Coupling aGrUM/pyAgrum with external libraries: an application to Copula Bayesian Networks

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Copula Bayesian Networks (CBNs)

- **Compact** representation of a joint probability distribution over a set of variables $\boldsymbol{X}$ using :

Bayesian Networks

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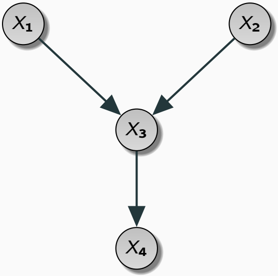
  - A Directed Acyclic Graph (*DAG*),



$$\mathcal{I}_l(\mathcal{G}) = \{(X_i \perp \mathrm{ND}_i | \mathrm{Pa}_i)\}.$$

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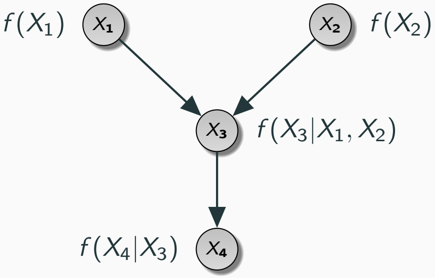

$$f(\boldsymbol{x}) = \prod_{i=1}^{n} f(x_i|\mathbf{pa}_i)$$

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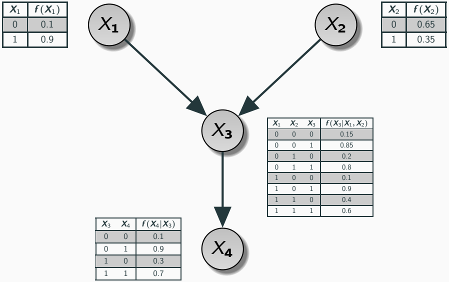

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X_2	$f(X_2)$
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X_1	X_2	X_3	$f(X_3 \mid X_1, X_2)$
0	0	0	0.15
0	0	1	0.85
0	1	0	0.2
0	1	1	0.8
1	0	0	0.1
1	0	1	0.9
1	1	0	0.4
1	1	1	0.6

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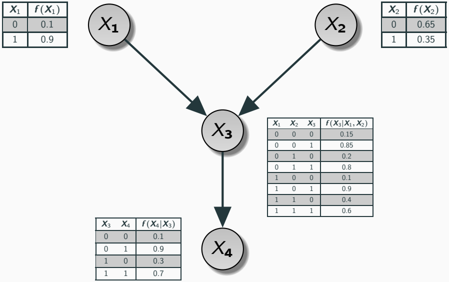

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Continuous case : ???

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- **Mixture models:** Langseth et al. 2012; Cortijo et al. 2016
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  2. Bad: Hard to learn

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Definition (Copula Nelsen 2007)

A copula function is a cumulative distribution function on $[0,1]^n$:

$$C(u_1, \ldots, u_n) = \mathbb{P}(U_1 \leq u_1, \ldots, U_n \leq u_n)$$

with **uniform** one-dimensional marginals :

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- If C is **absolutely continuous**, a copula density function c exists :

$$c(\mathrm{x}) = \frac{\partial^n C}{\partial x_1 \cdots \partial x_n}(x_1, \cdots, x_n)$$

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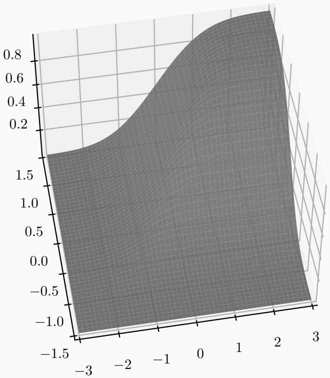
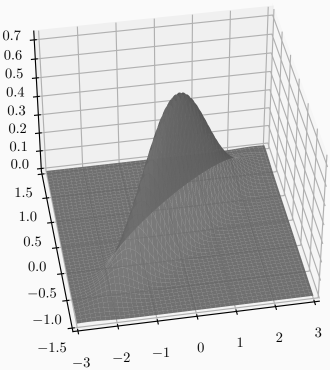
- Solution: use the BN framework over the copula function → Copula Bayesian Networks (CBNs) (Elidan 2010)

Example : Gaussian copula



(a) Gaussian CDF



(b) Gaussian PDF

- $(X_1, X_2) \backsim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, with $\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $\Sigma = \begin{pmatrix} 1 & 0.45 \\ 0.45 & 0.25 \end{pmatrix}$

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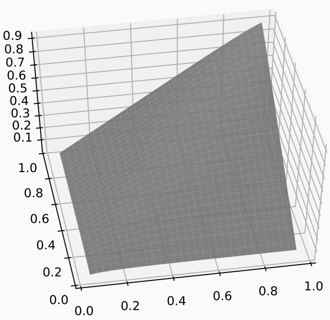
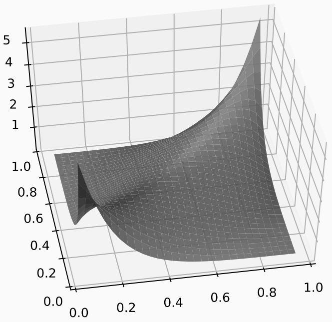


(a) Copula function



(b) Copula density function

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- $\Big(U_1 = \Phi_{0,1}(X_1),\ U_2 = \Phi_{0,\frac{1}{2}}(X_2)\Big) \backsim C_{\mathcal{N}}(R)$ with $R = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$

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- Same graphical language than classical BNs (same independences)
- Classic algorithms can be adapted for structural learning.

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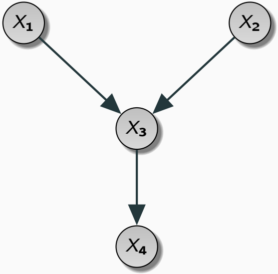

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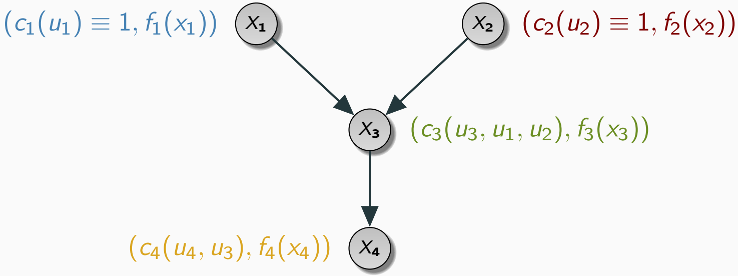

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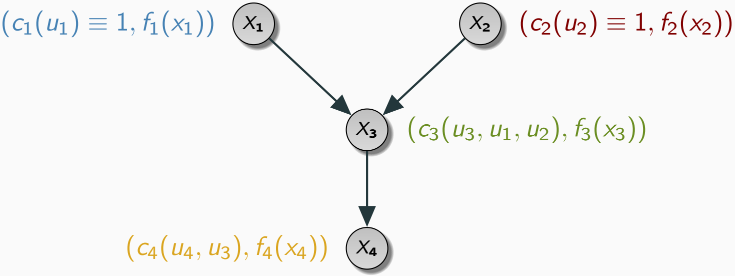

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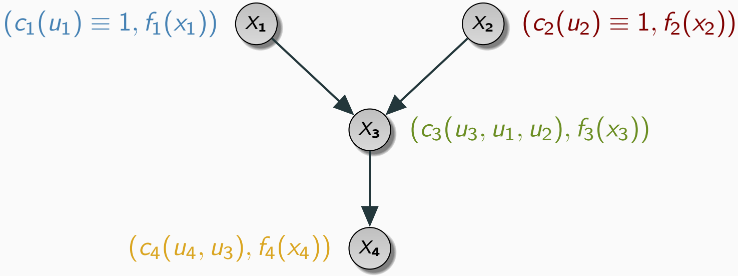

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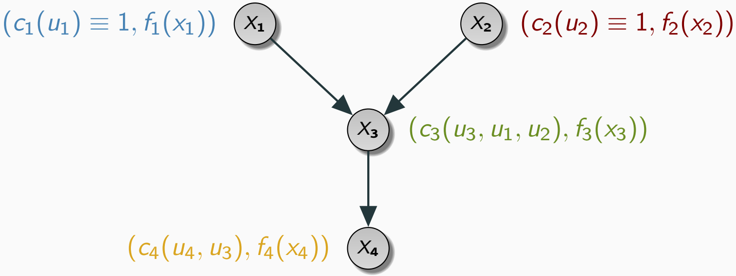

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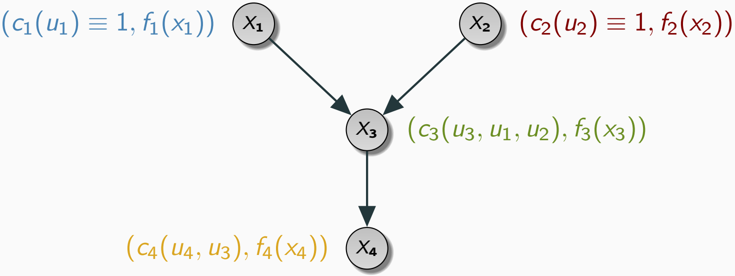

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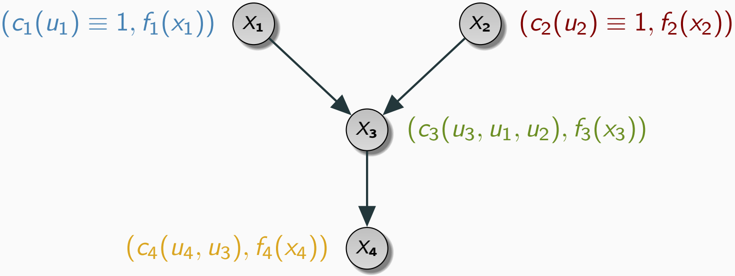

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- Non-parametric copulas: Empirical Bernstein Copula (EBC)

Non-parametric estimation : empirical Bernstein copula

- Sample $\mathcal{D} = \{\boldsymbol{x}[1], \dots, \boldsymbol{x}[m]\} \rightarrow$ Copula sample $\mathcal{C} = \{\boldsymbol{u}[1], \dots, \boldsymbol{u}[m]\}$ with $\boldsymbol{u}[m] = (u_1[m], \dots, u_n[m])$, $u_i[m] = F_i(x_i[m])$

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- Empirical Bernstein copula (EBC) $\hat{C}_B$:

$$\hat{C}^B_{K,m}(\boldsymbol{u}) = \sum_{v_1=0}^{K} \cdots \sum_{v_n=0}^{K} \hat{C}_m(\frac{v_1}{K}, \ldots, \frac{v_n}{K}) \prod_{i=1}^{n} B_{v_i,K}(u_i),$$

Non-parametric estimation : empirical Bernstein copula

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$$\hat{C}^B_{K,m}(\boldsymbol{u}) = \frac{1}{m} \sum_{i=1}^{m} \prod_{j=1}^{n} I_{r_j[i], s_j[i]}(u_j)$$

with $r_j[i] = \lceil K u_j[i] \rceil$, $s_j[i] = K - r_j[i] + 1$ and $I_{\alpha,\beta}$ the cumulative function of beta distribution,

Non-parametric estimation : empirical Bernstein copula

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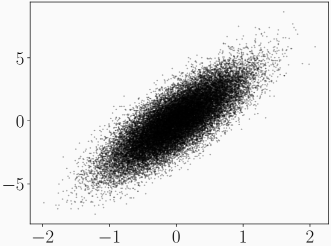
  with $r_j[i] = \lceil K u_j[i] \rceil$, $s_j[i] = K - r_j[i] + 1$ and $I_{\alpha,\beta}$ the cumulative function of beta distribution,
- Empirical Bernstein copula (EBC) density $\hat{c}_B$ by differentiation:

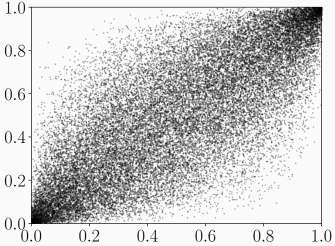
$$\hat{c}_B(\boldsymbol{u}) = \frac{1}{m} \sum_{i=1}^{m} \prod_{j=1}^{n} \beta_{r_j[i], s_j[i]}(u_j)$$

Non-parametric estimation : empirical Bernstein copula



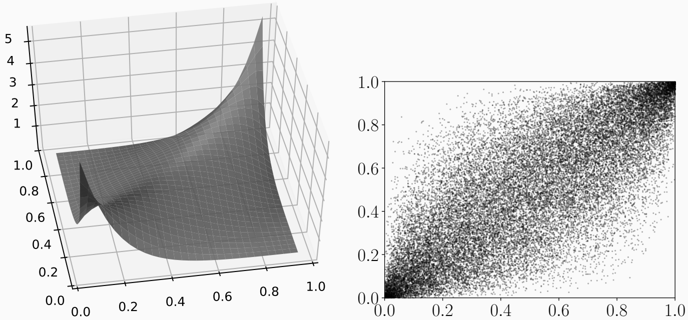
(a) Gaussian sample

Non-parametric estimation : empirical Bernstein copula



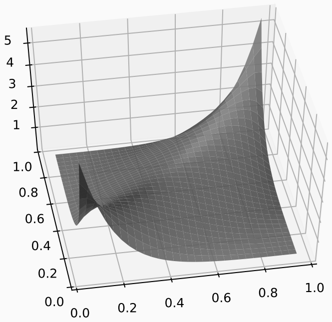
(a) Gaussian copula density sample

Non-parametric estimation : empirical Bernstein copula

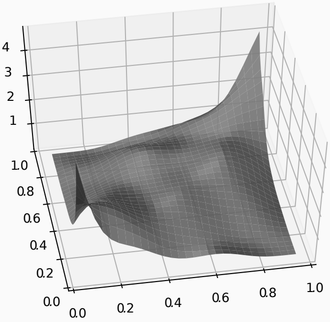


(a) Gaussian copula density **(b)** Gaussian copula density sample

Non-parametric estimation : empirical Bernstein copula

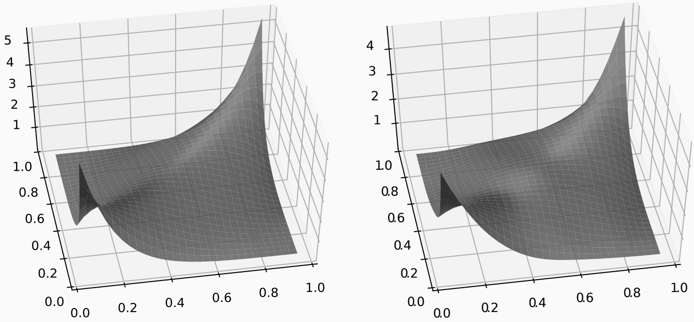


(a) Gaussian copula density

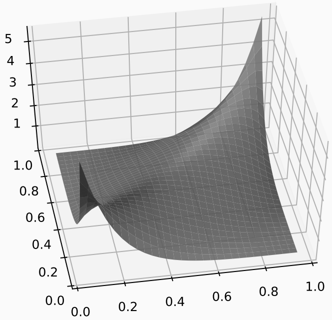


(b) Bernstein copula: $m = 10^2$

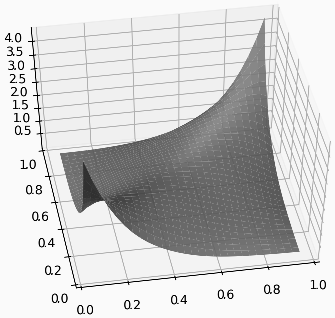
Non-parametric estimation : empirical Bernstein copula



(a) Gaussian copula density **(b)** Bernstein copula: $m = 10^3$



(a) Gaussian copula density



(b) Bernstein copula: $m = 10^4$

The otagrum module

otagrum: an open source library to learn CBNs

Two similar libraries (C++, python wrappers, open source):

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A module to rule them all: **otagrum**.

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- A CBN class,
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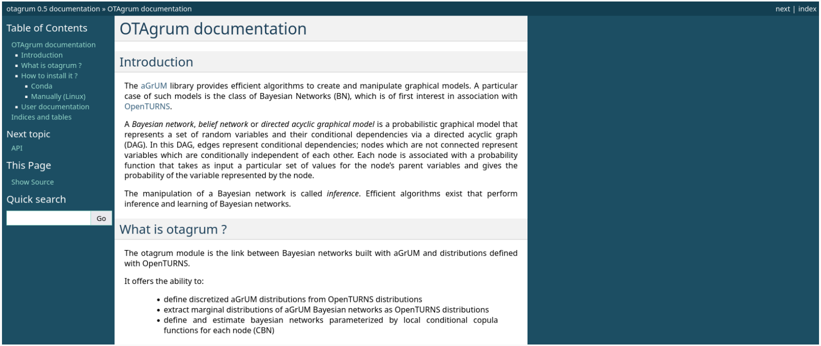
Where to find it ?

- Module : openturns/otagrum (GitHub)
- Experiments : MLasserre/otagrum-experiments (GitHub)

otagrum: installation

- Online website : `https://openturns.github.io/otagrum/master/index.html`



otagrum 0.5 documentation » OTAgrum documentation

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OTAgrum documentation

Introduction

The aGrUM library provides efficient algorithms to create and manipulate graphical models. A particular case of such models is the class of Bayesian Networks (BN), which is of first interest in association with OpenTURNS.

A *Bayesian network*, *belief network* or *directed acyclic graphical model* is a probabilistic graphical model that represents a set of random variables and their conditional dependencies via a directed acyclic graph (DAG). In this DAG, edges represent conditional dependencies; nodes which are not connected represent variables which are conditionally independent of each other. Each node is associated with a probability function that takes as input a particular set of values for the node's parent variables and gives the probability of the variable represented by the node.

The manipulation of a Bayesian network is called *inference*. Efficient algorithms exist that perform inference and learning of Bayesian networks.

What is otagrum ?

The otagrum module is the link between Bayesian networks built with aGrUM and distributions defined with OpenTURNS.

It offers the ability to:

- define discretized aGrUM distributions from OpenTURNS distributions
- extract marginal distributions of aGrUM Bayesian networks as OpenTURNS distributions
- define and estimate bayesian networks parameterized by local conditional copula functions for each node (CBN)

- Can be easily installed using conda:

```
$ conda install -c conda-forge otagrum
```

- Or manually to have the development version.

otagrum: an example of use

Using OTaGrUM: The wine data set

Importing modules

Entrée [1]:
```
import openturns as ot
import openturns.viewer as otv

import pyAgrum as gum
import pyAgrum.lib.notebook as gnb

import otagrum as otagr
```

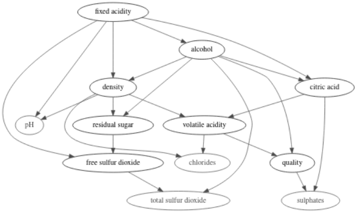
Loading data

Entrée [2]:
```
data_ref = ot.Sample.ImportFromTextFile('winequality-red.csv', ";")
```

otagrum: an example of use

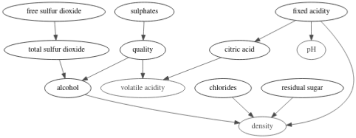
Structure learning with CBIC algorithm

Entrée [3]:
```
learner = otagr.TabuList(data_ref, 2, 10, 2) # Creating a TabuList learner
cbic_dag = learner.learnDAG()                # Learning DAG
gnb.showDot(cbic_dag.toDot())
```



Structure learning with CPC algorithm

Entrée [4]:
```
learner = otagr.ContinuousPC(data_ref, 4, 0.05) # Using a CPC learner
cpc_dag = learner.learnDAG()                    # Learning DAG
gnb.showDot(cpc_dag.toDot())
```

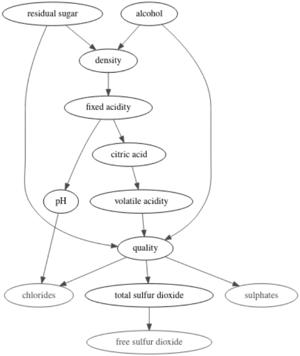


otagrum: an example of use

Structure learning with CMIIC algorithm

Entrée [5]:

```
learner = otagr.ContinuousMIIC(data_ref) # Using a CMIIC learner
learner.setAlpha(0.04)                   # Setting the value of alpha
cmiic_dag = learner.learnDAG()           # Learning DAG
gnb.showDot(cmiic_dag.toDot())
```



otagrum: an example of use

Parameter learning

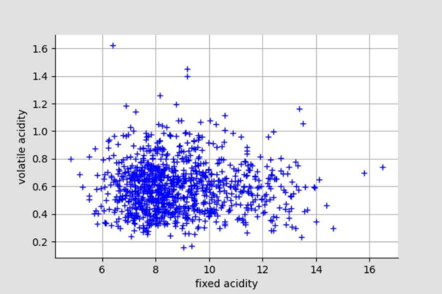
Entrée [7]:
```
cpc_cbn = otagr.ContinuousBayesianNetworkFactory(ot.KernelSmoothing(ot.Histogram()),
                                                 ot.BernsteinCopulaFactory(),
                                                 cpc_dag,
                                                 0.05,
                                                 4,
                                                 False).build(data_ref)
```

otagrum: an example of use

Sampling the CBN

Entrée [9]:
```
sample = cpc_cbn.getSample(1000)
ot.VisualTest.DrawPairs(sample.getMarginal([0,1]))
```

Out[9]:



Structure learning for CBNs

Learning algorithms

- CPC a continuous PC algorithm based on an independence test using Hellinger distance:
  - M. Lasserre et al. (May 2020). "Constraint-Based Learning for Non-Parametric Continuous Bayesian Networks". In: *FLAIRS 33 - 33rd Florida Artificial Intelligence Research Society Conference*. Miami, United States: AAAI, pp. 581–586
  - M. Lasserre et al. (2021a). "Constraint-based learning for non-parametric continuous bayesian networks". In: *Annals of Mathematics and Artificial Intelligence*, pp. 1–18
- CMIIC, an algorithm based on information theory:
  - M. Lasserre et al. (2021b). "Learning Continuous High-Dimensional Models using Mutual Information and Copula Bayesian Networks". In: *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 35. 13, pp. 12139–12146
- Improvement of the state of the art algorithm (CBIC) by using mutual information to speed up the calculations.

Comparison method

1. A reference structure is chosen : ALARM or random,
2. Copulas are parametrized : Gaussian, Student or Dirichlet,
3. Samples are generated from the CBN : forward-sampling,
4. A structure is learned from the generated data,
5. Structural scores are computed : F-score et SHD.

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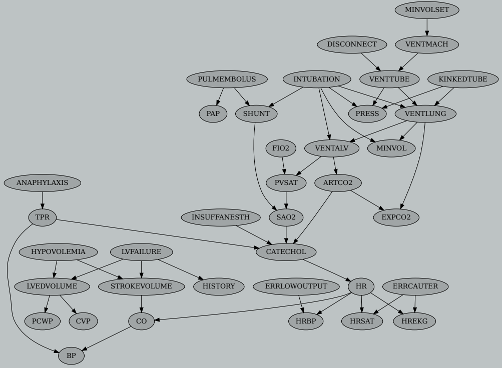

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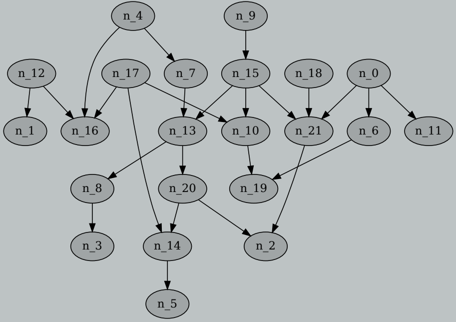

Number of nodes : n $\Longrightarrow$ Number of arcs : $\lfloor 1.2 \times n \rfloor$

Comparison method

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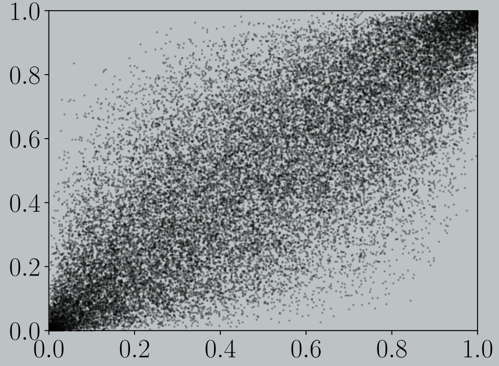

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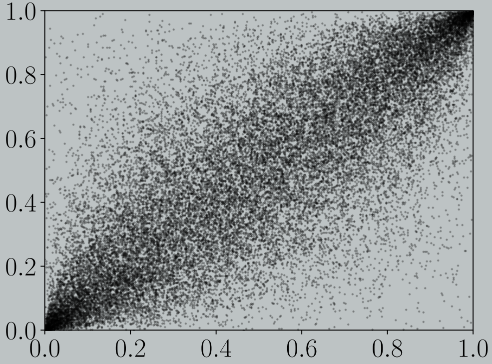

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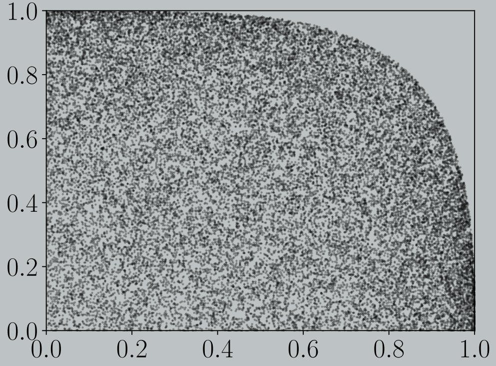

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Comparison method

1. A reference structure is chosen : ALARM or random,
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→ 5. Structural scores are computed : F-score et SHD.

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$\rightarrow$ 5. Structural scores are computed : **F-score** et SHD.

- **F-score** : skeleton (undirected structure)

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- **F-score** : skeleton (undirected structure)
  - Skeleton perfectly retrieved : **F-score = 1**

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- **Structural Hamming Distance** (SHD) : CPDAG (skeleton + v-structures)

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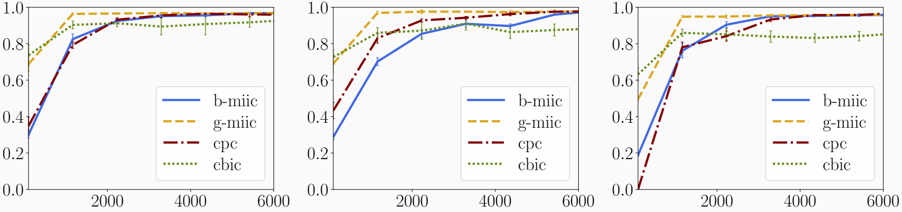
- **F-score** : skeleton (undirected structure)
  - Skeleton perfectly retrieved : **F-score = 1**
- **Structural Hamming Distance** (SHD) : CPDAG (skeleton + v-structures)
  - CPDAG perfectly retrieved : **SHD = 0**

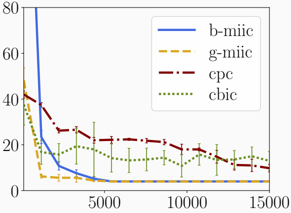
F-score evolution : ALARM structure



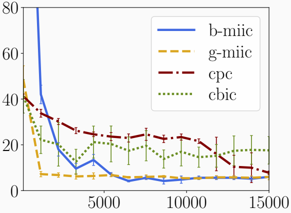
(a) Gaussian case **(b)** Student Case **(c)** Dirichlet case

F-score evolution for **CBIC**, **CPC**, **G-CMIIC** and **B-CMIIC** methods with respect to the **sample size**. For a given size, the results are averaged over 5 different samples generated from the **ALARM** structure.

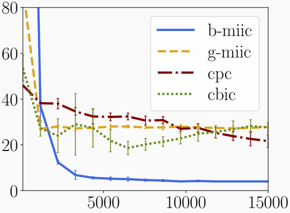
SHD evolution : ALARM structure



(a) Gaussian case



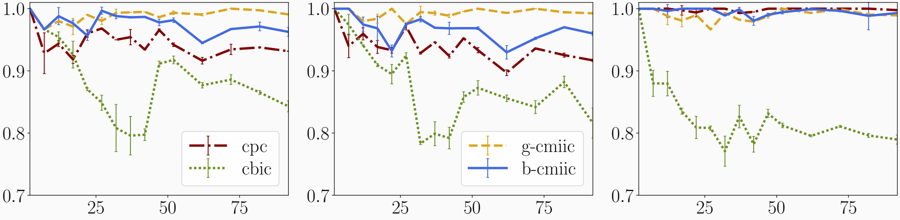
(b) Student case



(c) Dirichlet case

SHD evolution for **CBIC**, **CPC**, **G-MIIC** and **B-MIIC** methods with respect to the sample size. For a given size, the results are averaged over 5 different samples generated from the **ALARM** structure.

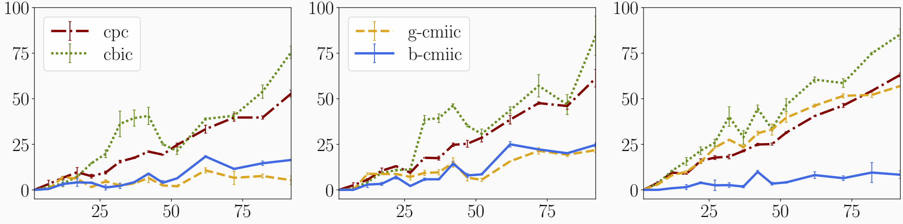
F-score evolution : random structures



(a) Gaussian case **(b)** Student case **(c)** Dirichlet case

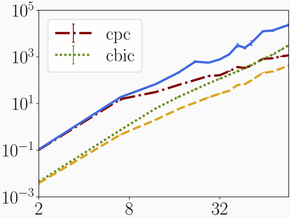
F-score evolution for **CBIC**, **CPC**, **G-MIIC** and **B-MIIC** methods with respect to the **dimension** of the random structures. The results are averaged over 2 random structures of same dimension and over 5 different samples of size $m = 10^4$.

SHD evolution : random structures

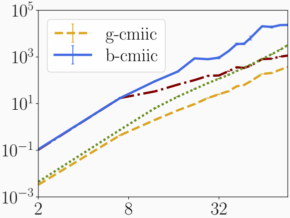


(a) Gaussian case **(b)** Student case **(c)** Dirichlet case

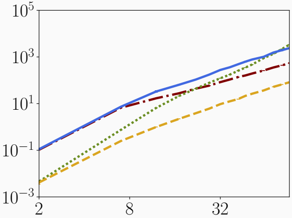
SHD evolution for **CBIC**, **CPC**, **G-CMIIC** and **B-CMIIC** methods with respect to the **dimension** of the random structure. The results are averaged over 2 different structures of same dimension and over 5 different samples of size $m = 10^4$.



(a) Gaussian case



(b) Student case



(c) Dirichlet case

Learning time in seconds for CBIC, CPC, G-CMIIC et B-CMIIC with respect to the **dimension** of the random structures. The results are averaged over 2 different **random structures** of same dimension and over 5 different samples of size $m = 10^4$.

Thank you for your attention !

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