However, it is advisable to use graphical tools to assess whether the fit is adequate, therefore, the fit criteria must be confirmed using the histogram, the cumulative histogram and the cumulative distribution function.

4. Parametric copula estimation and model fitting: This step uses the results obtained in step 3 and the bivariate samples to estimate and select the best Archimedean copula model. The estimation is developed using maximum likelihood (MLE), Kendall inversion τ (ITau) and Spearman inversion ρ (IRho) (Hofert *et al.*, 2019).
5. Well-log simulation uses the joint probability distribution function using simulated annealing.
6. Compare the statistics and the spatial distribution between the variables (step 1) and the simulated variables obtained in step 5.

This algorithm is implemented using the RGEOSTAD tools (M. A. Díaz-Viera *et al.*, 2021) and GSLIB (Deutsch & Journel, 1998).

4. Method validation

To implement the stochastic simulation using parametric, semi-parametric and non-parametric copulas, the Lakach-1 geophysical well logs are taken. This well crosses the Miocene turbiditic system. This system is important due to unassociated fields discovered in this unit; the unit is divided into three sections: Lower Miocene, Middle Miocene and Upper Miocene. The age of interest of this implementation is the Lower Miocene, in this zone the flow goes from southwest to northeast with some dominant channel systems. The rocks are medium-grained sandstones; evidence of volcanic material, feldspars, quartz and some metamorphic fragments were also found. The rock is poorly consolidated and mineralogically immature; the porosity ranges from 12 to 28% (Arreguin-Lopez *et al.*, 2011). The interval to be evaluated is from 3035 to 3404.5 meters with a sampling interval of 0.1 meters.

4.1 Exploratory data analysis

Analyzing the geophysical well logs, the best option is the bivariate case (I_p, ϕ_i). The Figure 1 shows the well log plots.

The statistics are in Table 1, both well-logs have 3696 samples. The total porosity well-log (ϕ_i) has difference between the mean and the median is -0.0075, which is very low. Regarding the box plot (Figure 2, green histogram), most of the outliers are to the left of the graph. Meanwhile the impedance acoustic well log (I_p), the difference between

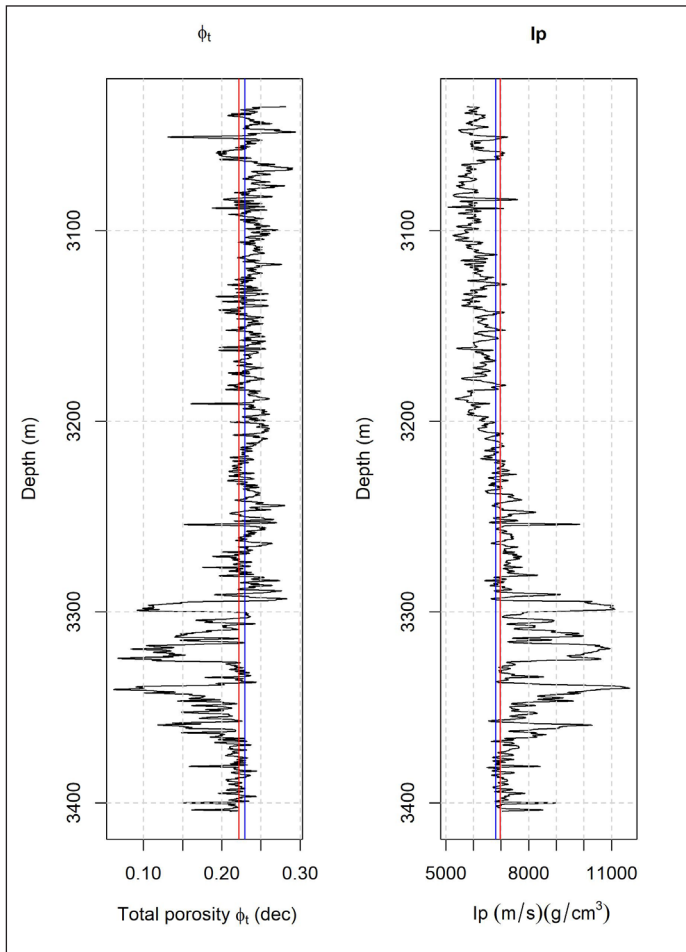


Figure 1. ϕ_t (left) and I_p (right) geophysical well logs.

the mean and the median is 158.7265, it indicates that it has positive skewness, which is possibly caused by the large number of outliers located to the right of the graph (Figure 2, blue histogram).

Table 1. Basic statistics of total porosity (ϕ_t) and acoustic impedance (I_p).

Statistics	ϕ_t	I_p
Samples	3696	3696
Minimum	0.0620	5086.0072
1 st quartile	0.2147	6157.0051
Median	0.2295	6809.5573
Mean	0.2219	6968.2838
3 rd quartile	0.2414	7321.6169
Maximum	0.2939	11661.4642
Range	0.2319	6575.4569
Interquartile range	0.0267	1164.6118
Variance	0.0011	1310302.94
Standard deviation	0.0337	1144.6846
Skewness	-1.8109	1.5616
Kurtosis	6.9969	5.7657

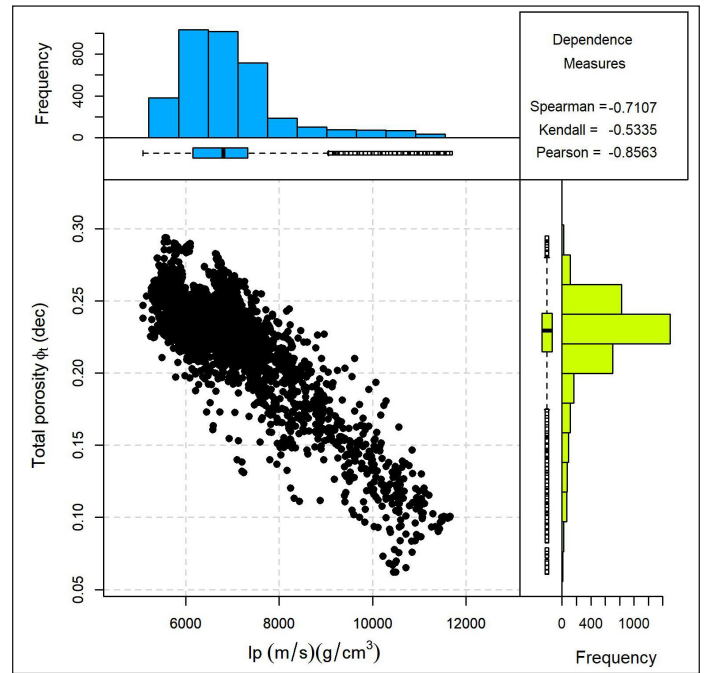


Figure 2. (I_p , ϕ_t) scatter plot and dependence measures.

The dependency measures and the scatter plot of (I_p , ϕ_t) is in Figure 2, this shows good dependence. The Spearman measure is -0.7107, Kendall -0.5335 and Pearson -0.8563

4.2 Variographic analysis

In this step the variogram of ϕ_t is estimated using three models: exponential, Gaussian, and spherical. The best model selected is spherical with sill 0.0011, range 16 meters and nugget 0 (Figure 3). This model will be used to obtain the simulations using the simulated annealing method.

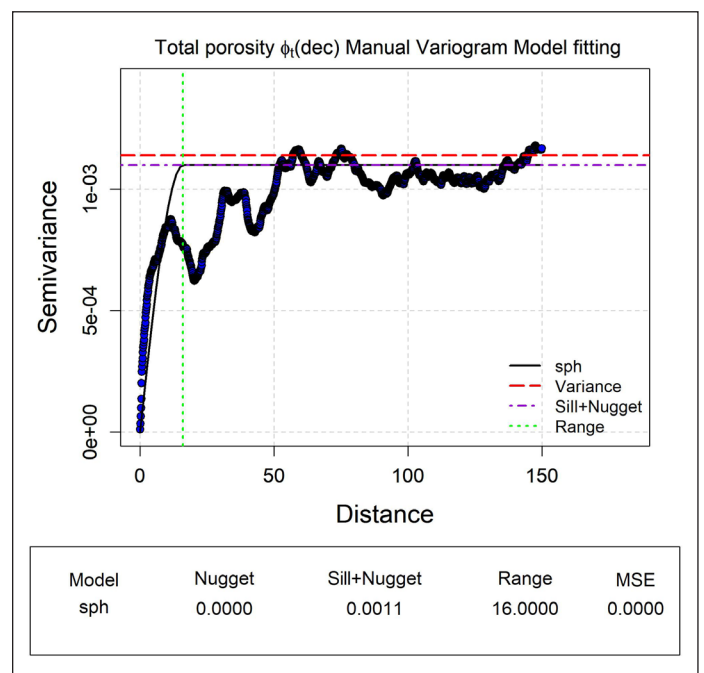


Figure 3. ϕ_t variogram model

4.3 Parametric modeling of the marginal CDF

The (I_p, ϕ_i) samples are fitted in parametric probability distribution function that allows to represent it. The Akaike information criteria (AIC), Bayesian information criteria (BIC) and log-likelihood are used to select the best option.

4.3.1 Total porosity CDF modeling

For this variable, the gamma, beta, normal, logistic, lognormal and Weibull functions were tested. The goodness of fit results for ϕ_i is in Table 2 which shows the best option is Weibull function, followed by the normal function. As can see in the Figure 4, the functions cannot cover the entire histogram, only a large part of the central area, the lower values

located to the left of the histogram are omitted Figure 4(A). This is confirmed in the cumulative histogram Figure 4(B), so it is possible that the results obtained in the simulation give greater importance to the largest values and not so much to the minimum values reported during the univariate analysis.

4.3.2 Acoustic impedance CDF modeling

This estimation uses the following functions: gamma, normal, logistic, lognormal and Weibull, the goodness of fit results for I_p is in Table 3, the best function for I_p is lognormal, gamma function is very close to lognormal and maybe that function could be a good option, however, the lognormal function is taken.

Table 2. Goodness of fit results for ϕ_i

Function	Parameter	Error	Parameter	Error	Likelihood	AIC	BIC
Weibull	$\alpha = 5.164$	0.129	$\lambda = 0.220$	0.0010	1791.958	-3579.91	-3569.90
Normal	$\mu = 0.205$	0.001	$\sigma = 0.040$	0.0010	1747.720	-3491.45	-3481.43
Logistics	$\mu = 0.210$	0.001	$\beta = 0.028$	0.0002	1735.720	-3467.45	-3457.44
Beta	$\alpha = 11.662$	0.489	$\beta = 45.080$	1.9240	1685.870	-3367.75	-3357.74
Gamma	$k = 13.994$	0.588	$\beta = 67.980$	2.9130	1660.400	-3316.80	-3306.79
Lognormal	$Log\mu = -1.610$	0.008	$Log\sigma = 0.280$	0.0060	1598.540	-3193.09	-3183.08

Table 3. Goodness of fit results for I_p

Function	Parameter	Error	Parameter	Error	Likelihood	AIC	BIC
Lognormal	$Log\mu = 8.905$	0.005	$Log\sigma = 0.190$	0.004	-9562.235	19128.47	19138.48
Gamma	$k = 26.558$	0.411	$\beta = 0.003$	$5.03e-5$	-9586.137	19176.27	19186.28
Normal	$\mu = 7513.696$	45.850	$\sigma = 1521.670$	32.406	-9647.394	19298.79	19308.80
Logistics	$\mu = 7317.655$	45.170	$\beta = 858.563$	21.770	-9653.742	19311.48	19321.50
Weibull	$\alpha = 4.963$	0.108	$\lambda = 8153.500$	52.592	-9710.083	19424.17	19434.18

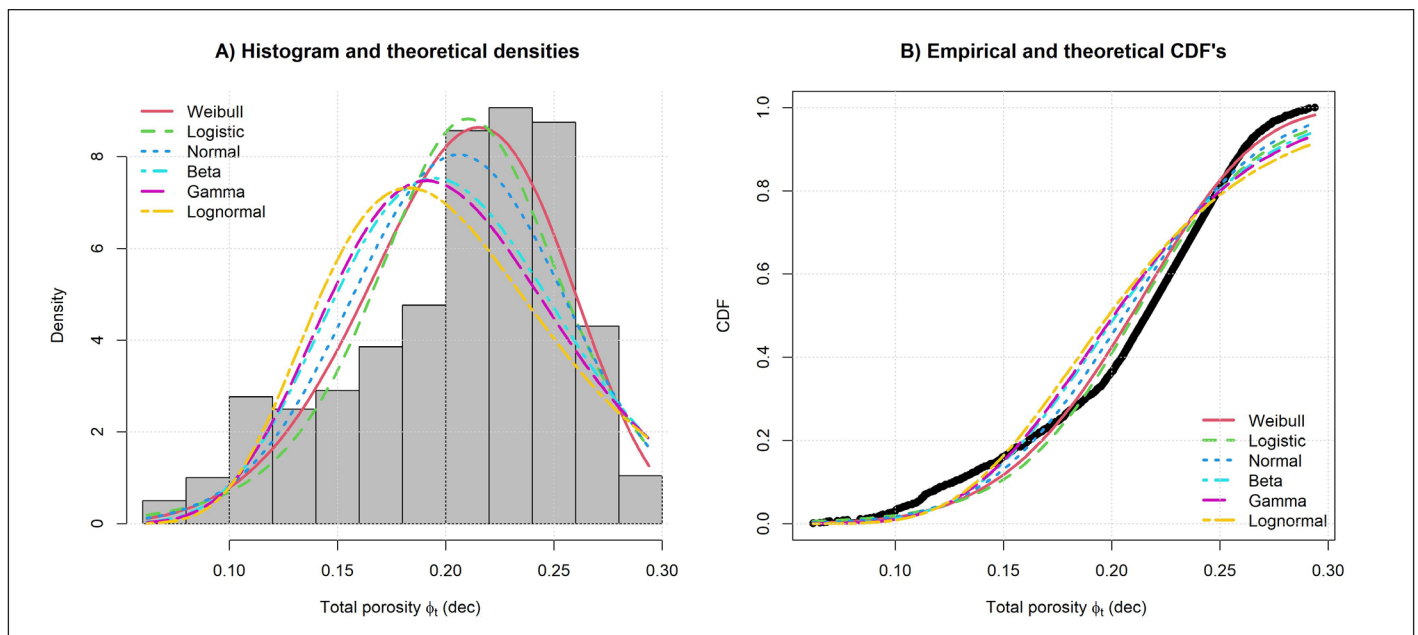


Figure 4. Histogram (A) and empirical CDF (B) with the best-fit probability functions for the total porosity ϕ_i

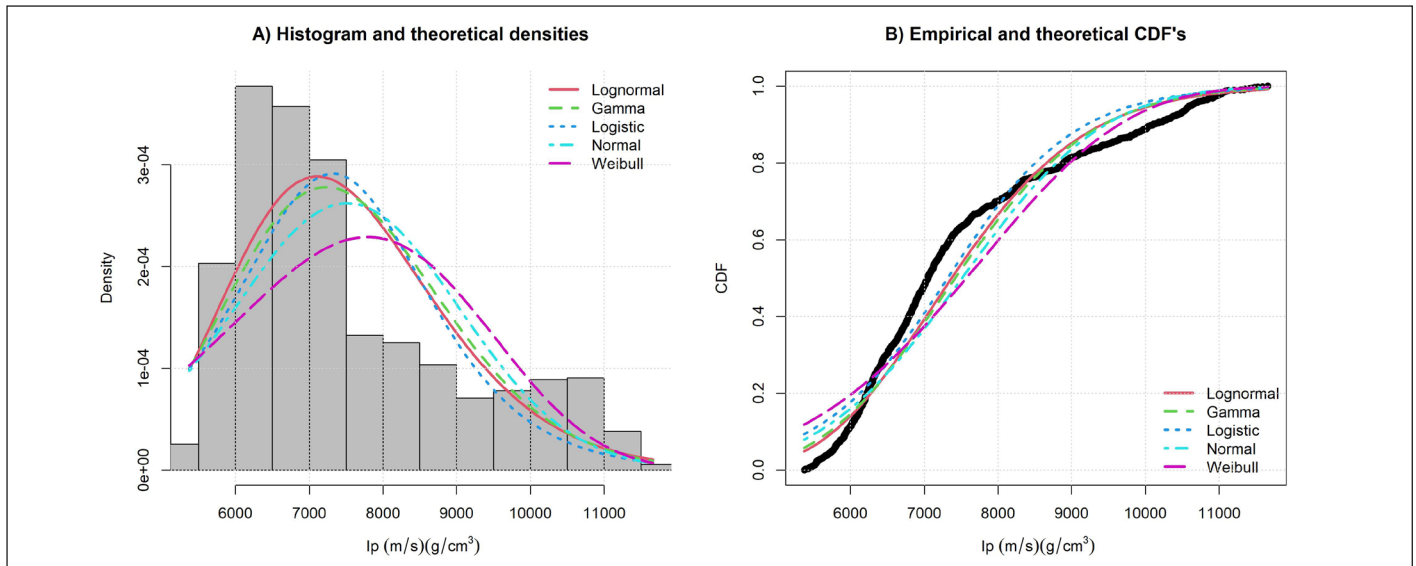


Figure 5. Histogram (A) and the empirical CDF (B) with the best-fit probability functions for the acoustic impedance I_p

Table 4. Fitted values for parameter θ

Copula	Method	Parameter θ	Error
Clayton	ITau	-0.86	0.006
Clayton	IRho	-0.92	0.006
Frank	ITau	-15.22	0.030
Frank	MLE	-15.04	0.443
Frank	IRho	-14.03	0.664

As ϕ_i variable, all functions fail to cover the entire histogram Figure 5(A). Notice that the highest values are not covered. If the cumulative histogram in Figure 5(B) is examined, the interval 6000 to 7000 has good approximation to empirical function.

4.4 Copula parametric modeling

After selecting the best-fit marginal probability functions, the best-fit parametric copula is sought. Considering the dependence model has negative dependencies, it is necessary to omit the Gumbel-Hougaard copula because it is not valid on negative dependencies, Clayton copula can be calculated in negative dependencies only if the parameter estimation method is semi-parametric, for this reason the Kendall inversion τ (ITau) and Spearman inversion ρ (IRho) is used. To select the best joint distribution function, the error or standard deviation and the graphs in the Figure 6 are used. Examining the information in Table 4, the best option is Clayton copula (Figure 6(A)). However, using this function could omit the values that are outside its coverage area, therefore the Frank's copula with the parameter estimated by maximum likelihood method (MLE) is used (Figure 6(B)).

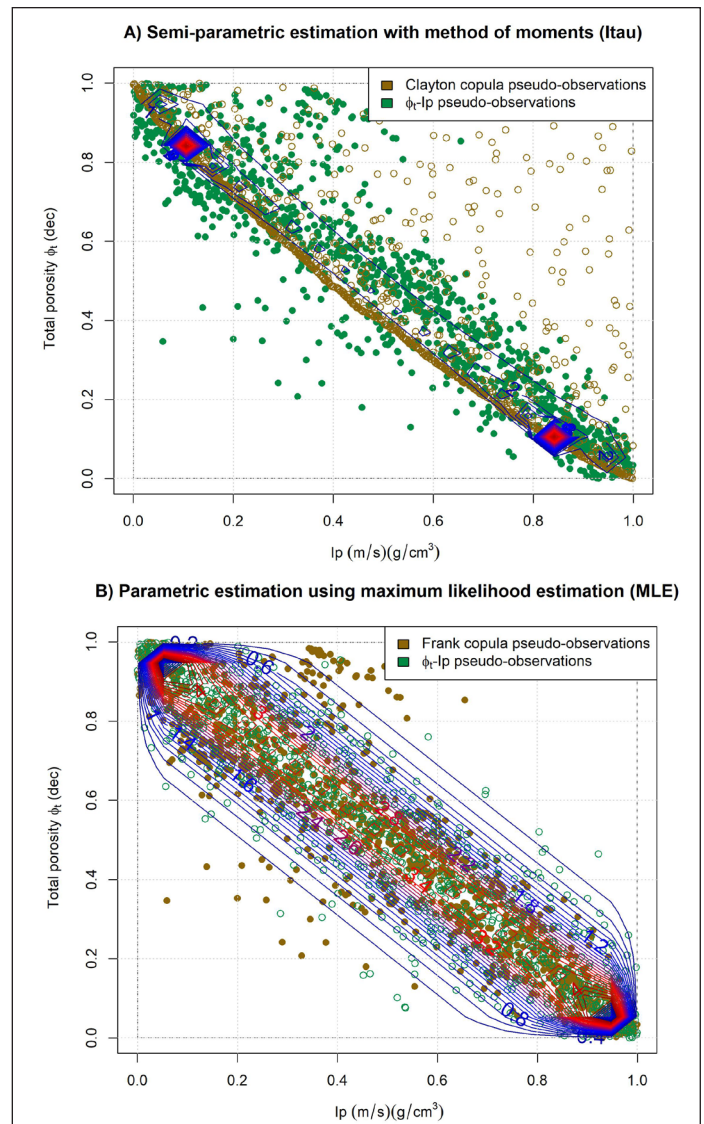


Figure 6. (A) Clayton copula, (B) Frank copula obtained with semi-parametric and parametric estimation.

4.5 Conditional joint simulation of total porosity with acoustic impedance.

After selecting the best parameters for the joint probability distribution function, a considerable number of pairs (I_p, ϕ_t) are simulated, it is proposed to simulate 40,000 observations based on the best estimate selected. The simulation samples under the parametric approach are very fast, less than a second. Considering the information in comparative Table 5, the case of ϕ_t simulated and ϕ_t variable has difference in the minimum values of 0.01 and maximum 0.007; in the case of mean and median, their differences are even lower. Therefore, it can be considered that the probability distribution function is representative. With the case of I_p ,

the difference in the minimum and maximum values have considerable differences, however, the mean and median values are very close to each other.

In comparison, the dependency measures obtained from the simulated samples appear to be quasi linear, however this may be due to the large number of samples. Regarding the comparison in the scatter plots (Figure 7), it is noted that the joint probability distribution function fails to adequately sample the area located in the interval I_p (10000,12000) ϕ_t (0.05,0.15). Sampling is abundant in the central part of the data sample (red dots), which is to be expected given the properties of Frank's copula (black dots).

Table 5. Comparative between (I_p, ϕ_t) data sample and simulated using parametric copula approach.

Statistics	ϕ_t	ϕ_t simulated	I_p	I_p simulated
Samples	3696	40000	3696	40000
Minimum	0.0620	0.0316	5086.0072	3018.2752
1 st quartile	0.2147	0.1767	6157.0051	6492.1272
Median	0.2295	0.2089	6809.5573	7376.3306
Mean	0.2219	0.2065	6968.2838	7511.1841
3 rd quartile	0.2414	0.2388	7321.6169	8377.4856
Maximum	0.2939	0.3548	11661.4642	15836.6388
Range	0.2319	0.3233	6575.4569	12818.3636
Interquartile range	0.0267	0.0620	1164.6118	1885.3584
Variance	0.0011	0.0020	1310302.9400	2099141.1700
STD	0.0337	0.0455	1144.6846	1448.8413
Skewness	-1.8109	-0.2597	1.5616	0.6097
Kurtosis	6.9969	2.9036	5.7657	3.7259

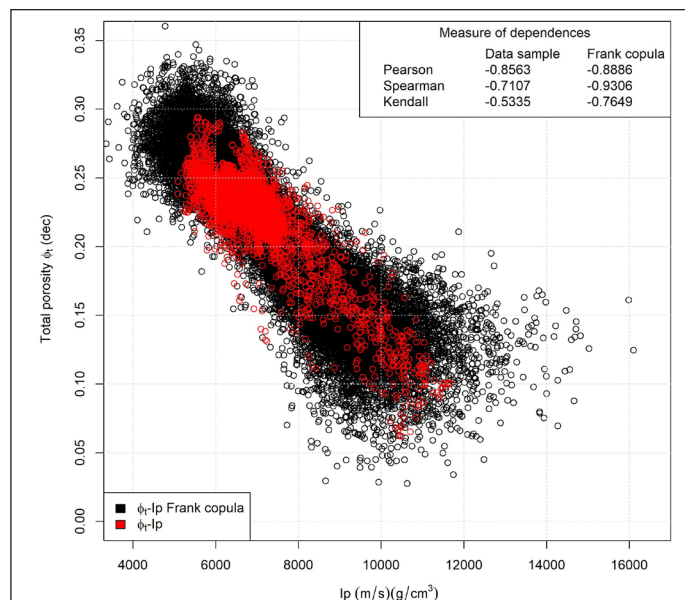


Figure 7. (I_p, ϕ_t) samples (red dots), (I_p, ϕ_t) simulated using parametric copula approach (black dots).

4.6 Total porosity spatial simulation

The total porosity ϕ_t is simulated using simulated annealing method, the GSLIB package (Deutsch & Journel, 1998) was used for the implementation. The variogram estimated for ϕ_t (Figure 3) is used as objective function and considered 100 realizations. The results are shown in the comparative Table 6. The minimum, maximum, mean and median values have low differences, not greater than 0.01.

Superimposing all realizations (Figure 8 (A)) dispersion in the interval 3200 to 3330 meters is noted.

5. Comparison between parametric, non-parametric and semi-parametric based copula simulations.

5.1 Non-parametric copula simulation.

The comparison with the non-parametric approach is made using a Bernstein copula for the estimation of the joint probability distribution function. The same data set (I_p, ϕ_t) is used for its implementation. As in the parametric case,

Table 6. Statistics obtained from ϕ_i data sample, 100 realizations, best realization and their differences using parametric approach.

Statistics	ϕ_i data sample	ϕ_i 100 realizations	Difference 100 realizations	ϕ_i best realization	Difference best realization
Samples	3696	369600		3696	
Minimum	0.0620	0.0541	0.0079	0.0707	-0.0087
1 st quartile	0.2147	0.2071	0.0076	0.2071	0.0075
Median	0.2295	0.2284	0.0011	0.2284	0.0010
Mean	0.2220	0.2244	-0.0020	0.2244	-0.0024
3 rd quartile	0.2414	0.2489	-0.0070	0.2487	-0.0072
Maximum	0.2939	0.3338	-0.0400	0.3102	-0.0162
Range	0.2319	0.2798	-0.0480	0.2394	-0.0075
Interquartile range	0.0267	0.0418	-0.0150	0.0416	-0.0148
Variance	0.0011	0.0014	-0.0003	0.0014	-0.0002
STD	0.0338	0.0375	-0.0040	0.0375	-0.0037
Skewness	-1.8110	-0.8640	-0.9470	-0.8750	-0.9364
Kurtosis	6.9970	4.2437	2.7533	4.2437	2.7532

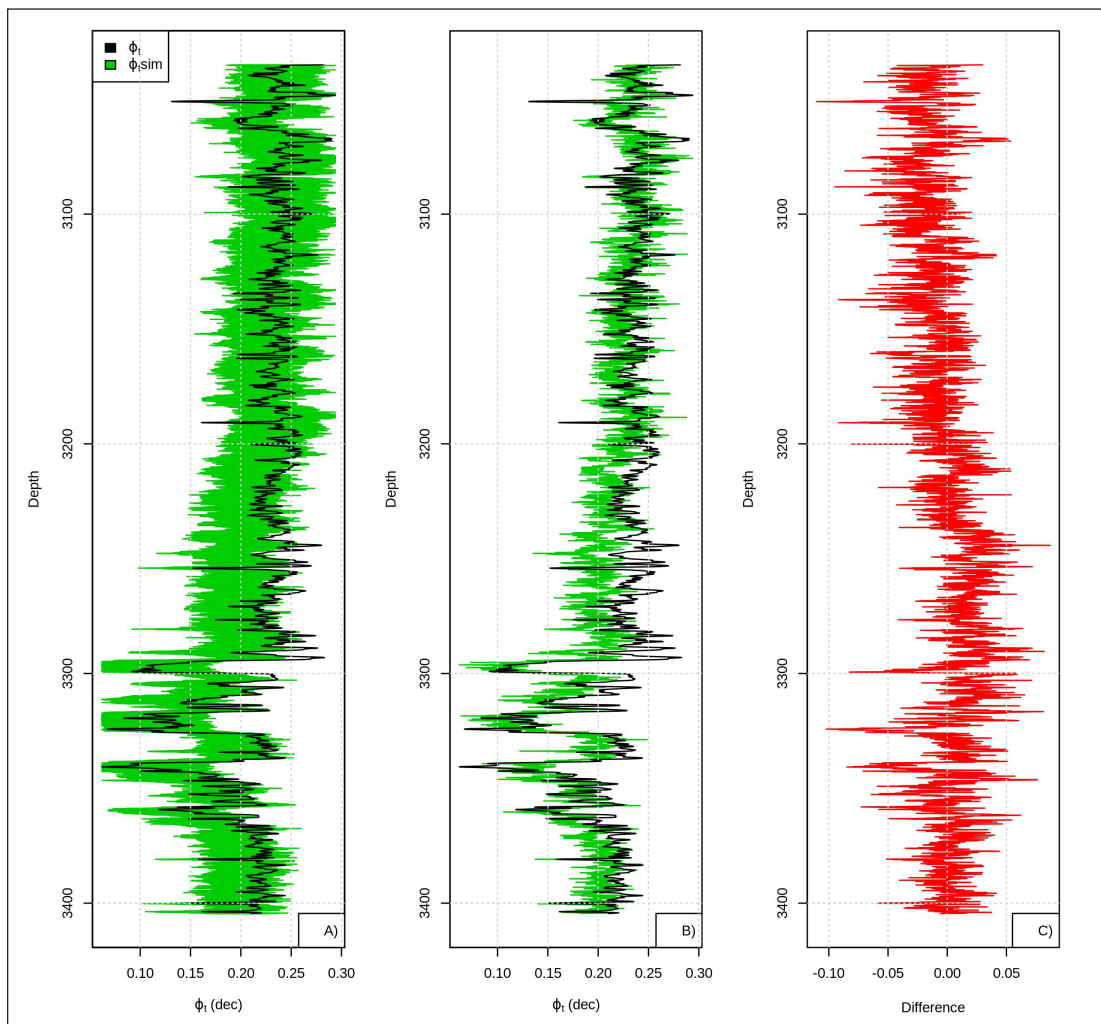
**Figure 8.** Well-log plots of A) 100 realizations of ϕ_i (green lines) with the well-log data values (black line), B) the ϕ_i best realization (green line) and C) the difference of the ϕ_i best realization with respect to the well-log data.

Table 7. Comparative between (I_p , ϕ_i) data samples and data simulated using non-parametric approach.

Statistics	ϕ_i	ϕ_i simulated	I_p	I_p simulated
Samples	3696	40000	3696	40000
Minimum	0.0620	0.0620	5086.0072	5086.0072
1 st quartile	0.2147	0.2147	6157.0051	6157.0052
Median	0.2295	0.2295	6809.5573	6809.5574
Mean	0.2219	0.2220	6968.2838	6968.2839
3 rd quartile	0.2414	0.2415	7321.6169	7321.6170
Maximum	0.2939	0.2938	11661.4642	11661.4642
Range	0.2319	0.2318	6575.4569	6575.4570
Interquartile range	0.0267	0.0268	1164.6118	1164.6118
Variance	0.0011	0.0011	1310302.9400	1309980.6378
Standard deviation	0.0337	0.0338	1144.6846	1144.5439
Skewness	-1.8109	-1.8212	1.5616	1.5617
Kurtosis	6.9969	7.0257	5.7657	5.7657

Table 8. Statistics obtained from ϕ_i data sample, 100 realizations, best realization and their differences using non-parametric approach.

Statistics	ϕ_i data sample	ϕ_i 100 realizations	Difference 100 realizations	ϕ_i best realization	Difference best realization
Samples	3696	369600		3696	
Minimum	0.0620	0.0620	0	0.0622	-0.0002
1 st quartile	0.2147	0.2154	-0.0006	0.2154	-0.0006
Median	0.2295	0.2295	0	0.2294	0.0001
Mean	0.2220	0.2220	0	0.2220	0
3 rd quartile	0.2414	0.2413	0.0001	0.2412	0.0002
Maximum	0.2939	0.2938	0.0001	0.2868	0.0071
Range	0.2319	0.2318	0.0001	0.2246	0.0072
Interquartile range	0.0267	0.0259	0.0008	0.0258	0.0009
Variance	0.0011	0.0011	0	0.0011	0
STD	0.0338	0.0330	0.0008	0.033	0.0008
Skewness	-1.8111	-1.9460	0.1349	-1.97	0.1590
Kurtosis	6.9970	7.4361	-0.4391	7.5698	-0.5728

40,000 samples using the Bernstein joint distribution function are simulated (Figure 11).

Each step takes around 10 hours, which compared to the time of parametric copula estimate, is too much. However, the statistics obtained from this estimate are very close to data samples (Table 7), this is confirmed in the Figure 11, the samples simulated using Bernstein copula (green dots) are close to data sample.

100 simulations using the samples obtained from Bernstein copula are made. As shown, the spatial distributions (Figure 9) obtained using the Bernstein copula are even closer

to the data sample distribution. However, the computational cost is high, the simulation of 40,000 samples can take hours.

5.2 Semi-parametric copula simulation.

This is formed using Bernstein copula and parametric marginals, the marginals are Lognormal (I_p) and Weibull (ϕ_i). The statistics obtained are close for I_p ; ϕ_i has differences, especially in minimum and maximum (Table 9). Comparing the scatter plot (Figure 11) the samples obtained with semi-parametric joint distribution function are between Frank copula and Bernstein copula. The computational cost

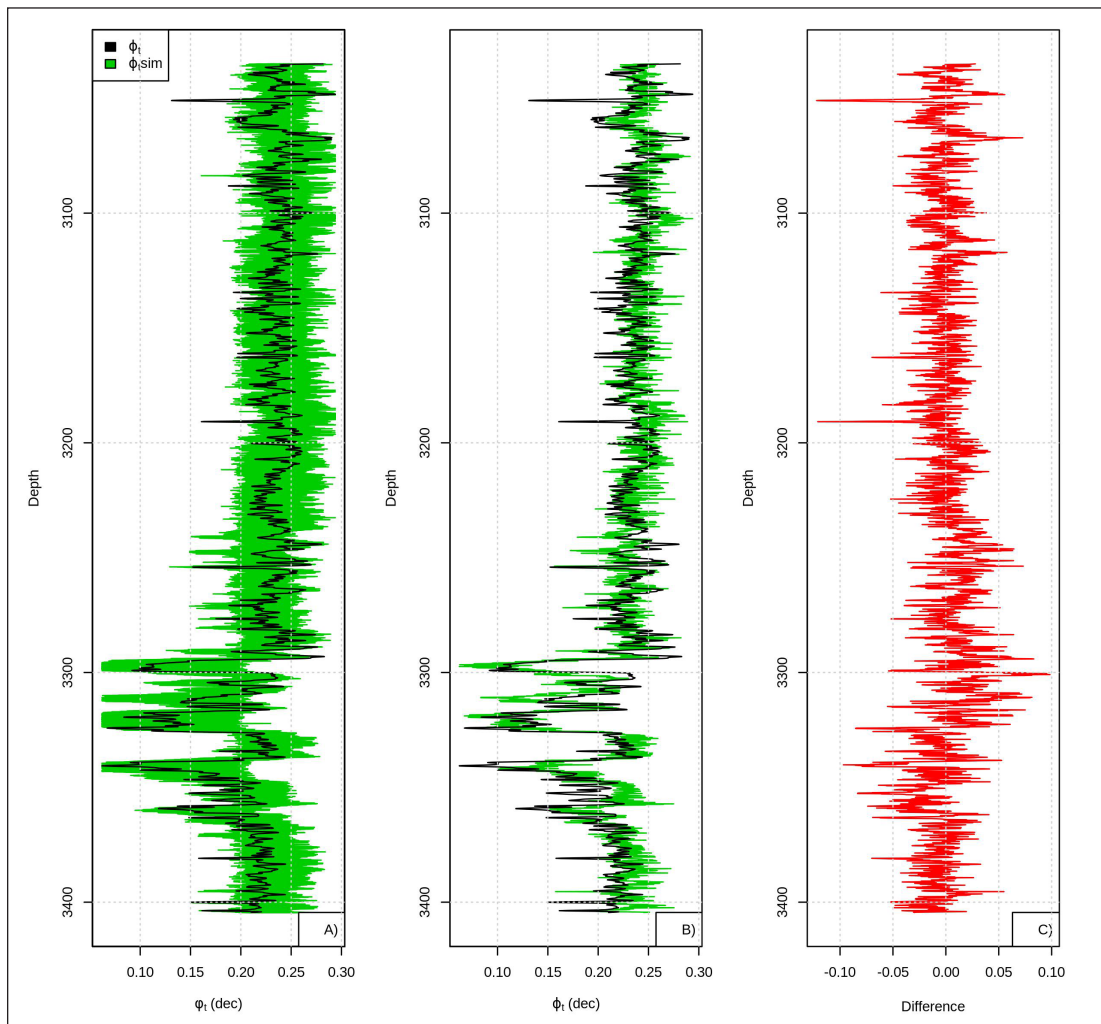


Figure 9. Realizations (green) superimposing over ϕ_r (black), B) Best realization obtained and C) difference between well-log ϕ_r and best simulated ϕ_r .

Table 9. Comparative between (I_p, ϕ_r) data sample and data simulated using semi-parametric approach.

Statistics	ϕ_r	ϕ_r simulated	I_p	I_p simulated
Samples	3696	40000	3696	40000
Minimum	0.0620	0.0298	5086.0072	5086.0072
1 st quartile	0.2147	0.1967	6157.0051	6157.0052
Median	0.2295	0.2217	6809.5573	6809.5574
Mean	0.2219	0.2183	6968.2838	6968.2839
3rd quartile	0.2414	0.2459	7321.6169	7321.6170
Maximum	0.2939	0.3340	11661.4642	11661.4642
Range	0.2319	0.3042	6575.4569	6575.4570
Interquartile range	0.0267	0.0492	1164.6118	1164.6118
Variance	0.0011	0.0017	1310302.9400	1309983.8600
STD	0.0337	0.0411	1144.6846	1144.5453
Skewness	-1.8109	-0.6140	1.5616	1.5617
Kurtosis	6.9969	3.8246	5.7657	5.7657

is 10% less than the Bernstein copula, but the statistics are not the same.

Comparing the 100 ϕ_i simulations (Figure 10), the realizations are centered, this does not happen with the realiza-

tions obtained using Frank copula samples, but have more dispersion than the realizations obtained using the Bernstein copula samples, the statistics between data sample and data simulation are very close (Table 10).

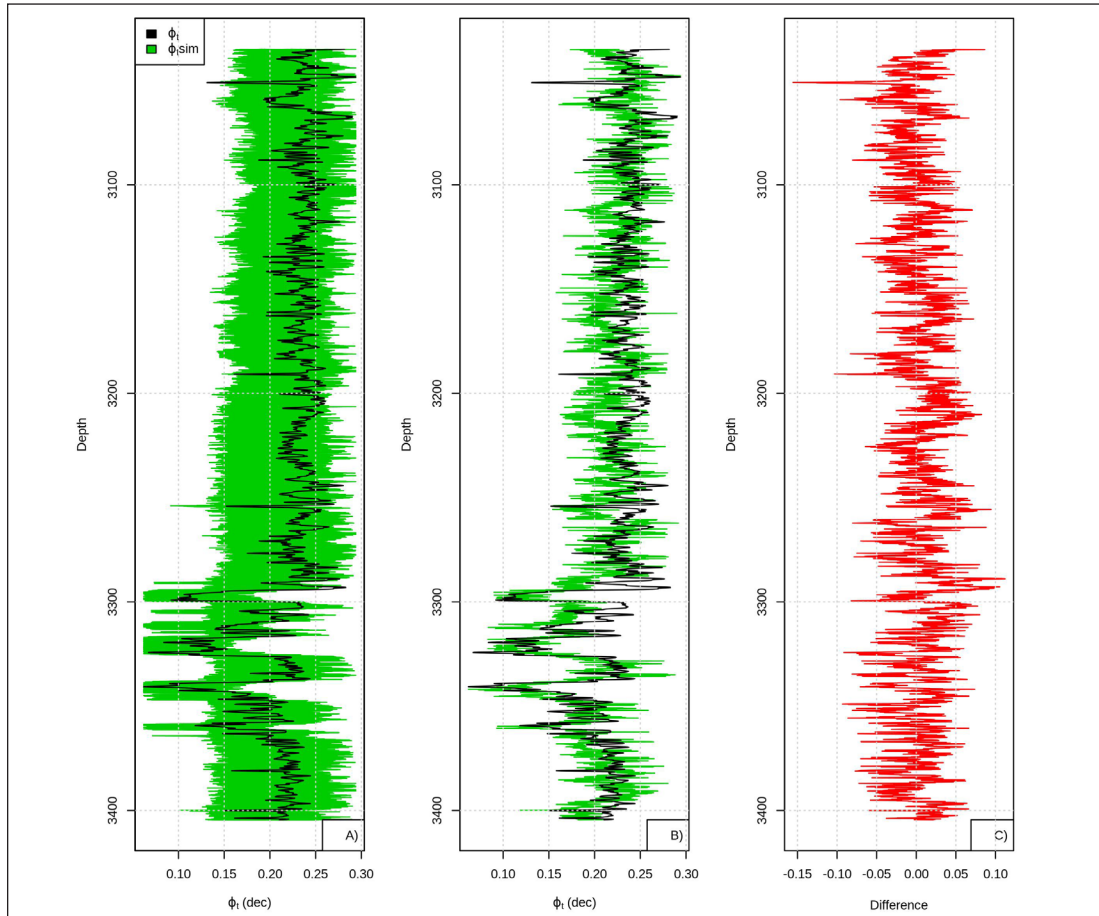


Figure 10. Realizations (green) superimposing over ϕ_i (black), B) Best realization obtained and C) difference between well-log ϕ_i and best simulated ϕ_i .

Table 10. Statistics obtained from ϕ_i data sample, 100 realizations, best realization and their differences using semi-parametric approach.

Statistics	ϕ_i data sample	ϕ_i 100 realizations	Difference 100 realizations	ϕ_i best realization	Difference best realization
Samples	3696	369600		3696	3696
Minimum	0.0620	0.0608	0.0012	0.0637	-0.0017
1 st quartile	0.2147	0.1979	0.0168	0.1978	0.0169
Median	0.2295	0.2216	0.0079	0.2215	0.0080
Mean	0.222	0.2182	0.0038	0.2181	0.0039
3 rd quartile	0.2414	0.2453	-0.0039	0.2456	-0.0042
Maximum	0.2939	0.3226	-0.0287	0.3054	-0.0115
Range	0.2319	0.2617	-0.0298	0.2418	-0.0099
Interquartile range	0.0267	0.0474	-0.0207	0.0479	-0.0212
Variance	0.0011	0.0015	-0.0004	0.0015	-0.0004
STD	0.0338	0.0383	-0.0045	0.0382	-0.0044
Skewness	-1.8110	-0.7330	-1.0780	-0.751	-1.0600
Kurtosis	6.9970	3.7493	3.2477	3.7789	3.2181

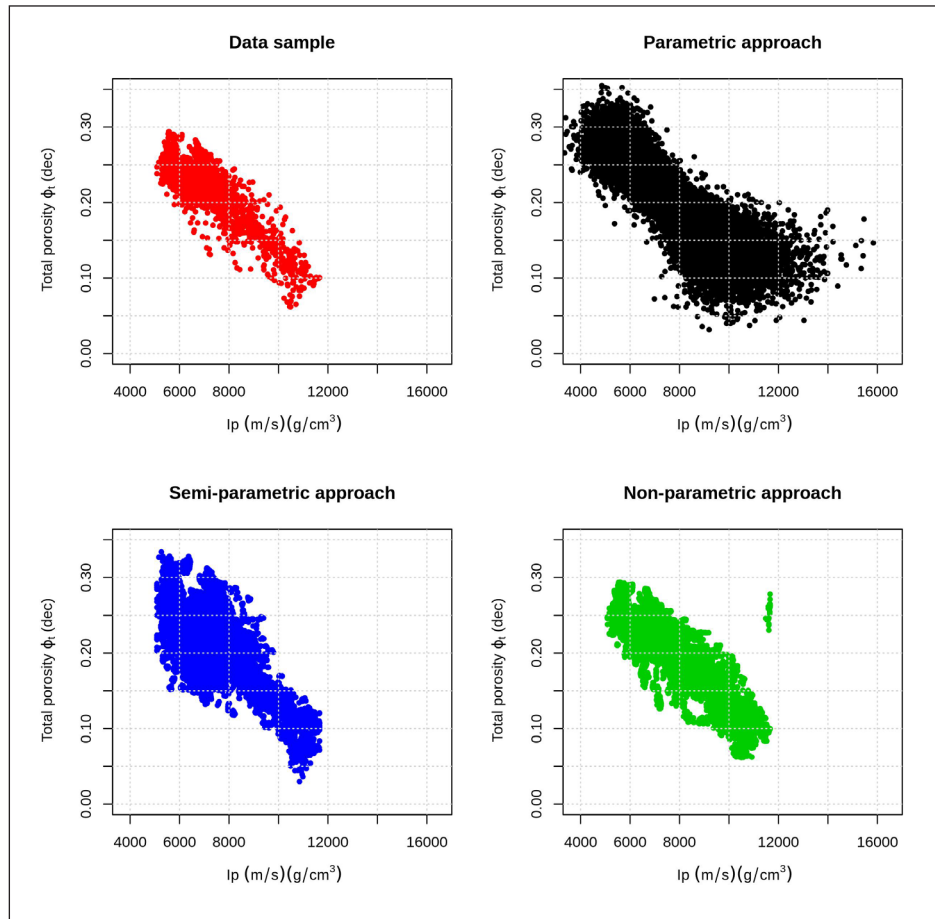


Figure 11. (I_p, ϕ_t) data samples (red dots), (I_p, ϕ_t) simulated using parametric copula (black dots), (I_p, ϕ_t) simulated using Semiparametric copula (blue dots) and (I_p, ϕ_t) simulated using non-parametric copula (green dots).

As shown in Table 11, the non-parametric approach almost perfectly reproduces the existing dependency relationship in the data sample, while the parametric and semi-parametric approaches either overestimate or underestimate it, respectively.

6. Application to case study: density vs. P- wave velocity

This example uses (V_p, ρ) well logs. The statistics (Table 15) and the histograms of V_p (Figure 12, blue histogram)

Table 11. Comparison of (I_p, ϕ_t) dependency measures among the parametric, semi-parametric and non-parametric approaches with respect to the data samples.

	Pearson	Spearman	Kendall
Data sample	-0.8563	-0.7107	-0.5335
Parametric approach	-0.8886	-0.9306	-0.7649
Semiparametric approach	-0.6780	-0.5074	-0.3671
Non-parametric approach	-0.8481	-0.7073	-0.5303

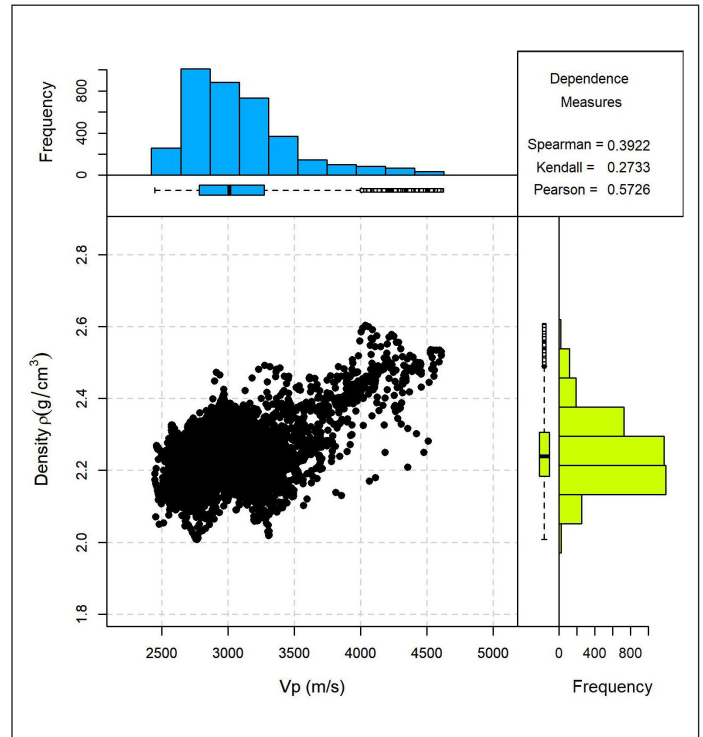


Figure 12. (V_p, ρ) Scatter plot, V_p histogram (blue) and ρ histogram (green).

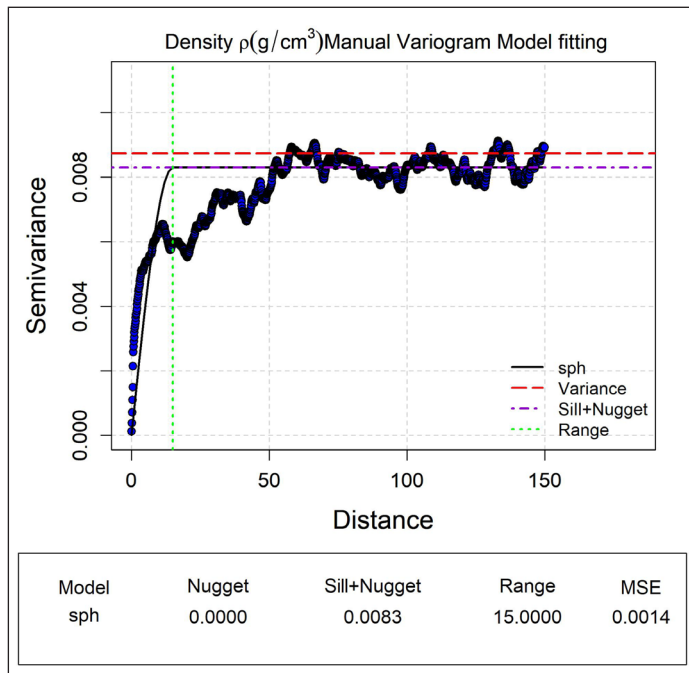


Figure 13. ρ variogram model

Table 12. Goodness of fit results for ρ

Function	Parameter	Error	Parameter	Error	Likelihood	AIC	BIC
Lognormal	$Log\mu = 0.8130$	0.009	$Log\sigma = 0.04$	0.006	1845.260	-3686.52	-3675.11
Gamma	$k = 455.2500$	13.650	$\beta = 201.60$	6.050	1838.346	-3672.69	-3661.28
Normal	$\mu = 2.2581$	0.002	$\sigma = 0.10$	0.001	1822.310	-3640.63	-3629.22
Logistics	$\mu = 2.2524$	0.002	$\beta = 0.06$	0.001	1804.600	-3605.21	-3593.80
Weibull	$\alpha = 20.278$	0.303	$\lambda = 2.31$	0.002	1568.410	-3132.83	-3121.42

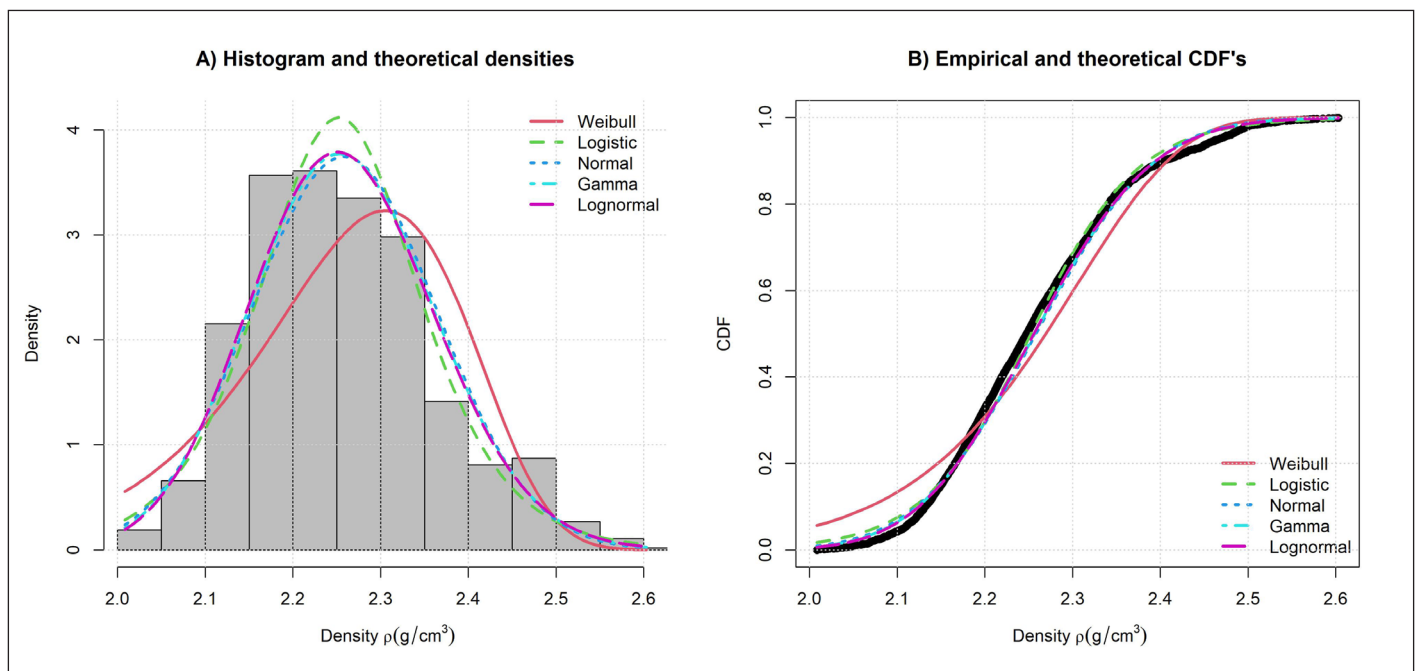


Figure 14. Histogram and theoretical densities (A) and empirical and theoretical CDF's (B) of Goodness of fit results for ρ

and ρ (Figure 12, green histogram) show high asymmetry although the difference between median and median is low in both variables. This case has positive dependence (Figure 12), but the dependence is less compared with the $(I\rho, \phi_i)$ case. So, the use of Frank, Gumbel, Clayton and Joe copula is allowed.

The variogram model estimated for ρ (Figure 13) is spherical with sill 0.0083, range 15 meters and nugget effect 0.

The parametric estimation for ρ (Table 12) suggests the lognormal function as best option, but the cumulative distribution functions in Figure 14 (B) shows all functions, except Weibull function has good fit. Gamma and normal functions have likelihood, AIC and BIC very close to lognormal.

Now, the $V\rho$ variable goodness of fit results in Table 13 shows gamma function as best option, Logistic and lognormal are close to gamma function results, and the graphs in Figure 15 demonstrate that gamma and lognormal functions have similar fitted.

Table 13. Goodness of fit results for V_p

Function	Parameter	Error	Parameter	Error	Likelihood	AIC	BIC
Gamma	$k = 58.244$	1.440	$\beta = 0.018$	0.0004	-16500.00	33004.01	33015.42
Logistic	$\mu = 3069.300$	8.140	$\beta = 224.63$	4.0810	-16523.25	33050.51	33061.92
Lognormal	$\text{Log}\mu = 8.039$	0.002	$\text{Log}\sigma = 0.12$	4.0800	-16523.44	32902.89	32914.30
Normal	$\mu = 3128.730$	9.117	$\sigma = 429.69$	6.4470	-16617.57	33239.13	33250.54
Weibull	$\alpha = 6.628$	0.096	$\lambda = 3325.87$	11.3400	-16903.62	33811.24	33822.65

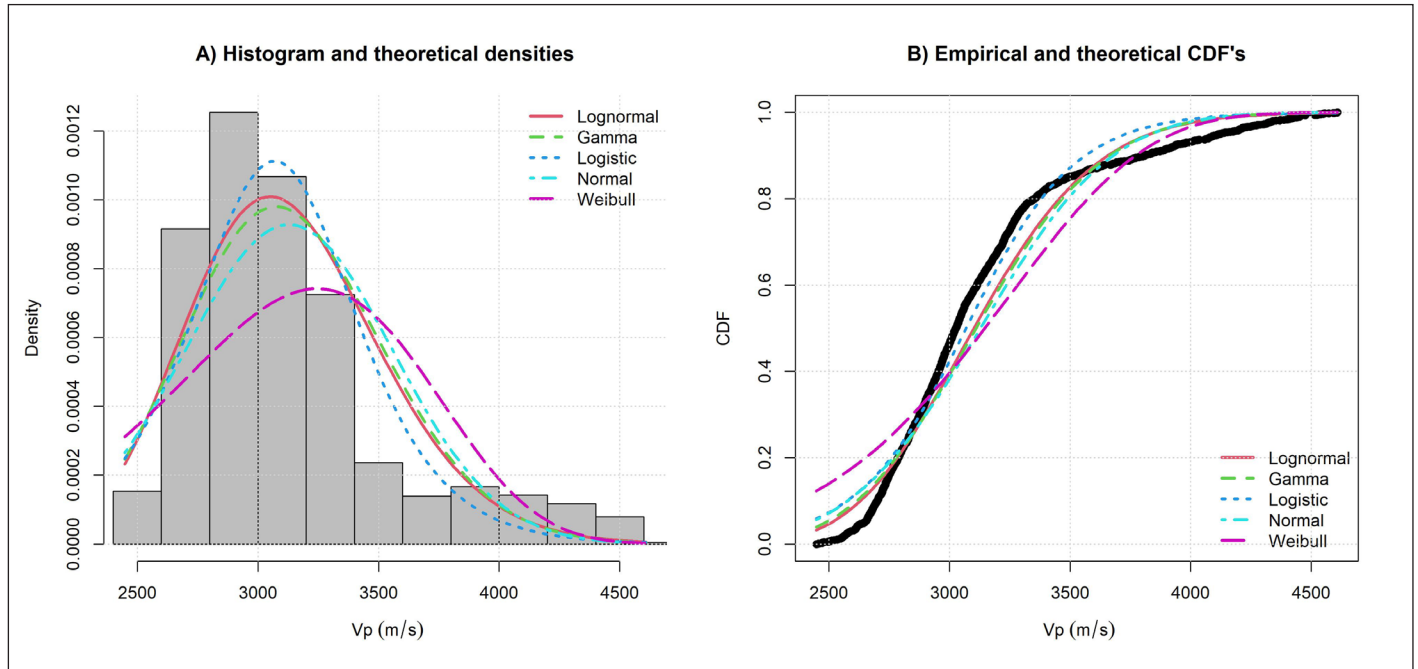


Figure 15. Histogram and theoretical densities (A) and empirical and theoretical CDF's (B) of Goodness of fit results for V_p

Table 14. Fitted values for parameter θ

Copula	Method	Parameter θ	Error	Loglikelihood
Joe	MLE	2.038	0.044	550.6
Gumbel	MLE	1.643	0.028	522.6
Frank	MLE	3.671	0.141	342.4
Clayton	MLE	0.570	0.035	170.2

The fit copula results show Joe copula model as best option (Table 14). Gumbel copula could be a good option, but Joe copula can cover the pseudo-observations, especially the samples in the extremes (Figure 16).

Simulating 40,000 samples from Joe copula, superimposing the results (Figure 17) the drop form of Joe copula samples is evident. The measures of dependences show Pearson values have difference of 0.02, but Spearman and Kendall measures are high. Other characteristic is the scatter of Joe copula samples, simulated samples are near to data samples. Comparing the variance and standard deviation in

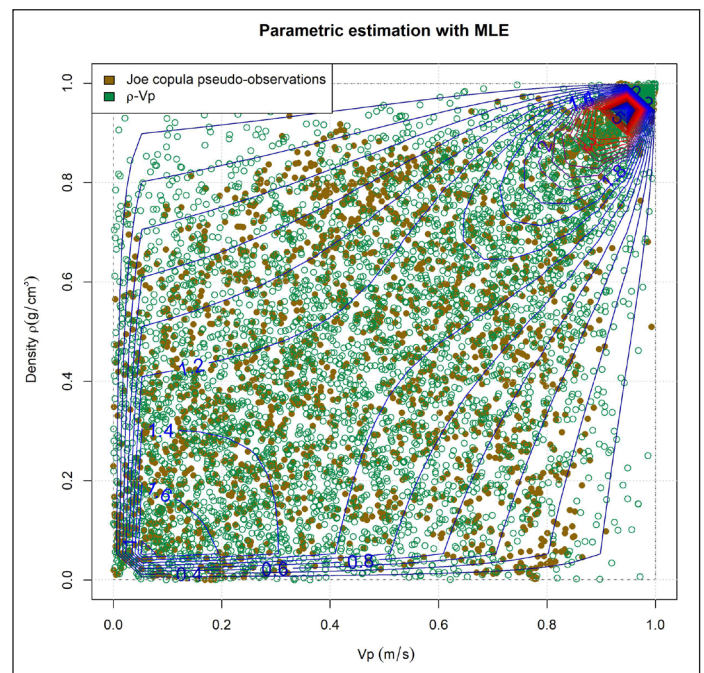


Figure 16. Joe copula estimated for (V_p, ρ)

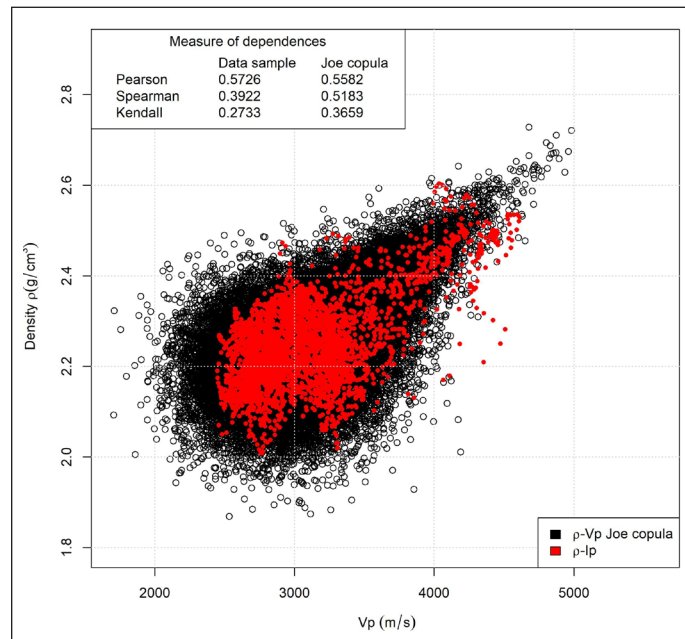


Figure 17. (Vp, ρ) samples (red dots), (Vp, ρ) simulated using Joe copula (black dots)

Table 15. Comparative between (Vp, ρ) data samples and simulated using Joe copula.

Statistics	Vp	Vp simulated	ρ	ρ simulated
Samples	3696	40000	3696	40000
Minimum	2448.0983	1619.7990	2.0085	1.8630
1 st quartile	2785.1214	2843.1401	2.1835	2.1873
Median	3011.4426	3112.6668	2.2395	2.2568
Mean	3088.0889	3129.2969	2.2494	2.2590
3 rd quartile	3273.1712	3398.5189	2.3062	2.3276
Maximum	4608.5457	5038.7143	2.6031	2.7328
Range	2160.4473	3418.9152	0.5946	0.8697
Interquartile range	488.0498	555.3788	0.1227	0.1402
Variance	165004.4920	168551.6370	0.0087	0.0110
Standard deviation	406.2074	410.5504	0.0934	0.1050
Skewness	1.2392	0.2460	0.6631	0.1302
Kurtosis	4.5799	3.0456	3.5973	3.0462

Table 15, the values are very close, this is not the same with the validation case, this could be an advantage of positive dependence.

The spatial distributions obtained to 100 simulations (Figure 18) show good covering except in the interval 3350-3400, the variance in that range is high.

7. Conclusions

In the comparison between parametric, semi-parametric and non-parametric approaches of the spatial stochastic simulation method based on copulas, it is concluded that the parametric approach has a very low computational cost, since its execution lasts only a few seconds; while the

semi-parametric and non-parametric approach can take up to hours. Given that the first approach involves analytic functions in the calculation, while the second approach requires the calculation of the joint probability distribution function through the numerical approximation of the copula and its marginals with Bernstein polynomials.

When comparing the numerical results, it can be verified that the parametric approach does not reproduce data statistics such as minimum, maximum, skewness and kurtosis with the same precision as the semi-parametric and non-parametric approach. The parametric approach presents a greater dispersion expressed by its variance, which means more uncertainty. This fact is due to it is practically im-

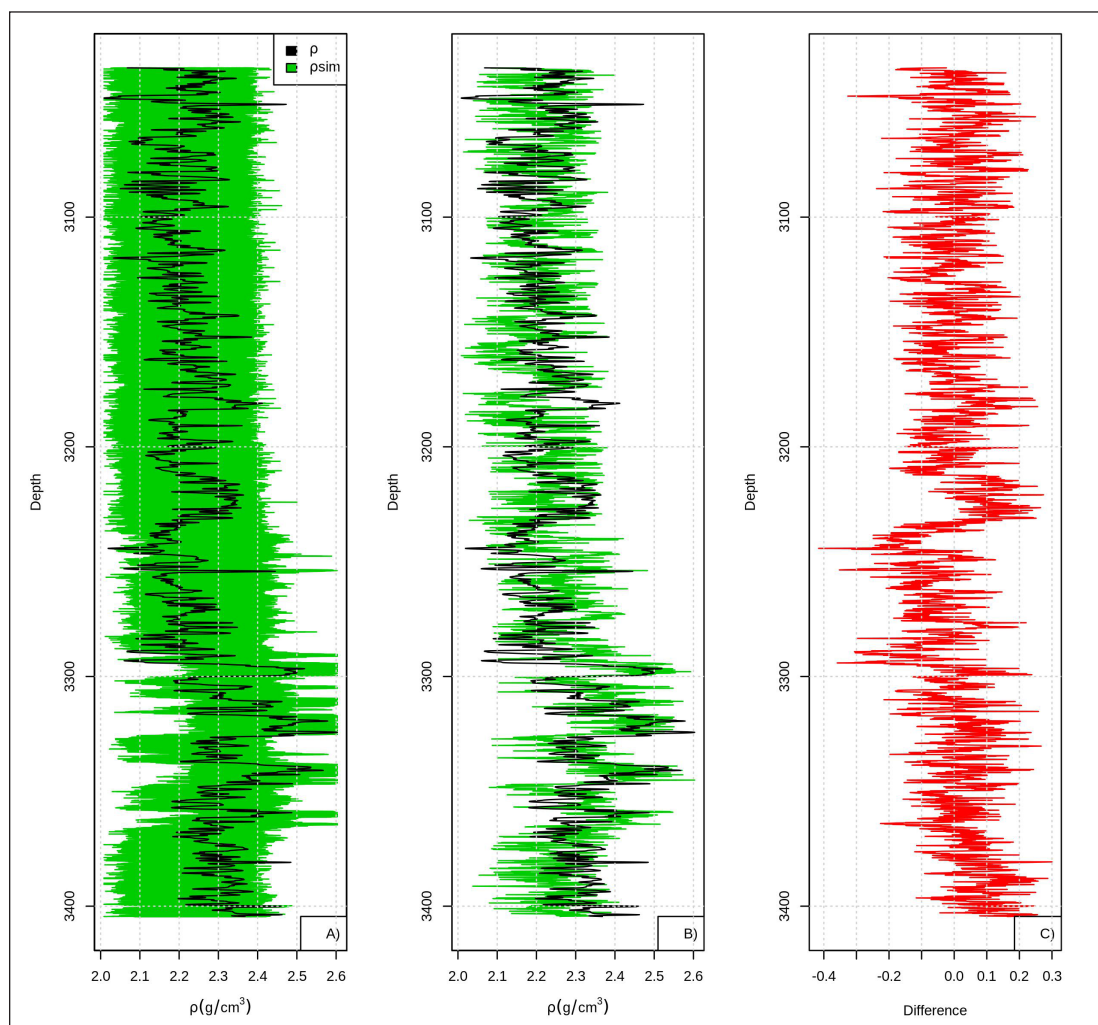


Figure 18. Realizations (green) superimposing over ρ (black), B) Best realization obtained and C) difference between well-log ρ and best simulated ρ .

possible to be able to represent the underlying dependence complexity between data with a parametric model, since the data is forced to fitting an analytical model depending of a single parameter, whereas the objective is to represent the real dependence complexity existing in the data, the latter only could be done by the non-parametric approach.

This indicates that it is advisable to use the parametric approach in cases with large data samples and limited computing capabilities. This problem would be expected to occur when the method is applied in three spatial dimensions and when more than two variables are included in the multivariate joint estimation as well. However, the non-parametric approach could be applied if the appropriate computational capabilities are available and predictions with less uncertainty are required.

8. Acknowledgments

The data were provided by the National Hydrocarbons Commission of Mexico, according to appendix C of the license to use the information in favor of Universidad Nacional

Autónoma de México, dated December 11, 2017, under the nomenclature CNIH-C-00417.305. This reference information is the property of Mexico and its collection, safekeeping, use, administration and updating, as well as its publication is only authorized to the National Hydrocarbons Commission.

9. Supplementary material

A pdf version of Jupyter notebook in R language is available in <https://github.com/esmg-mx/Copula-Base-modelling>

10. Appendix

10.1 Appendix A: Copula definition and basic properties

As defined by Nelsen (2006), a copula is “a function that joins or couples multivariate distribution functions to their one-dimensional marginal distribution functions”. If want to use copulas in the field of statistics, use Sklar's theorem. Sklar's theorem is defined as: *Let H be a joint distribution function with margins F and G . Then there exists a copula C such that for all (x, y) in \mathcal{R} .*

$$H(x,y)=C(F(x),G(y)) \tag{Eq. A1}$$

If $u=F(x)$ and $v=G(y)$ are marginal distribution functions and $C(u,v)=C(F(x),G(y))$ is a valid distribution function, then for any copula $C(u,v)$ its partial derivatives are $\frac{\partial C}{\partial u}$ and $\frac{\partial C}{\partial v}$ exist for almost all (u,v) in $[0;1]$. Then $\frac{\partial^2 C}{\partial u \partial v}$ and $\frac{\partial^2 C}{\partial v \partial u}$ exist and are continuous on I^2 . If this is true, the density function of the copula is

$$C(u,v) = \frac{\partial^2 C}{\partial u \partial v} \tag{Eq. A2}$$

And the joint probability density function of x and y is:

$$f(x,y) = \frac{\partial^2(C)}{\partial u \partial v} \cdot \frac{dF}{dx} \cdot \frac{dG}{dy} \tag{Eq. A3}$$

10.2 Appendix B: Bernstein copula simulation method

The Bernstein copula provides an estimate to the copula using the empirical copula and the Bernstein polynomials. If $F(x)$ and $G(y)$ are continuous, by elementary probability it is known that $U=F(X)$ and $V=G(Y)$ are continuous Uniform(0,1) random variables, and the underlying copula C for the random vector (U, V) is the same copula corresponding to (X, Y) , and by Sklar's Theorem the joint probability distribution function for (U, V) is equal to $F_{UV}(u,v)=C(F(u),G(v))=C(u,v)$. Therefore, in case $F(x)$ and $G(y)$ are known and F_{XY} is unknown, if $\{(x_1, y_1), \dots, (x_n, y_n)\}$ is an observed random sample from (X, Y) , the set $\{(u_k, v_k) = (F_X(x_k), F_Y(y_k)) : k=1, \dots, n\}$ would be an observed random sample from (U, V) with the same underlying copula C as (X, Y) , and since $C=F_{UV}$ may use the (u_k, v_k) values (called copula observations) to estimate C as a joint empirical distribution:

$$\hat{C}(u,v) = \frac{1}{n} \sum_{k=1}^n 1_{\{u_k \leq u, v_k \leq v\}} \tag{Eq. B1}$$

Strictly speaking, the estimation \hat{C} is not a copula since it is discontinuous and copulas are always continuous. If $F_X, F_Y,$ and F_{XY} are all unknown (the usual case), then F_X and F_Y are estimated by univariate empirical distribution functions:

$$\hat{F}_x(x) = \frac{1}{n} \sum_{k=1}^n 1_{\{x_k \leq x\}} \quad \hat{F}_y(y) = \frac{1}{n} \sum_{k=1}^n 1_{\{y_k \leq y\}} \tag{Eq. B2}$$

Now the set of pairs $\{(u_k, v_k) = (\hat{F}_x(x_k), \hat{F}_y(y_k)) : k = 1, \dots, n\}$ is referred to as copula pseudo-observations. It is straightforward to verify that $\hat{F}_x(x_k) = \frac{1}{n} rank(x_k)$ and $\hat{F}_y(y_k) = \frac{1}{n} rank(y_k)$. In this case the concept of empirical copula, see (Nelsen, 2006), is defined as the following function $C_n : I_n^2 \rightarrow [0,1]$, where $I_n = \left\{ \frac{i}{n} : i = 0, \dots, n \right\}$, given by:

$$C_n \left(\frac{i}{n}, \frac{j}{n} \right) = \frac{1}{n} \sum_{k=1}^n 1_{\{rank(x_k) \leq i, rank(y_k) \leq j\}} \tag{Eq. B3}$$

Again, C_n is not a copula but it is an estimation of the underlying copula C on the grid that may be extended to a copula on $[0,1]^2$ by means of, for example, Bernstein polynomials, as proposed and studied in Sancetta & Satchell (2004), which leads to what is known as a Bernstein copula non-parametric estimation $\tilde{C} : [0,1]^2 \rightarrow [0,1]$ given by:

$$\tilde{C}(u,v) = \sum_{i=0}^n \sum_{j=0}^n C_n \left(\frac{i}{n}, \frac{j}{n} \right) \binom{n}{i} u^i (1-u)^{n-i} \binom{n}{j} v^j (1-v)^{n-j} \tag{Eq. B4}$$

As summarized in Erdely & Diaz-Viera (2010) in order to simulate replications from the random vector (X, Y) with the dependence structure inferred from the observed data $\{(x_1, y_1), \dots, (x_n, y_n)\}$ it has the following:

Algorithm 1

1. Generate two independent and continuous Uniform(0,1) random variates u and t .
2. Set $v = c_u^{-1}(t)$ where $c_u(v) = \frac{\partial C(u,v)}{\partial u}$.
3. The desired pair is $(x,y) = (Q_n(u), R_n(v))$ where Q_n and R_n are empirical quantile functions for X and Y , respectively.

For a value x in the range of the random variable X and a given $0 < \alpha < 1$ let $y = \varphi_\alpha(x)$ denote the solution to the equation $P(Y \leq y | X = x) = \alpha$. Then the graph of $y = \varphi_\alpha(x)$ is the α -quantile regression curve of Y conditional on $X = x$. In Nelsen (2006) is proven that:

$$P(Y \leq y | X = x) = C_u(v) \Big|_{u=F_X(x), v=F_Y(y)} \tag{Eq. B5}$$

This result leads to the following algorithm to obtain the α -quantile regression curve of Y conditional on $X = x$:

Algorithm 2

1. Set $c_u(v) = \alpha$.
2. Solve for v the regression curve, say $v = g_\alpha(u)$.
3. Replace u by $Q_n^{-1}(x)$ and v by $R_n^{-1}(y)$.
4. Solve for y the regression curve, say $y = \varphi_\alpha(x)$.

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