The plugin otagrum: learning nonparametric Copula Bayesian Networks

Marvin LASSERRE

supervised by Pierre-Henri WUILLEMIN (LIP6) and Régis LEBRUN (Airbus CRT)

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- **Challenge:** Various non-parametric models exists to estimate a density but they are limited to a **few dimensions** (~ 5 variables),
- **Solution**: Use of Probabilistic Graphical Models (PGM) to break the joint distribution into a product of conditional distributions of **lesser dimensions**.

Modeling with copulas

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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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⚠ C becomes hard to model for high dimensions !

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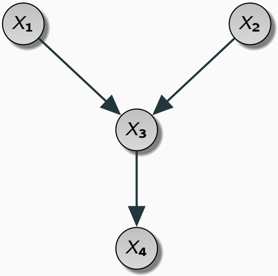

$$\mathcal{I}_l(\mathcal{G}) = \{(X_i \perp \mathrm{ND}_i | \mathrm{Pa}_i)\}.$$

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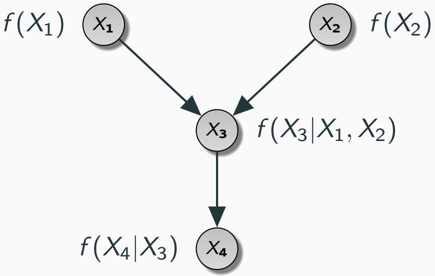

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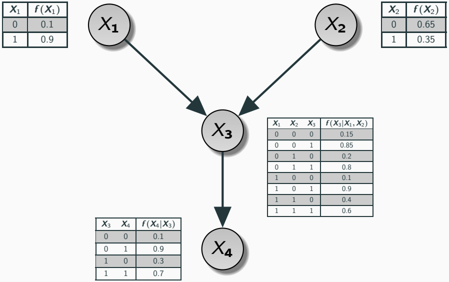

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1	0.35

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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Discrete case : Conditional Probability Tables.

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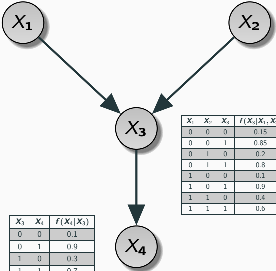

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Continuous case : ???

Bayesian Networks and continuous data

- **Discretization** :
  1. Limited to only a few bins for fast inference and learning algorithms.
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- **Linear Gaussian Bayesian Networks (LGBN)** Lauritzen et al. 1989: $f(y|\boldsymbol{x}) = \mathcal{N}(y; \beta_0 + \sum_{i=1}^{k} \beta_i x_i, \sigma_y^2)$
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- **Mixture models:** Langseth et al. 2012; Cortijo et al. 2016
  1. Good: Expressive models,
  2. Bad: Hard to learn

Copula Bayesian Networks (CBNs)

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

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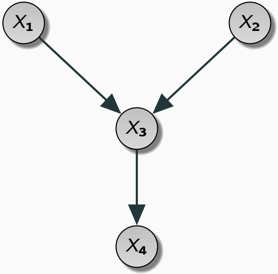

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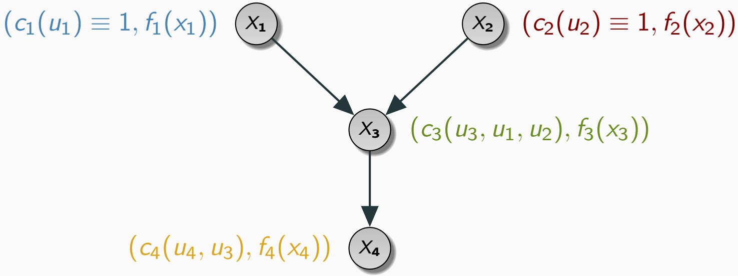

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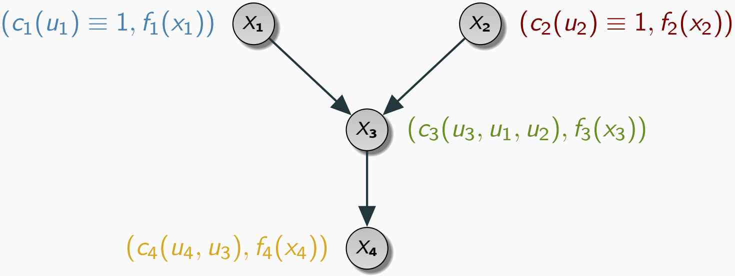

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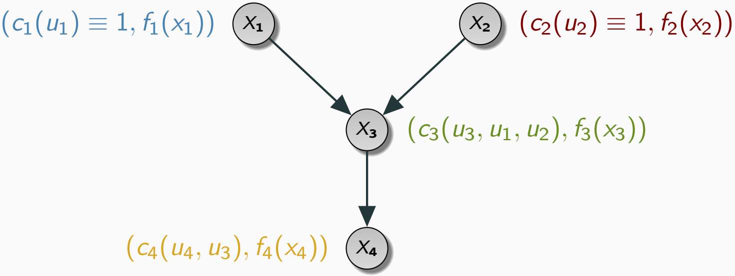

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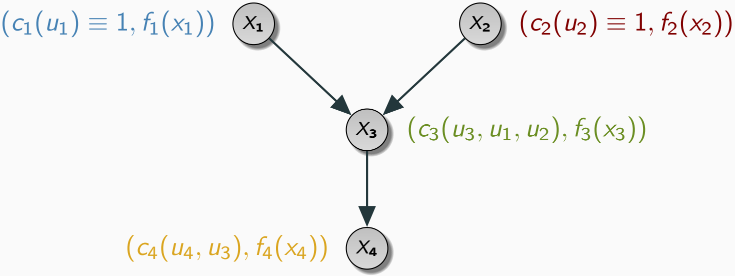

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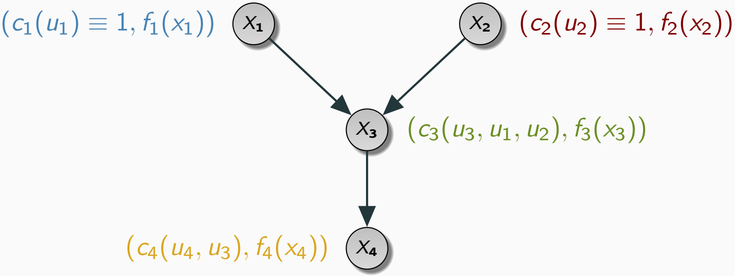

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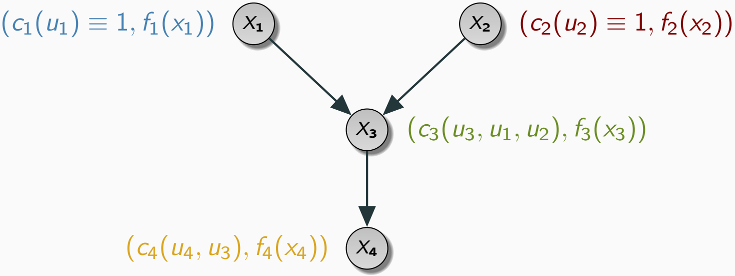

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- Parametric copulas: Gaussian, Student, Dirichlet, ...
- Non-parametric copulas: Empirical Bernstein Copula (EBC)

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
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- Improvement of the state of the art algorithm (CBIC) by using mutual information to speed up the calculations.

Comparison method

1. We generate random reference structures,
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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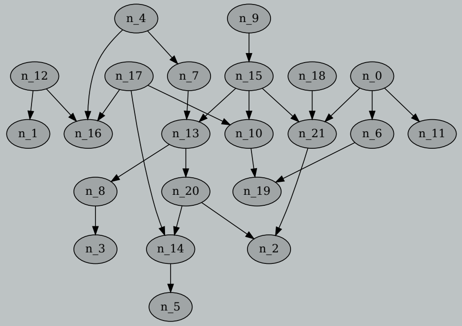

Number of nodes : n $\Longrightarrow$ Number of arcs : $\lfloor 1.2 \times n \rfloor$

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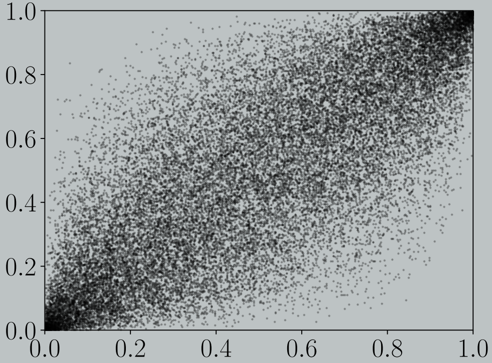

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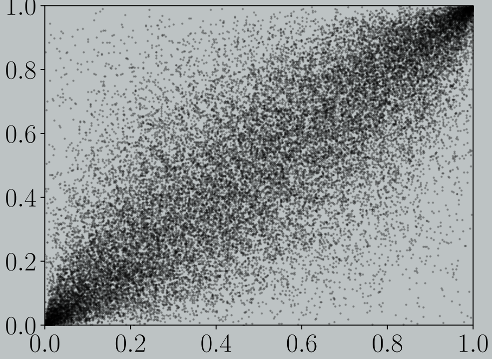
3. Samples are generated from the CBN : forward-sampling,
4. A structure is learned from the generated data,
5. Structural scores are computed : F-score et SHD.



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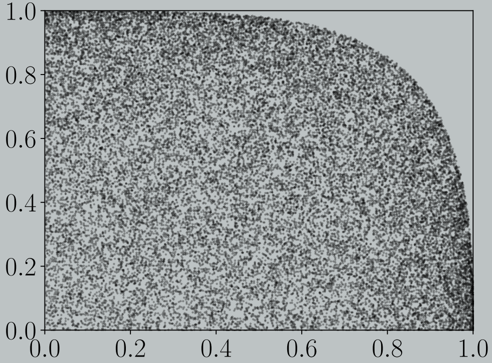

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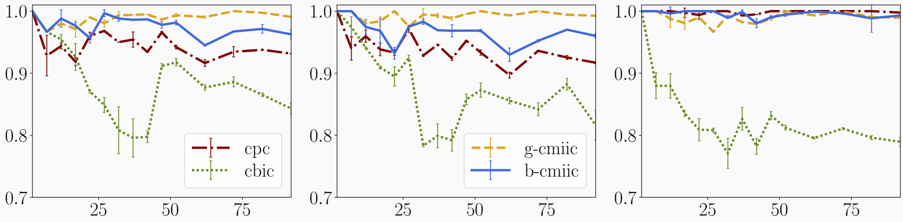
  - CPDAG perfectly retrieved : **SHD = 0**

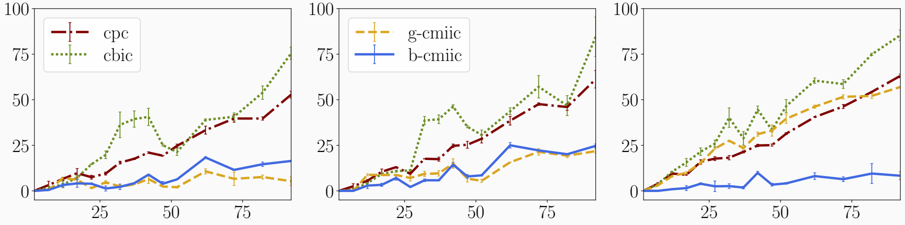
F-score evolution : random structures



(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 **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



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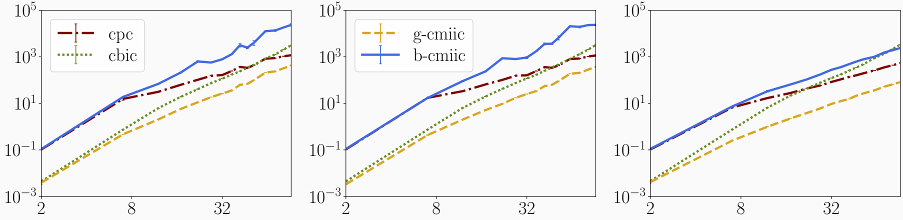
SHD evolution for CBIC, CPC, G-CMIIC and B-CMIIC methods with respect to the **dimension** of the random structure. The results are averaged over 2 different structures of same dimension and over 5 different samples of size $m = 10^4$.

Temporal complexity



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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 $m = 10^4$.

The otagrum module

otagrum: an open source library to learn CBNs

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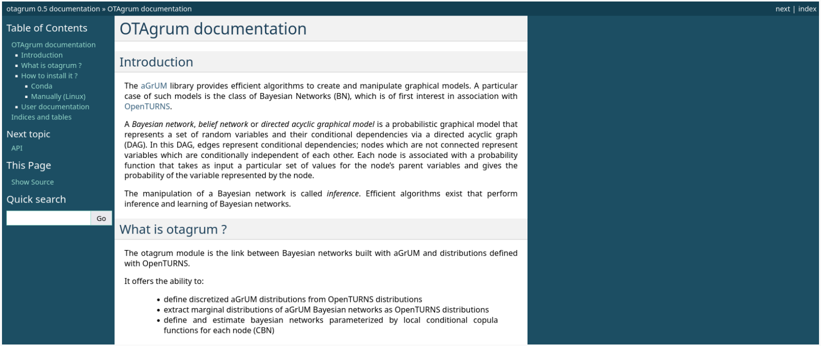
- Experiments : MLasserre/otagrum-experiments (GitHub)

otagrum: installation

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



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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

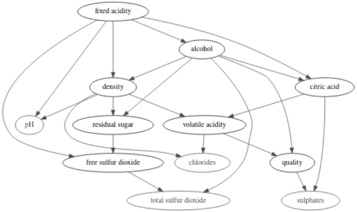
Entrée [2]:

```
data_ref = ot.Sample.ImportFromTextFile('winequality-red.csv', ";")
```

otagrum: an example of use

Structure learning with CBIC algorithm

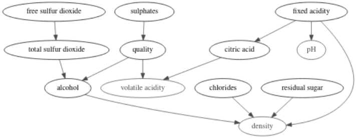
Entrée [3]:
```
learner = otagr.TabuList(data_ref, 2, 10, 2) # Creating a TabuList learner
cbic_dag = learner.learnDAG()                 # Learning DAG
gnb.showDot(cbic_dag.toDot())
```



otagrum: an example of use

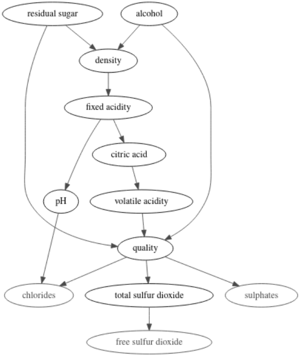
Structure learning with CPC algorithm

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())
```



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

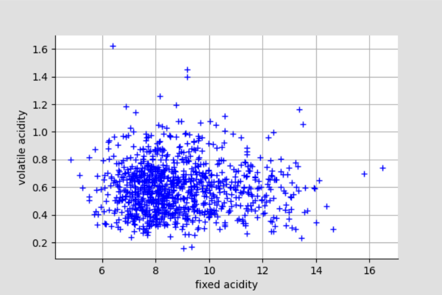
Parameter learning

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

Sampling the CBN

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

Out[9]:



Conclusion & Future Works

Conclusion

Summary:

- CBNs allow to take advantage of conditional independences to reduce the global complexity,
- Using the Empirical Bernstein Copula we obtained non-parametric independence tests and non-parametric CBNs,
- We implemented learning algorithms for CBNs in the plugin otagrum,

Future works : Inference in CBNs

- It consists in finding:
$$f(\boldsymbol{T}|\boldsymbol{E}=\boldsymbol{e})$$
where $\boldsymbol{T}, \boldsymbol{E} \subset \boldsymbol{X}$ such that $\boldsymbol{T} \cap \boldsymbol{E}$.
- Use of sampling to make approximate inferences,
- Use of junction trees to make numerical integrations.

Thank you for your attention !

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