Modeling high-dimensional system inputs with copulas for uncertainty quantification problems

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The general problem

A system is subject to stochastic input $\boldsymbol{X} = (X_1, X_2, \ldots, X_d) \in \mathbb{R}^d$ with joint pdf $f(\boldsymbol{x})$ and joint cdf $F(\boldsymbol{x})$.

$\hookrightarrow$ produces a response $Y = \mathcal{M}(\boldsymbol{X})$. Goal: find $\mathcal{M}(\cdot)$.

1. Computational model of $\mathcal{M}$ (e.g.: finite element model, FEM). Often though: expensive ...
2. Surrogate model of $\mathcal{M}$ (e.g.: polynomial chaos expansion, PCE). Inexpensive to evaluate, but requires the knowledge of $f(\cdot)$

   $\hookrightarrow$ determine $f(\cdot)$

Outline

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Copula of independent variables

"Two random variables (r.v.s) are independent if and only if their joint probability distribution is the product of their marginal distributions"

$$X \perp\!\!\!\perp Y \Leftrightarrow F_{XY}(X,Y) = F_X(X) \cdot F_Y(Y).$$

In other (more complicated?) words:

$$X \perp\!\!\!\perp Y \Leftrightarrow F_{XY}(x,y) = C(F_X(x), F_Y(y)) \quad \forall (x,y) \in \mathcal{D}_X \times \mathcal{D}_Y$$

where $C : [0,1] \times [0,1] \,/\, C(u,v) = u \cdot v$.

Note: C is a bivariate cumulative distribution function (cdf):

- C is 2-increasing
- $C(u,0) = C(0,v) = 0 \quad \forall u,v$ (grounded) and $C(1,1) = 1$

Besides, C has uniform margins: $C(u,1) = u$, $C(1,v) = v$.

Density: $$c(u,v) = \frac{\partial C(u,v)}{\partial u \partial v} = 1 \quad \forall u,v.$$

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Upper Frechet-Hoeffding bound

What if $Y = \alpha(X)$, α monotone increasing?

$$\begin{aligned} F_{XY}(x,y) &= \mathbb{P}(X < x,\, \alpha(X) < y) \\ &= \mathbb{P}(X < x,\, X < \alpha^{-1}(X)) \\ &= F_X\left(\min(x,\, \alpha^{-1}(y))\right) \\ &= \min\left(F_X(x),\, F_X(\alpha^{-1}(y))\right) \\ &= \min\left(F_X(x), F_Y(y)\right) \end{aligned}$$

$\Rightarrow F_{XY}(x,y) = C(F_X(x), F_Y(y))$, where

$$C : [0,1] \times [0,1] \,/\, C(u,v) = \min(u,v).$$

C: **upper Frechet-Hoeffding bound**, maximal positive dependence.

Note: C is a bivariate probability distribution over $[0,1] \times [0,1]$ with uniform margins:

$$C(u,1) = \min(u,1) = u, \qquad C(1,v) = \min(1,v) = v.$$

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Lower Frechet-Hoeffding bound

What if $Y = \beta(X)$, β monotone decreasing?

$$
\begin{aligned}
F_{XY}(x, y) &= \mathbb{P}(X < x,\, \beta(X) < y) \\
&= \dots \\
&= \max(0, F_X(x) + F_Y(y) - 1)
\end{aligned}
$$

$\Rightarrow F_{XY}(x, y) = C(F_X(x), F_Y(y))$, where

$$C : [0, 1] \times [0, 1] \,/\, C(u, v) = \max(0, u + v - 1).$$

C: **lower Frechet-Hoeffding bound**, maximal negative dependence.

Note: C is a bivariate probability distribution over $[0, 1] \times [0, 1]$ with uniform margins:

$$C(u, 1) = \max(0, u) = u, \qquad C(1, v) = \max(0, v) = v.$$

Sklar's theorem

So far: We could write $\boxed{F_{XY}(x,y) = C(F_X(x), F_Y(y))}$, with C bivariate distribution on $[0,1]\times[0,1]$ with uniform margins, when:

- $\boldsymbol{X \perp\!\!\!\perp Y}$ **:** $C(u,v) = u \cdot v$
- $\boldsymbol{Y = \alpha(X)}$**,** $\boldsymbol{\alpha}$ **increasing:** $C(u,v) = \min(u,v)$
- $\boldsymbol{Y = \beta(X)}$**,** $\boldsymbol{\beta}$ **decreasing:** $C(u,v) = \max(0, u+v-1)$

Is it always possible to decompose a joint cdf F_{XY} in a cdf C on $[0,1]\times[0,1]$ with uniform margins applied to F_X and F_Y?

Theorem (Sklar, 1959)

*Yes (under very general conditions). C: **copula** between X and Y. C is unique if F_X, F_Y are continuous: $C(u,v) = F_{XY}(F_X^{-1}(u), F_X^{-1}(v))$. Besides, for any copula C and univariate cdfs F_X, F_Y, the function $C(F_X, F_Y)$ is a joint cdf with margins F_X, F_Y.*

Valid for any dimension d.

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Valid for any dimension d.

Copulas in d dimensions

Just like any multidimensional distributions:

- Copulas generalize to any dimension
- Multidimensional copulas of specific families rarely fit data well

Example:

(X_1, X_2, X_3) such that

- X_1, X_2: negative correlated, no tail dependence (Gaussian copula?)
- X_2, X_3: positive correlated, upper tail dependence (Gumbel copula?)
- X_1, X_3: something else

Copula of (X_1, X_2, X_3)?

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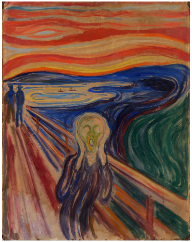
In large dimensions:



Outline

High-dim copula factorization

A d-copula, $d \geq 3$, can be factorized into $\binom{d}{2}$ conditional pair-copulas: **vine construction***

Remember the **law of total probability**:

$$f_{12\ldots d}(x_1, x_2, \ldots, x_d) = f_{1|2\ldots d}(x_1|x_2, \ldots, x_d) \cdot f_{2|3\ldots d}(x_2|x_3, \ldots, x_d) \cdot \ldots \cdot f_{d-1|d}(x_{d-1}|x_d) \cdot f_d(x_d)$$

$$\text{LHS:} \quad f_{1\ldots d}(x_1, \ldots, x_d) = c(F_1(x_1), \ldots, F_d(x_d)) \cdot \prod_{i=1}^{d} f_i(x_i)$$

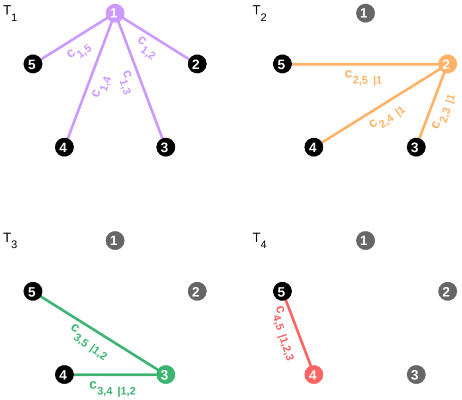
$$\text{RHS:} \quad f(x|\boldsymbol{v}) = c_{xv_j|\boldsymbol{v}_{-j}}\left(F(x|\boldsymbol{v}_{-j}), F(v_j|\boldsymbol{v}_{-j})\right) \cdot f_{x|\boldsymbol{v}_{-j}}(x|\boldsymbol{v}_{-j})$$

$$= \ldots = \prod(\text{pair-copulas}) \cdot \prod_{i=1}^{d} f_i(x_i)$$

* see Bedford and Cooke, 2002. The Annals of Statistics 30(4):1031-68

C-(anonical) vines

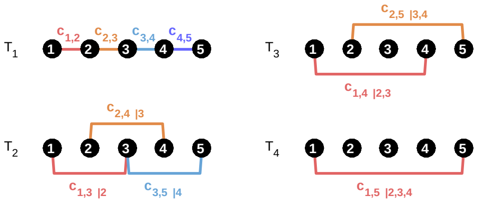
$$c_{12345} = c_{12} \cdot c_{13} \cdot c_{14} \cdot c_{15} \cdot$$
$$c_{23|1} \cdot c_{24|1} \cdot c_{25|1} \cdot$$
$$c_{34|12} \cdot c_{35|12} \cdot$$
$$c_{45|123}$$



For d variables: $d!$ different C-vines

D-(rawable) vines

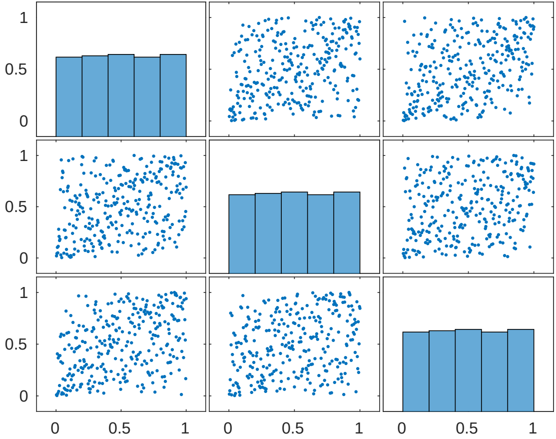
$$c_{12345} = c_{12} \cdot c_{23} \cdot c_{34} \cdot c_{45} \cdot c_{13|2} \cdot c_{24|3} \cdot c_{35|4} \cdot c_{14|23} \cdot c_{25|34} \cdot c_{15|234}$$



For d variables: $d!$ different D-vines

Example 1

(X_1, X_2, X_3): Gaussian copula ($\rho = 0.3$), $X_i \sim U([-i, i])$. 300 samples



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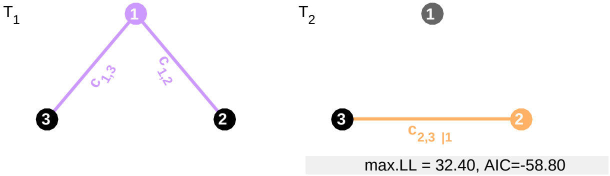
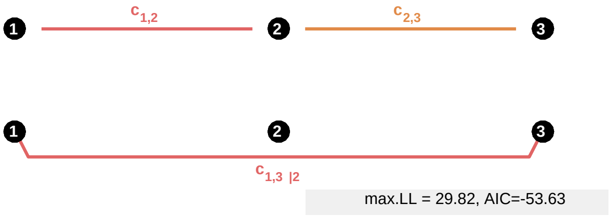
C-Vine:



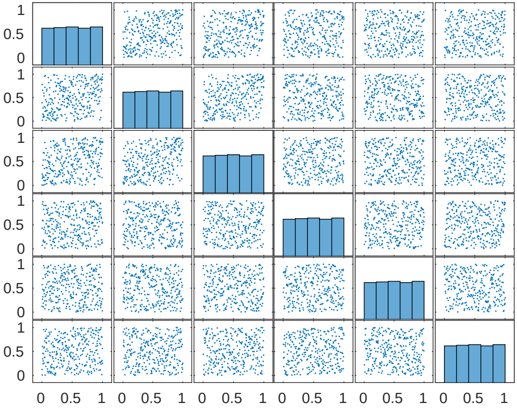
D-Vine:



For $d = 3$, C-vines are D-vines and vice versa.

Example 2

- (X_1, X_2, X_3): Gaussian copula $(\rho = 0.3)$, $X_i \sim U([-i, i])$
- $X_{5(6)} = X_4 + U_{1(2)}, \quad U_1 \perp\!\!\!\perp U_2 \qquad \Rightarrow X_5 \perp\!\!\!\perp X_6 | X_4 \; (\rho = 0.3)$
- $(X_1, X_2, X_3) \perp\!\!\!\perp (X_4, X_5, X_6)$ (300 samples)



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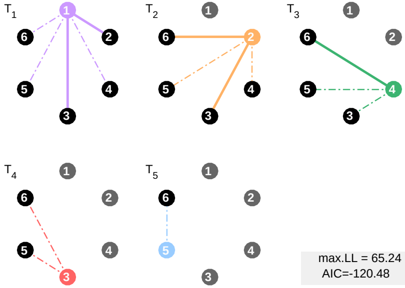
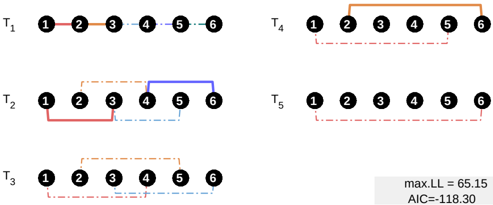


max.LL = 65.24
AIC=-120.48

$$(X_1, X_2, X_3) \perp\!\!\!\perp (X_4, X_5, X_6)$$
$$X_5 \perp\!\!\!\perp X_6 | X_4$$

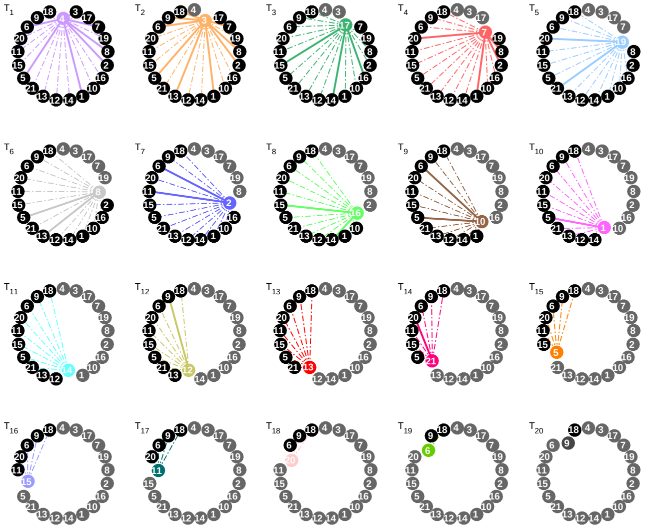
$\leftarrow$ C-Vine

D-Vine $\rightarrow$



max.LL = 65.15
AIC=-118.30

Example 3: 21 variables, 5 mutually independent groups



max.LL = 353.24, AIC=-604.48

$$\underbrace{(X_1, \ldots, X_8)}_{C^{\mathcal{G}}}$$

$$\perp\!\!\!\perp$$

$$\underbrace{(X_9, \ldots, X_{13})}_{X_i = X_9 + U_i, i \geq 10}$$

$$\perp\!\!\!\perp$$

$$\underbrace{(X_{14}, \ldots, X_{17})}_{C^{\mathcal{G}}}$$

$$\perp\!\!\!\perp$$

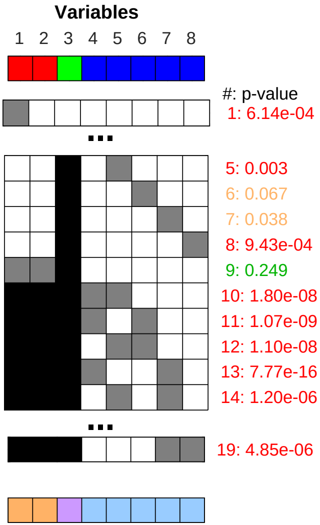
$$X_{18}$$

$$\perp\!\!\!\perp$$

$$\underbrace{(X_{19}, X_{20}, X_{21})}_{C^{\mathcal{G}}}$$

Outline

Identification of independent components



Input variables form independent sub-groups:

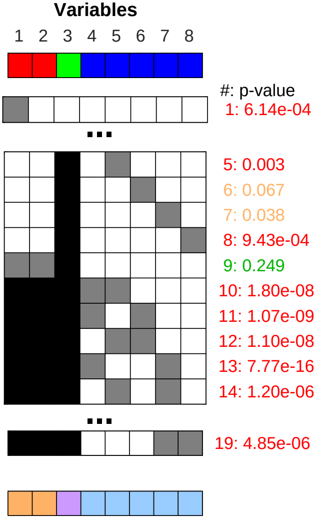
$$(X_1, X_2) \perp X_3 \perp (X_4, \ldots, X_8)$$

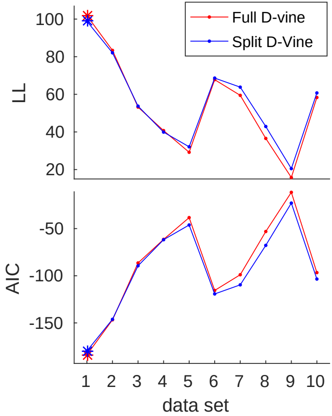
Then:

- Search for these groups first, via hierarchical testing
- Fit vine to each subgroup individually:

$$\begin{aligned} \mathcal{V}_{1\ldots8} &= \mathcal{V}_{1,2} \cdot \mathcal{V}_{3} \cdot \mathcal{V}_{4\ldots8} \\ &= C_{1,2} \cdot 1 \cdot \mathcal{V}_{4\ldots8} \end{aligned}$$

Vine fitting to independent components





Conclusions

To model the stochastic input $\boldsymbol{X} = (X_1, \ldots, X_d)$ to a system, we can

- Decompose the joint cdf $F_{12\ldots,d}$ in the **copula** (dependence structure) $C_{12\ldots d}$ applied to the margins $F_1, F_2, \ldots, F_d$:

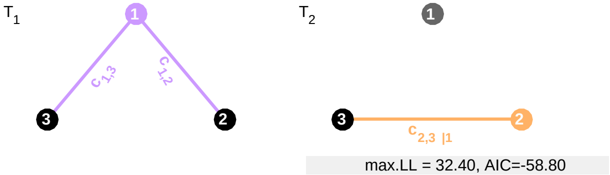
$$F_{12\ldots,d}(x_1, x_2, \ldots, x_d) = C_{12\ldots d}\left(F_1(x_1), F_2(x_2), \ldots, F_d(x_d)\right)$$

- Fit margins and copula separately $\Rightarrow$ much greater flexibility
- Model $C_{12\ldots d}$ as a **vine**, i.e. a product of pair copulas:
  - First fit $d-1$ unconditional copulas C_{ij} (tree T_1), e.g. by ML
  - Given the trees T_1 up to T_{i-1}, model the conditional copulas of T_i
  - Re-fit full vine by global log-likelihood maximization
- ...Or first separate $\boldsymbol{X}$ into independent components, and then fit a vine to each component
- Rosenblatt-transform the data into independent variables $\boldsymbol{X'} = (X'_1, X'_2, \ldots, X'_d)$
- Apply surrogate methods (e.g. PCE) to find $\boldsymbol{Y} = \mathcal{M}(\boldsymbol{X'})$

Example 1: algorithm

(X_1, X_2, X_3): Gaussian copula ($\rho = 0.3$), $X_i \sim U([-i, i])$. 300 samples

C-Vine:



- Tree T_1: choose $c_{1,2}$ and $c_{1,3}$ and fit to the data
- Tree T_2: obtain $c_{2,3|1}\left(F_{2|1}(x_2|x_1), F_{3|1}(x_3|x_1)\right)$ as follows:
    - Obtain $F_{2|1} = \partial C_{12}(F_1, F_2)/\partial F_1$ and $F_{3|1} = \partial C_{13}(F_1, F_3)/\partial F_1$ (from the previous tree)
    - Transform the data $x_i \to x_i' = F_{i|1}(x_i|x_1)$, $i = 2, 3$
    - Obtain $C_{2,3|1}$ as the copula between x_2' and x_3', fitted to the data. **under the simplifying assumption:** $C_{2,3|1}$ does not depend on x_1

This procedure generalizes to larger trees by iteration.

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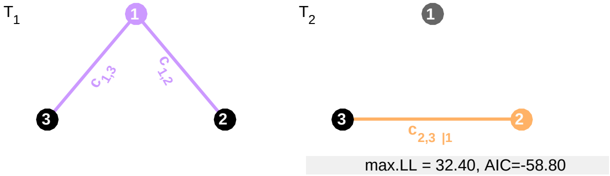

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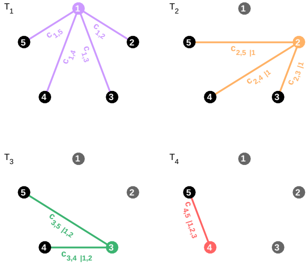
  - Transform the data $x_i \to x'_i = F_{i|1}(x_i|x_1)$, $i = 2, 3$
  - Obtain $C_{2,3|1}$ as the copula between x'_2 and x'_3, fitted to the data. **under the simplifying assumption:** $C_{2,3|1}$ does not depend on x_1

This procedure generalizes to larger trees by iteration.

Simplifying assumption

$C_{i,j|k_1,\dots,k_l}(u_i, u_j | u_{k_1}, \dots, u_{k_l})$ does not depend on $u_{k_1}, \dots, u_{k_l}$, $k_h \neq i, j$.

Used to estimate $C_{i,j|k_1,\dots,k_l}$ as the 2-copula between $F_{i|k_1,\dots,k_l}(u_i | u_{k_1}, \dots, u_{k_l})$ and $F_{j|k_1,\dots,k_l}(u_j | u_{k_1}, \dots, u_{k_l})$, obtained from previous trees.



Holds for (See Joe, 2015, *Dependence Modeling with Copulas*, p.118):

- Gaussian copula:

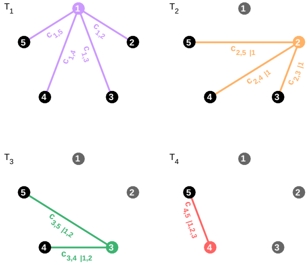
$$C_{i,j|k_1,k_2,\dots,k_l}(u_i, u_j | u_{k_1}, \dots, u_{k_l}) = \Phi_2(\Phi^{-1}(u_i), \Phi^{-1}(u_j); \rho_{i,j|k_1,k_2,\dots,k_l}) \\ = C^{\mathcal{G}}(u_i, u_j; \rho_{i,j|k_1,k_2,\dots,k_l})$$

  where $\rho_{i,j|k_1,k_2,\dots,k_l}$ is a partial correlation coefficient, a function of all correlation coefficients $\rho_{n,m}$.

Simplifying assumption

$C_{i,j|k_1,\ldots,k_l}(u_i, u_j | u_{k_1}, \ldots, u_{k_l})$ does not depend on $u_{k_1}, \ldots, u_{k_l}$, $k_h \neq i, j$.

Used to estimate $C_{i,j|k_1,\ldots,k_l}$ as the 2-copula between $F_{i|k_1,\ldots,k_l}(u_i | u_{k_1}, \ldots, u_{k_l})$ and $F_{j|k_1,\ldots,k_l}(u_j | u_{k_1}, \ldots, u_{k_l})$, obtained from previous trees.



Holds for (See Joe, 2015, *Dependence Modeling with Copulas*, p.118):

- Gaussian copula
- Multivariate t copula, and extensions to elliptical distributions with finite support (and only those)
- Archimedean copulas based on gamma LT and their extensions to negative dependence (and those only)
- GB2 copula, Dirichlet copula, ...
- Several other families, though often only for specific vines

Rosenblatt transform

Goal: transform input r.v.s $(X_1, \ldots, X_d)$ into mutually independent r.v.s $(X'_1, \ldots, X'_d)$ such that $X'_i \perp\!\!\!\perp X'_j \quad \forall i \neq j$.

Remember again:

$$F_{12\ldots d}(x_1, x_2, \ldots, x_d) = F_1(x_1) \cdot F_{2|1}(x_2|x_1) \cdot F_{3|2,1}(x_3|x_2, x_1) \cdot \ldots \cdot F_{d|d-1,\ldots,1}(x_d|x_{d-1}, \ldots, x_1)$$

Theorem (Rosenblatt transform)

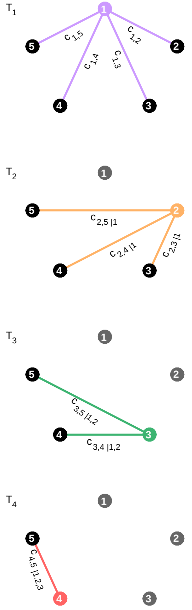
The r.v.s

$$\begin{cases} X'_1 = F_1(X_1) \\ X'_2 = F_{2|1}(X_2|X_1) \\ \ldots \\ X'_d = F_{d|d-1,\ldots,1}(X_d|X_{d-1}, \ldots, X_1) \end{cases}$$

are mutually independent.

Rosenblatt transform of C-vines

$$
\begin{cases}
F_1(x_1) : \text{obtained from data} \\[2ex]
F_{2|1}(x_2|x_1) = \underbrace{C_{2|1}}_{\partial_1 C_{12}} (F_1(x_1), F_2(x_2)) \text{ (from tree 1)} \\[2ex]
F_{3|2,1}(x_3|x_2,x_1) = \underbrace{\underbrace{C_{3|2,1}}_{\partial_1 C_{23|1}}}_{\text{from tree 2}} \underbrace{\left(\underbrace{F_{3|1}(x_3|x_1)}_{\partial_1 C_{13}} \middle| \underbrace{F_{2|1}(x_2|x_1)}_{\partial_1 C_{12}} \right)}_{\text{from tree 1}} \\[2ex]
F_{4|3,2,1}(x_4|x_3,x_2,x_1) = \\
\quad = \underbrace{\underbrace{C_{4|3,2,1}}_{\partial_1 C_{34|12}}}_{\text{from tree 3}} \underbrace{\left(\underbrace{F_{4|2,1}(x_4|x_2,x_1)}_{\partial_1 C_{24|1}(F_{2|1},F_{4|1})} \middle| \underbrace{F_{3|2,1}(x_3|x_2,x_1)}_{\partial_1 C_{23|1}(F_{2|1},F_{3|1})} \right)}_{\text{from tree 2 (and recursively 1)}} \\
\quad \vdots \\
F_{d|d-1,\ldots,1}(x_d|x_{d-1},\ldots,x_1) : \text{from trees } d-2, d-1
\end{cases}
$$



Analogously for D-vines (see Aas et al, 2009).