Dependence Modeling Using Copulas

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Measures of Dependence

Linear Correlation

$$Corr = \frac{Cov(X_1, X_2)}{\sqrt{Var(X_1) Var(X_2)}}$$

- Zero correlation implies independence only for normal distribution
- Invariant only to *linear* transformations,
 Example: log-normal RVs vs underlying normal RVs
- Interval of attainable correlations shrink with some distributions: Small correlation does not imply small degree of dependence.

Example:
$$X_1 \sim \mathcal{N}(0,1), X_2 = X_1^2$$
.
 $Cov(X_1, X_2) = E(X_1(X_1^2 - 1)) = E(X_1^3) - E(X_1) = 0$



Measures of Dependence

Rank Correlation

RVs X_1, X_2 with marginals F_1, F_2 , Spearman's rho:

$$\rho_s = Corr(F_1(X_1), F_2(X_2))$$

- CDF maps RV into a uniform variable Grade of X: $F_X(X) \sim \mathcal{U}_{[0,1]}$
- Sample–based estimate: $Corr(R(X_1), R(X_2))$, R: Rank transformation
- Measures monotonicity: ± 1 perfect monotonicity
- Other measures: Kendall's Tau, Mutual Information based measures...

Copulas

- Parametric models of dependence
- Can capture many different kinds of dependence, notably (a)symmetric tail dependence
- A *p*-dimensional copula is a multivariate distribution function (joint distribution of the grades)

$$C:[0,1]^p\mapsto [0,1]$$

$$C_U(u) = \mathcal{P}(F_{X_1}(X_1) \leq u_1, \ldots, F_{X_n}(X_n) \leq u_n)$$

Examples

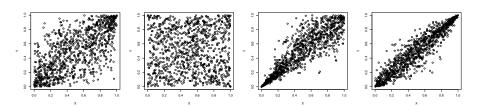


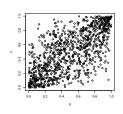
Figure: Gaussian, T, Clayton and Gumbel copulas (left to right).

Gaussian Copula

• For a given correlation matrix $R \in \mathbb{R}^{p \times p}$, the Gaussian copula is given by:

$$C_R^{\mathbf{N}}(u_1,\ldots,u_p) = \Phi_R\left(\Phi^{-1}(u_1),\ldots,\Phi^{-1}(u_p)\right)$$

- \bullet Φ^{-1} is the inverse cumulative distribution function (CDF) of a standard Normal
- Φ_R is the joint cumulative distribution function of a multivariate Normal distribution with mean vector zero and covariance matrix equal to the correlation matrix R



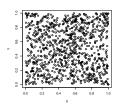


Student's t-copula

• For a correlation matrix Σ with ν degrees of freedom, the t-copula is defined as:

$$C_{\theta}(u_1,\ldots,u_p) = \mathbf{t}_{\nu,\Sigma}(t_{\nu}^{-1}(u_1),\ldots,t_{\nu}^{-1}(u_p))$$

- $\mathbf{t}_{\nu,\Sigma}$: multivariate Student's t distribution t_{ν} : univariate t distribution
- Allows for joint fat tails and increased probability of joint extreme events (compared to Gaussian copula)
- Additional parameter ν : increasing ν decreases the tendency to exhibit extreme co–movements.

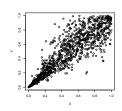




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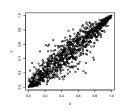
Clayton Copula

- $C_{\delta}(u,v) = (u^{-\delta} + v^{-\delta} 1)^{-1/\delta}$
- δ controls the dependence. perfect dependence: $\delta \longrightarrow \infty$, independence: $\delta \longrightarrow 0$
- Asymmetric: greater dependence in negative tail



Gumbel Copula

- $C_{\delta}(u, v) = exp(-[(-\log u)^{\delta} + (-\log v)^{\delta}]^{1/\delta})$
- \bullet δ controls the dependence. perfect dependence: $\delta \longrightarrow \infty$, independence: $\delta = 1$
- Assymetric: greater dependence in the positive tail



Sklar's Theorem

Theorem

Let F be a joint distribution function with marginals F_1, \ldots, F_p . Then there exists a copula $C: [0,1]^p \mapsto [0,1]$ such that

$$F(x_1,\ldots,x_p)=C(F_1(x_1),\ldots,F_p(x_p))$$

If the marginal distributions are continuous, then this copula is unique. Conversely, if C is a copula and F_1, \ldots, F_p are univariate distribution functions, then F as defined above is a multivariate distribution function with marginals F_1, \ldots, F_p .

- Model marginals and copula independently
- No constraints on marginals



Multivariate PDF

- Joint density: $f(x_1, ..., x_p) = C(F_1(x_1), ..., F_p(x_p)) \prod_{k=1}^p f_k(x_k)$
 - Absolutely continuous joint distribution F
 - Strictly increasing and continuous marginal distributions F_1, \ldots, F_p and densities f_1, \ldots, f_p
- The copula density can be expressed in terms of the joint density and the marginals:

$$C(F_1(x_1),\ldots,F_p(x_p)) = \frac{f(x_1,\ldots,x_p)}{\prod_{k=1}^p f_k(x_k)}.$$

Parameter Estimation

Many different methods exist Inference from Margins:

- Estimate marginals (e.g. maximum likelihood fit)
- Assume copula family, c
- Maximum likelihood estimate of copula parameter θ

$$l(\theta) = \sum_{1}^{n} \log \left[c_{\theta}(\hat{F}_{1}(X_{1}), \dots, \hat{F}_{n}(X_{n})) \right]$$

• Since copulas are invariant to monotonic transformations, a semi–parametric approach:

$$l(\theta) = \sum_{1}^{n} \log \left[c_{\theta}(R(X_1), \dots, R(X_n)) \right]$$

Parameter estimation algorithms can be improved



Gaussian Mixture Copula Model (GMCM)

• Tewari et al (2011) propose a Gaussian Mixture Copula Model:

$$C(u_{i1}, u_{i2}, ..., u_{ip} \mid \boldsymbol{\vartheta}) = \frac{\sum_{g=1}^{G} \pi_g \phi(\mathbf{y}_i \mid \boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)}{\prod_{j=1}^{p} \psi_j(y_{ij})}$$

 $y_{ij} = \Psi_j^{-1}(u_{ij})$: inverse distribution values ψ_j : marginal density of the GMM along the *j*-th dimension Ψ_j^{-1} : inverse distribution function of the GMM along the *j*-th dimension

- Dependence structure from GMM
- No distributional assumption on the marginal is required
- ullet Gradient-descent based heuristic: maximum-likelihood estimate of $oldsymbol{artheta}$
- Application: clustering



Gaussian Mixture Copula Model (GMCM)

• For a heterogenous dataset $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n)$,

$$\log \mathcal{L}\left(\boldsymbol{\vartheta} \mid \mathbf{u}_{1}, \mathbf{u}_{2}, ..., \mathbf{u}_{n}\right) = \sum_{i=1}^{n} \log \frac{\sum_{g=1}^{G} \pi_{g} \phi(\mathbf{y}_{i} \mid \boldsymbol{\mu}_{g}, \boldsymbol{\Sigma}_{g})}{\prod_{j=1}^{p} \psi_{j}(y_{ij})}$$

- $\pi_g > 0$, with $\sum_{g=1}^G \pi_g = 1$, are mixing proportions,
- $\phi(\mathbf{x} \mid \boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)$ is multivariate Gaussian density with mean $\boldsymbol{\mu}_g$ and covariance matrix $\boldsymbol{\Sigma}_g$,
- $\vartheta = (\pi_1, \ldots, \pi_G, \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_G, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_G),$
- $u_{ij} = F_j(x_{ij})$ and F_j is the unknown marginal distribution for the *j*-th dimension,
- $y_{ij} = \Psi_j^{-1}(u_{ij})$ where Ψ_j and ψ_j are the marginal CDF and marginal pdf of the GMM along the *j*-th dimension.



EM for GMM

Initialize $\mu_g, \Sigma_g, \pi_g > 0, \qquad g = 1, \dots, G.$

REPEAT

[E step]

$$z_{ig}^{(t)} = \frac{\pi_g^{(t)} \phi(\mathbf{x}_i \mid \boldsymbol{\mu}_g^{(t)}, \boldsymbol{\Sigma}_g^{(t)})}{\sum_{g=1}^{G} \pi_g^{(t)} \phi(\mathbf{x}_i \mid \boldsymbol{\mu}_g^{(t)}, \boldsymbol{\Sigma}_g^{(t)})}$$

• [M step] For each g, update μ_g , Σ_g , π_g that maximizes likelihood:

$$\begin{aligned} \bullet & \pi_g^{(t+1)} = \frac{\sum_{i=1}^n z_{ig}^{(t)}}{n} \\ \bullet & \mu_g^{(t+1)} = \frac{\sum_{i=1}^n z_{ig}^{(t)} \mathbf{x}_i}{\sum_{i=1}^n z_{ig}^{(t+1)}} \\ \bullet & \mathbf{\Sigma}_g^{(t+1)} = \frac{\sum_{i=1}^n z_{ig}^{(t+1)} \left(\mathbf{x}_i - \boldsymbol{\mu}_g^{(t+1)}\right)^T \left(\mathbf{x}_i - \boldsymbol{\mu}_g^{(t+1)}\right)}{\sum_{i=1}^n z_{ig}^{(t)}} \\ \bullet & \text{Likelihood,} \\ & L^{(t+1)} = \prod_{i=1}^n \sum_{g=1}^G \pi_g^{(t+1)} \frac{1}{\sqrt{\det(2\pi \mathbf{\Sigma}_g^{(t+1)})}} \times \\ & \exp\{-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_g^{(t+1)})^T \mathbf{\Sigma}_g^{(t+1)^{-1}} (\mathbf{x}_i - \boldsymbol{\mu}_g^{(t+1)})\} \end{aligned}$$

UNTIL termination criterion reached



A modified EM algorithm

- The y_{ij} values change at every iteration
- The conventional EM algorithm of a GMM, where the inputs remain fixed in each iteration, cannot be directly used here
- Our algorithm runs iteratively with the standard Expectation (E) and Maximization (M) steps and an additional step in each iteration
- The (E) and (M) steps update the parameters based on y_{ij}
- The additional step updates y_{ij} based on the parameters
- \bullet y_{ii} is truncated above to ensure convergence



A modified EM algorithm

- Initialize: Standardize the matrix $X = (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_p)$. Set $\boldsymbol{\vartheta}^{(0)}$ randomly or by K-means clustering under the constraints that $\pi_g^{(0)} > 0$, $\sum_{g=1}^G \pi_g^{(0)} = 1$ and $\boldsymbol{\Sigma}_g^{(0)}$ is positive definite, and set $\delta_i = \min_{g,j} |y_{ij}^{(0)} - 2\kappa^{(0)} \left(\left[\boldsymbol{\Sigma}_g^{(0)} + I \right]^{-1} \boldsymbol{\Sigma}_g^{(0)} \mathbf{1} \right)_i |$. Set $u_{ij} = F_j(x_{ij})$.
- **Quantized** Repeat the following steps until $||L^{(t+1)} L^{(t)}|| < \gamma$.
 - $\bullet \quad \text{Set } y_{ij}^{(t)} = \min \left(\Lambda_{ij}^{(t)}, \Gamma_{ij}^{(t)} \right) \text{ where } \Lambda_{ij}^{(t)} = \left(\sum_{g=1}^G \frac{\pi_g^{(t)}}{\sigma_{g,ij}^{(t)}} \right)^{-1} \left[u_{ij} + \frac{1}{\sqrt{2\pi}} \sum_{g=1}^G \frac{\pi_g^{(t)} \mu_{ij}^{(t)}}{\sigma_{g,ij}^{(t)}} \frac{1}{2} \right],$ $\Gamma_{ij}^{(t)} = \kappa^{(t)} \left(\left[S_i^{(t)} + I \right]^{-1} S_i^{(t)} \mathbf{1} \right)_j \frac{\delta_i}{2} (3 \frac{p}{m_i^{(t)} + p}), \\ \kappa^{(t)} = \max_{g,j} (\mu_{gj}^{(t)}), \\ S_i^{(t)} = \sum_{g=1}^G z_{ig}^{(t-1)} \mathbf{\Sigma}_g^{(t)}, \\ \text{ and } m_i^{(t)} \text{ is the sum of all elements of } S_i^{(t)}.$
 - E-Step: $z_{ig}^{(t)} = \frac{\pi_g^{(t)} \phi(\mathbf{y}_i^{(t)} | \boldsymbol{\mu}_g^{(t)}, \boldsymbol{\Sigma}_g^{(t)})}{\sum_{g=1}^G \pi_g^{(t)} \phi(\mathbf{y}_i^{(t)} | \boldsymbol{\mu}_g^{(t)}, \boldsymbol{\Sigma}_g^{(t)})}$.
 - M-Step:

$$\pi_g^{(t+1)} = \frac{\sum_{i=1}^n z_{ig}^{(t)}}{n}, \mu_g^{(t+1)} = \frac{\sum_{i=1}^n z_{ig}^{(t)} \mathbf{y}_i^{(t)}}{\sum_{i=1}^n z_{ig}^{(t)}}, \mathbf{\Sigma}_g^{(t+1)} = \frac{\sum_{i=1}^n z_{ig}^{(t+1)} \left(\mathbf{y}_i^{(t)} - \boldsymbol{\mu}_g^{(t+1)}\right)^t \left(\mathbf{y}_i^{(t)} - \boldsymbol{\mu}_g^{(t+1)}\right)}{\sum_{i=1}^n z_{ig}^{(t)}}$$

Likelihood:

$$\mathcal{L}^{(t+1)} = \prod_{i=1}^{n} \sum_{g=1}^{G} \pi_g^{(t+1)} \frac{1}{\sqrt{\det(2\pi \mathbf{\Sigma}_g^{(t+1)})}} \times \exp{-\frac{1}{2}(\mathbf{y}_i^{(t)} - \boldsymbol{\mu}_g^{(t+1)})^T \mathbf{\Sigma}_g^{(t+1)}^{-1}(\mathbf{y}_i^{(t)} - \boldsymbol{\mu}_g^{(t+1)})}$$



Theoretical results

Lemma

For each i and j, with probability more than 0.9975, y_{ij} can be approximated as

$$y_{ij} pprox \left(\sum_{g=1}^G rac{\pi_g}{\sqrt{\sigma_{g,ij}}}
ight)^{-1} \left[u_{ij} + rac{1}{\sqrt{2\pi}} \sum_{g=1}^G rac{\pi_g \mu_{gj}}{\sqrt{\sigma_{g,ij}}} - rac{1}{2}
ight].$$

Lemma

If
$$Max \mid y_{ij}^{(t+1)} - y_{ij}^{(t)} \mid \leq \delta_i$$
, then

$$\log \mathcal{C}(\boldsymbol{\vartheta}^{(t+1)}, \mathbf{y}_i^{(t+1)} \mid \mathbf{z}_i^{(t)}) \geq \log \mathcal{C}(\boldsymbol{\vartheta}^{(t+1)}, \mathbf{y}_i^{(t)} \mid \mathbf{z}_i^{(t)}).$$

Theorem

There exists t_0 such that $\mathcal{L}(\boldsymbol{\vartheta}^{(t+1)} \mid \mathbf{u}_1,...,\mathbf{u}_n) \geq \mathcal{L}(\boldsymbol{\vartheta}^{(t)} \mid \mathbf{u}_1,...,\mathbf{u}_n)$ for $t \geq t_0$.

PGMM

- Large number of parameters in the covariance matrices
- Constraints are imposed as $\Sigma_g = \Lambda_g \Lambda'_g + \Psi$ where Ψ is the matrix of white noise, Λ is a $p \times q$ matrix of factor loadings and q is the number of latent factors
- Mcnicholas and Murphy (2008) put constraints on the loading and noise structures to derive eight parsimonious covariance structures

Model ID	Λ_g	Ψ_g	$\Psi_g = \psi_g \mathbf{I}$	Cov. Parameters
CCC	Constrained	Constrained	Constrained	[pq - q(q-1)/2] + 1
CCU	Constrained	Constrained	Unconstrained	[pq - q(q-1)/2] + p
CUC	Constrained	Unconstrained	Constrained	[pq - q(q-1)/2] + G
CUU	Constrained	Unconstrained	Unconstrained	[pq - q(q-1)/2] + Gp
UCC	Unconstrained	Constrained	Constrained	G[pq - q(q-1)/2] + 1
UCU	Unconstrained	Constrained	Unconstrained	G[pq - q(q-1)/2] + p
UUC	Unconstrained	Unconstrained	Constrained	G[pq - q(q-1)/2] + G
UUU	Unconstrained	Unconstrained	Unconstrained	$G\{pq - q(q-1)/2\} + Gp$

The BIC

- The BIC (Schwartz, 1978) is used to select the best member of the PGMM family
- The BIC can be written

$$BIC = 2l(\mathbf{x}, \hat{\boldsymbol{\vartheta}}) - \rho \log n,$$

where $\hat{\vartheta}$ is the MLE of ϑ , ρ is the number of free parameters and n is the number of observations

 Keribin (1998, 2000) shows that the BIC gives consistent estimates of the number of mixture components under certain regularity conditions

Simulated data

- We generate 25 simulations each for eight different simulation settings
- Each simulation setting has 2-dimensional data points in four clusters
- Each data point is a product of a sample from a Multivariate Normal (MVN) distribution and another distribution as outlined in the table below
- In each simulation we generate the clusters by sampling from the distributions, f_i
- The tables in the next slide show the cluster distributions and sizes for each simulation setting

Simulation setup

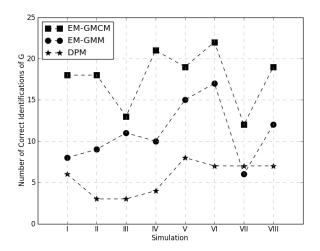
$$\begin{array}{l} f_1 = \text{MVN}(-5.5, I_2/2) \times \text{Unif}(0, 1) \\ f_2 = \text{MVN}(2, D_2) \times \text{t}(\text{df} = 9) \\ f_3 = \text{MVN}(3, \Delta) \times \text{C}(\text{loe} = 0, \text{sc} = 1) \\ f_4 = \text{MVN}(-5.5, I_2/2) \times \Gamma(\text{sh} = 0.5, \text{rt} = 1) \end{array}$$

Table: Parameter settings in each cluster; f_i : distribution in cluster $i=1,2,3,4,I_2$: 2×2 Identity matrix with, D_2 : 2×2 diagonal matrix with unequal diagonal elements and Δ : matrix with (i,j)-th element $0.9^{|i-j|}$. Abbreviations – C: Cauchy, loc: location, sc: scale, sh: shape, rt: rate.

Sim	$ c_1 $	c2	c ₃		Data size
I	400	300	300	500	1500
II	300	500	300	400	1500
III	300	300	500	400	1500
IV	500	400	300	300	1500
V	1200	900	900	1500	4500
VI	900	1500	900	1200	4500
VII	900	900	1500	1200	4500
VIII	1500	1200	900	900	4500

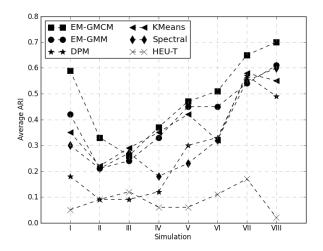
Table: Parameter settings for each simulation set: $|c_i|$ denotes size of cluster c_i for i = 1, 2, 3, 4.

Identification of right number of clusters





Classification Accuracy



Real data experiment I

- Cleveland Heart data set, obtained from UCI Repository.
- 297 patients.
- We extract five numerical features—age, resting blood pressure, serum cholesterol, maximum heart rate, ST depression induced by exercise.
- The task is to classify the individuals into two groups: those with and those without heart disease.
- we set the range of G (the number of clusters) and q (number of latent factors) in our algorithms to (1,2,3) and (1,2) respectively.
- For algorithms which do not estimate the number of clusters, such as K-means, Spectral clustering and HEU-T, we provide the correct number of clusters (2) as input.

Real data experiment I

- EM-GMCM detects the correct number of clusters, G = 2, with the CCU dependency structure and q = 1.
- EM-GMM incorrectly predicts 3 clusters with UCU dependence structure and q=2.

	Algorithm	EM-GMCM	EM-GMM	K-Means Spectral		HEU-T				
	Accuracy	70%	15%	57%	35%	50%				
EM-GMCM	EM-G	EM-GMM		K-Means		Spectral		HEU-T		
A B	A	B C	A	В	A	В		A	В	
A 137 23	A 19	69 72	A 110	50	A 64	96	A	114	46	
B 67 70	B 12	26 99	B 76	61	B 98	39	B	103	34	

Table: Above: Classification accuracy of the algorithms tested on the Cleveland Heart Disease Data. Below: Classification tables of the best models chosen by EM-GMCM and EM-GMM and of K-means, Spectral clustering and HEU-T for the Cleveland Heart data. *A*: group without heart disease, *B*: group with heart disease. EM-GMM erroneously estimates a third group *C*. True labels: horizontal, Estimated labels: vertical.

Real data experiment II

- Gamma Telescope data, obtained from UCI Repository.
- consists of features extracted from a preprocessed image of reconstructed radiation showers.
- 2000 observations with 10 features.
- The task is to statistically discriminate between two signals within the image: the primary gamma signal in Cherenkov radiation and background hadronic shower signal from cosmic rays in the upper atmosphere.
- We set the range of G (the number of clusters) and q (number of latent factors) in the algorithms to (1, 2, 3) and (1, 2, 3, 4) respectively.



V Moone Chaotrol

EM GMCM

Real data experiment II

- Both EM-GMCM and EM-GMM detect the correct number of clusters G=2 with the CCC dependency structure and number of latent factors, q = 3.
- However, EM-GMCM outperforms other methods in classification accuracy. EM CMM

			Augorium Em Ginem		Livi Giviivi It ivicans		Spectrar		IILC I					
			Acc	uracy	72%		59%	57%	54	1%	51%			
EM-GMCM			EM-GMM		K-Means		Spectral			HEU-T				
	A	В		A	В		A	В		A	В		A	В
A	814	186	A	731	269	A	857	143	A	1000	0	A	668	332
В	370	630	В	542	458	B	712	288	В	993	7	В	645	355

Table: Above: Classification accuracy of the algorithms tested on the Gamma Telescope Data. Below: Classification tables of the best models chosen by EM-GMCM and EM-GMM and of K-means, Spectral clustering and HEU-T. A: gamma signal, B: hadron showers (background). True labels: horizontal, Estimated labels: vertical.

Summary

- GMCM: models heterogeneous multimodal data where the dependence structure comes from a GMM
- GMCM based clustering outperforms popular approaches like GMM,
 K-means in our experiments
- Future work: high-dimensional, and categorical data

Research Challenges

- Better estimation algorithms
- Discrete Data
 - Sklar's Theorem: copula not unique
 - Hoff's extended rank likelihood approach
- High Dimensions

Copulas: higher dimensions

• A multivariate density may be decomposed into conditional densities:

$$f(x_1,...,x_n) = f_n(x_n).f(x_{n-1}|x_n)...f(x_1|x_2,...x_n)$$

 Each term in the above expression can be written as functions of bivariate copula densities:

$$f(x|v_1,\ldots,v_d) = c_{xv_j|v_{-j}}(F(x|v_{-j}),F(v_j|v_{-j})).f(x|v_{-j}),$$

where v_{-j} denotes the d-dimensional vector v excluding the j^{th} component.

• Example, $f(x_1|x_2,x_3) = c_{13|2}(F(x_1|x_2),F(x_3|x_2))f(x_1|x_2)$ and $f(x_2|x_3) = c_{23}(F(x_2),F(x_3)).f(x_2)$.



Copulas: higher dimensions

• The conditional distributions in the pair copula constructions, also called *h-functions*, are given by:

$$F(x|v) = \frac{\partial C_{x,v_j|v_{-j}}(F(x|v_{-j}), F(v_j|v_{-j}))}{\partial F(v_j|v_{-j})}.$$

 Analytic expressions for these h-functions have been derived for commonly used copulas. Thus all the densities in

$$f(x_1,...,x_n) = f_n(x_n).f(x_{n-1}|x_n)...f(x_1|x_2,...x_n)$$

may be expressed in terms of univariate marginals and bivariate copulas.

 This forms the basis of pair copula constructions for multivariate distributions.

Vines: hierarchical collection of copulas

A D-vine has n-1 hierarchical trees and n(n-1)/2 bivariate copulas for n random variables. For example,

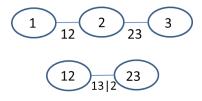


Figure: Three dimensional D Vine.

$$f(x_1, x_2, x_3) = f_1(x_1) f_2(x_2) f_3(x_3) c_{12}(F_1(x_1), F_2(x_2)) c_{23}(F_2(x_2), F_3(x_3)).$$

 $c_{13|2}(F(x_1|x_2), F(x_3|x_2))$



Thank you!

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