Introduction, introspection, illustration

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1. introduction
   - short history
   - components
   - opensource project
   - next

2. introspection : focus on 3 elementary Components

3. illustration
   - The model (Liessman Eric Sturlaugson, Montana, 2014)
     - dynamic Bayesian Network
     - Chaîne de Markov à temps continu
     - CTBN
   - Quick implementation of CTBNs using pyAgrum

aGrUM/pyAgrum

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($>$ 10 years) aGrUM's goals (as a tool for laboratory)

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- repository : svn$\rightarrow$local git$\rightarrow$local gitlab$\rightarrow$gitlab
- Open Source : GPL then LGPL.

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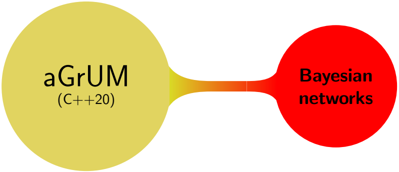

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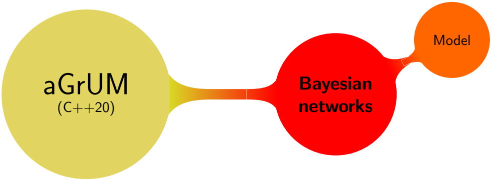

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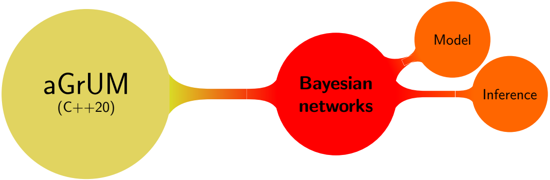

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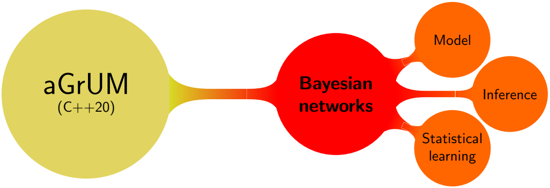

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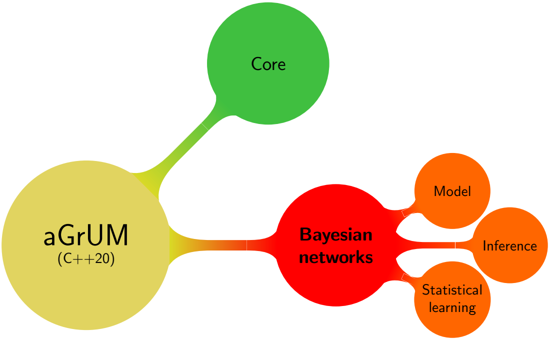

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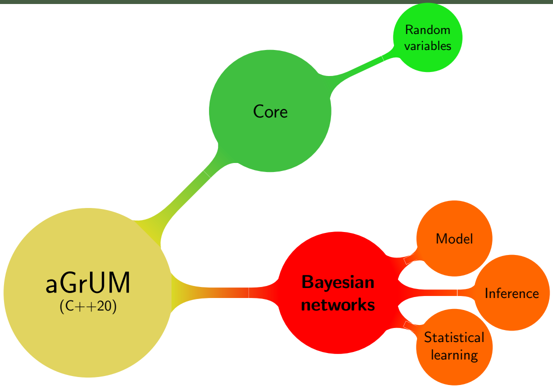

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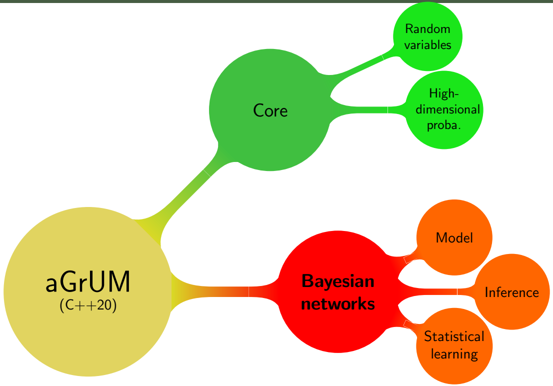

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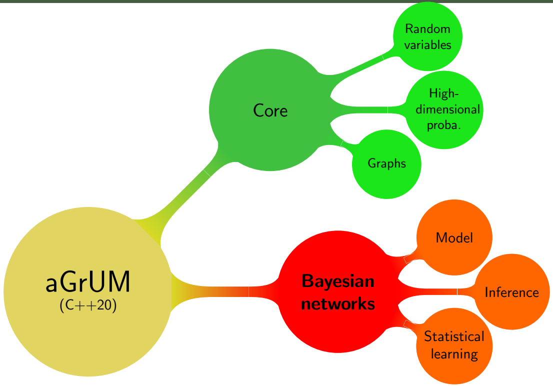

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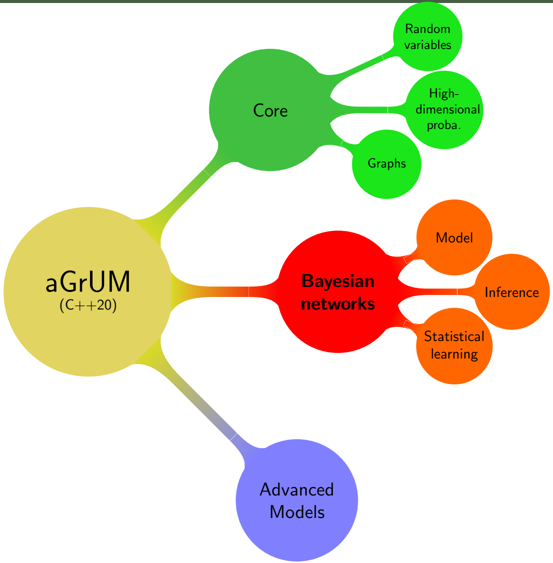

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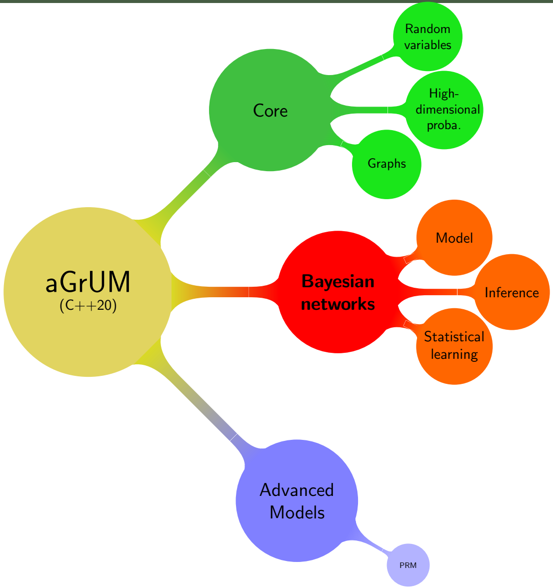

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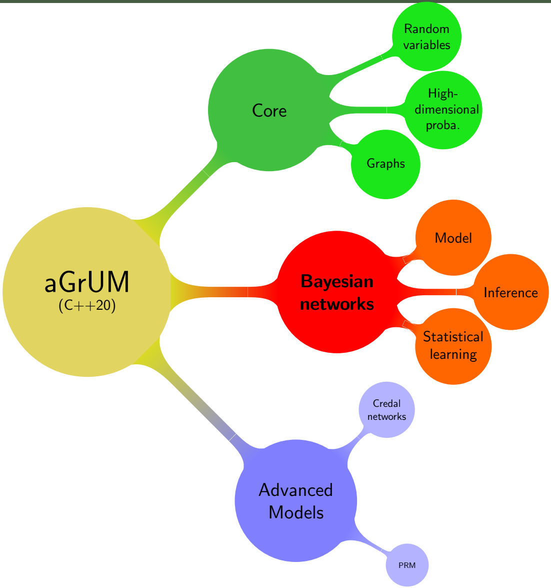

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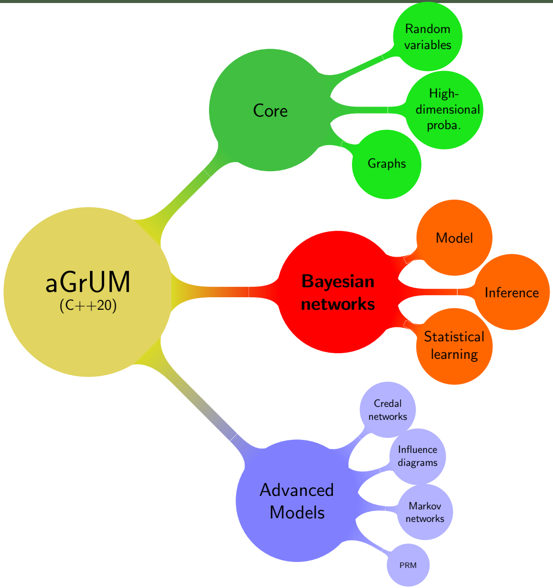

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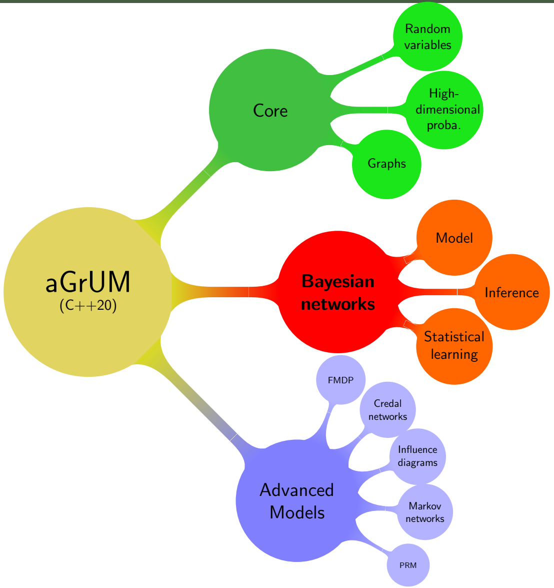

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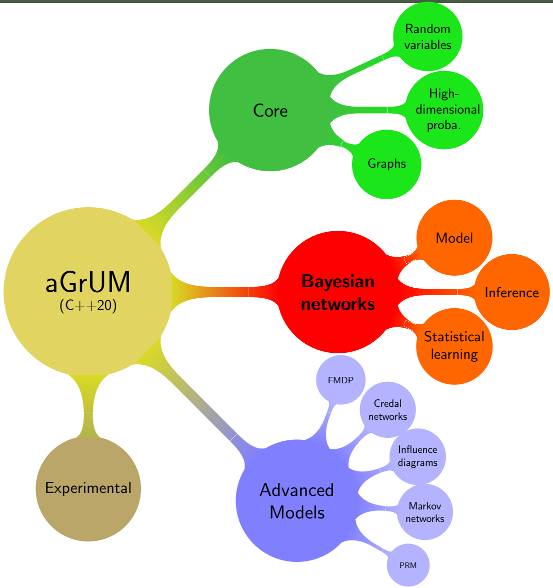

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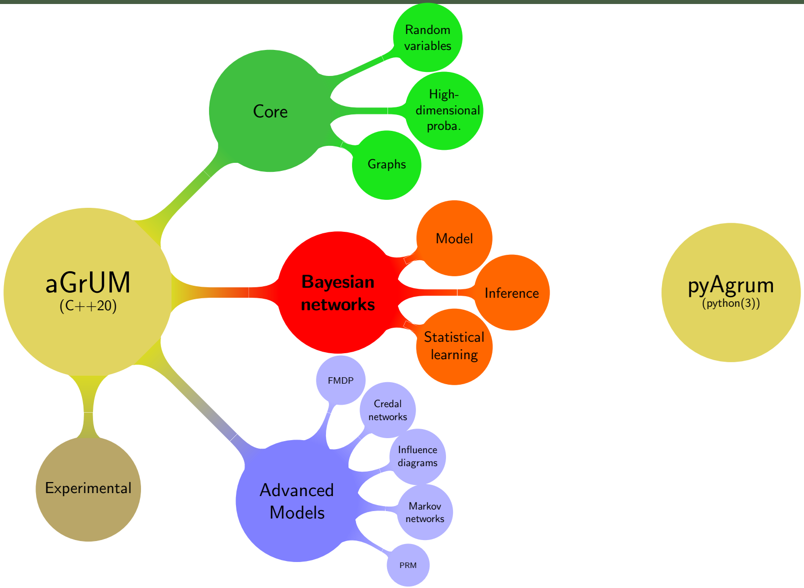

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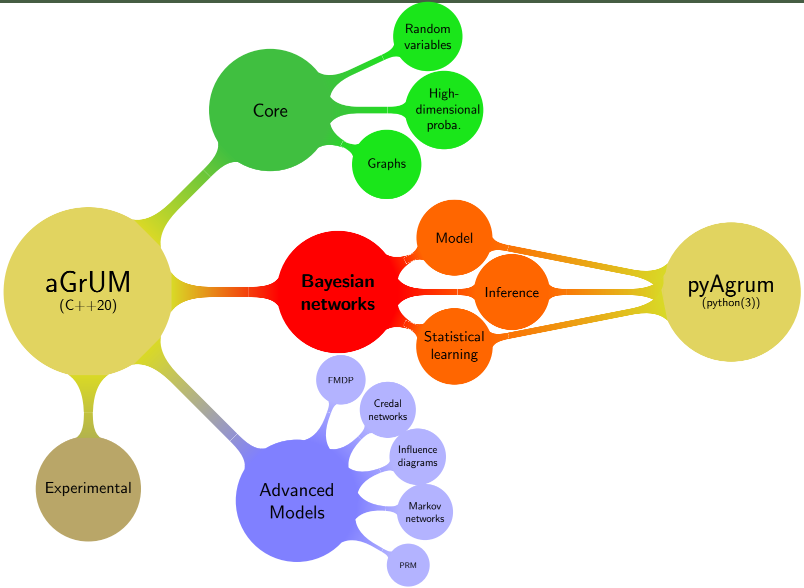

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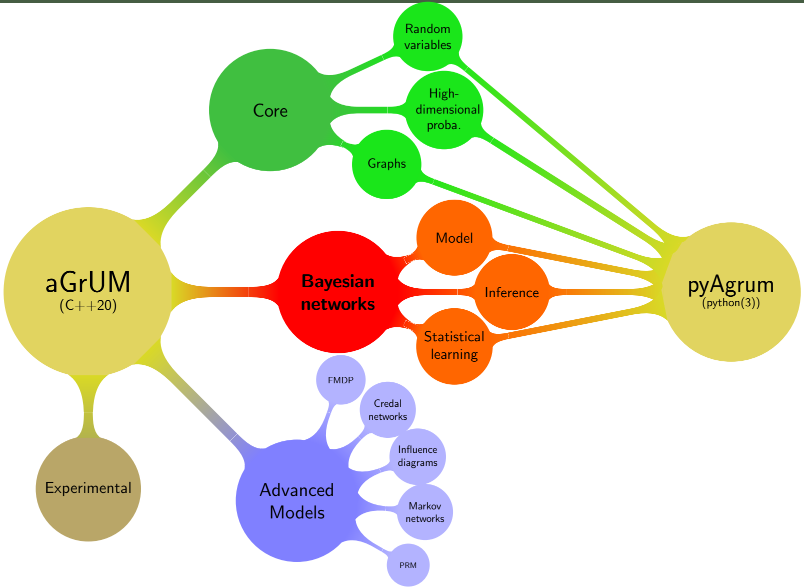

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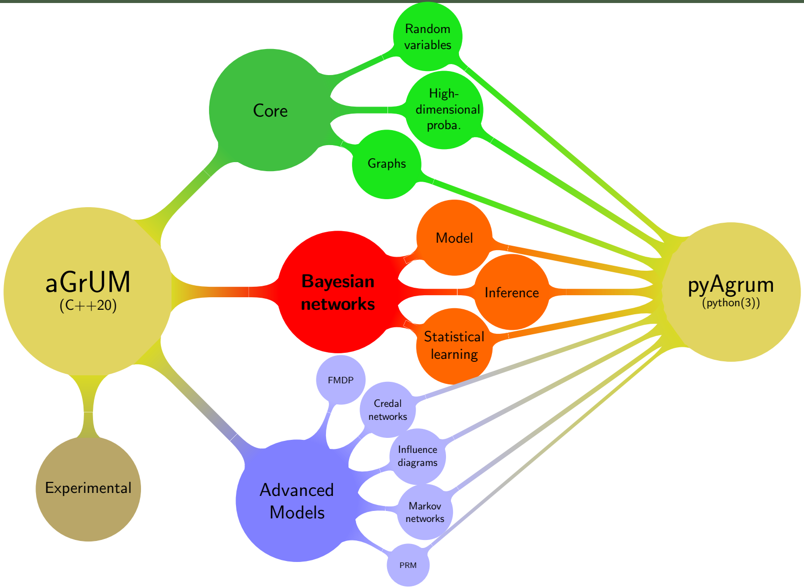

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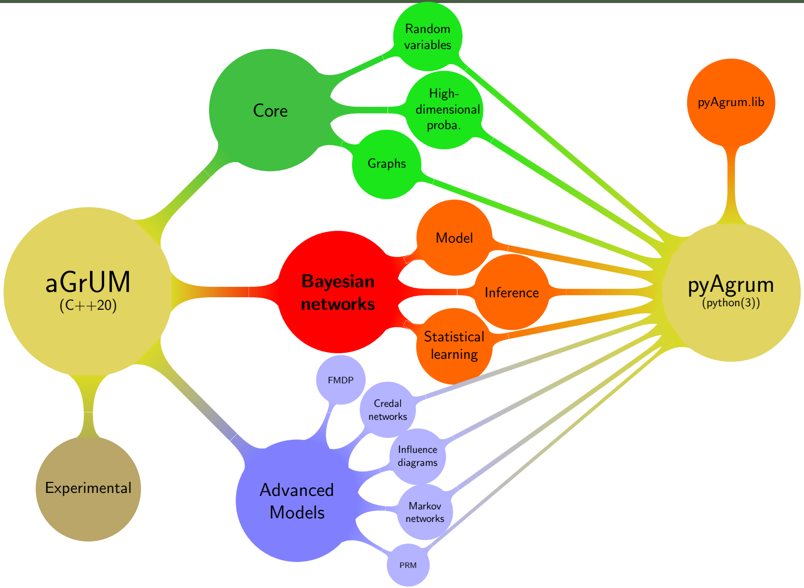

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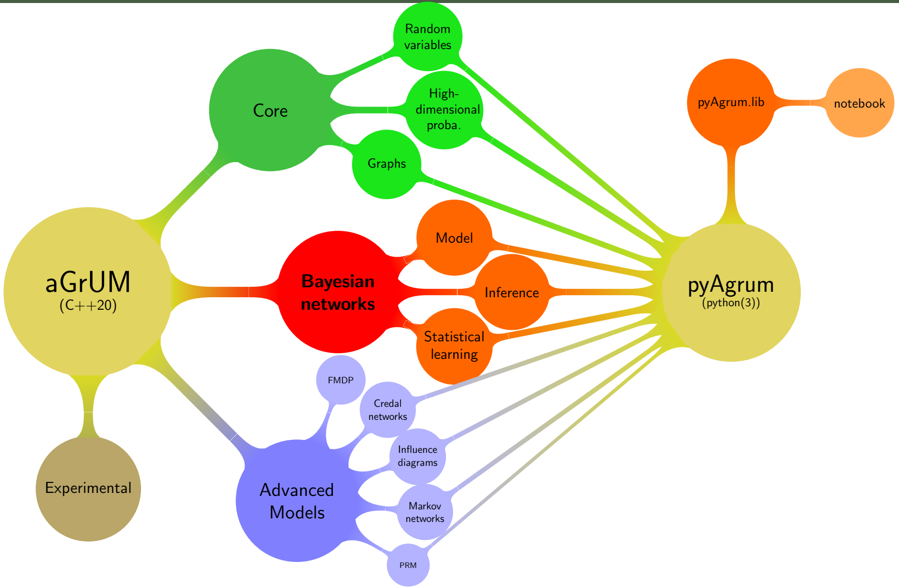

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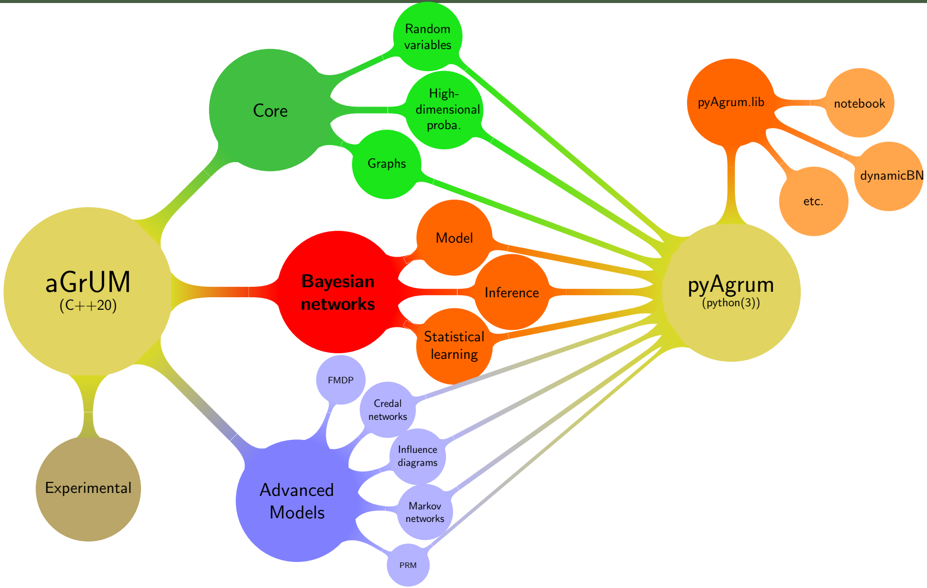

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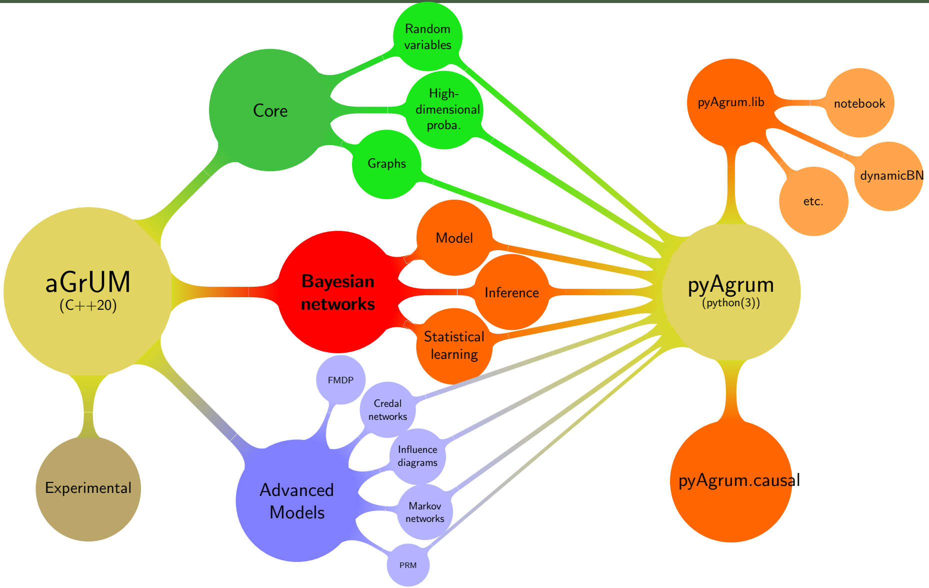

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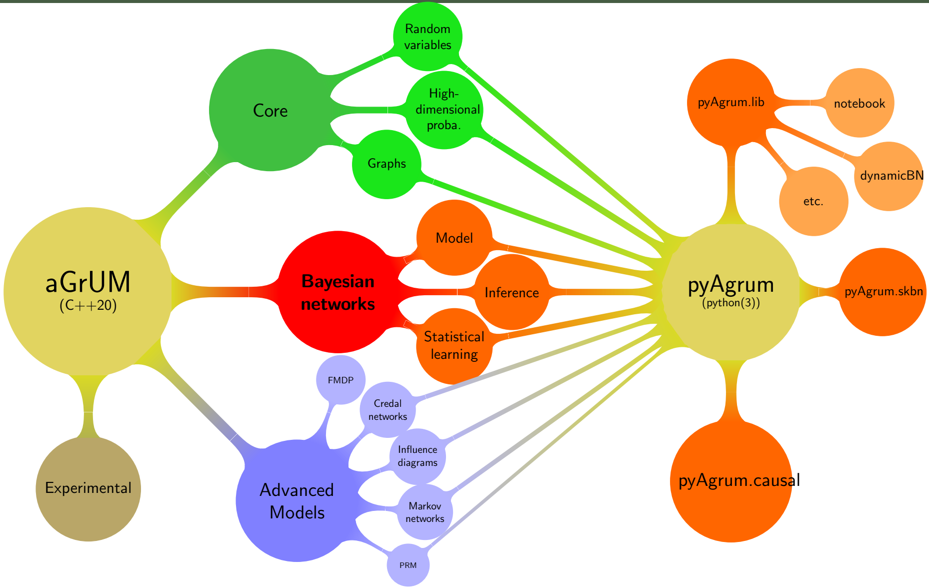
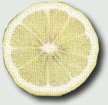
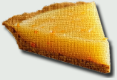




aGrUM/pyAgrum as OpenSource project



Contents
- aGrUM
- pyAgrum

Documentations
- aGrUM's doc
- pyAgrum's ReadTheDocs

Notebooks
- pyAgrum's Tutorials
- From The Book Of Why

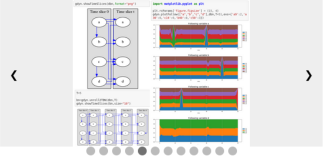
RECENT POSTS
- aGrUM/pyAgrum 0.22.8 released
- aGrUM/pyAgrum 0.22.7 released
- aGrUM/pyAgrum 0.22.6 released
- aGrum/pyAgrum in 2021

Stats on downloads

pypi package 0.22.8 | dwnlds 20.6k/month
Anaconda.org 0.22.8 | dwnlds 5.2k/month
aGrUM aGrUM aGrUM

aGrUM/pyAgrum

A GRaphical Universal Modeler (https://gitlab.com/agrumery/aGrUM)



aGrUM

aGrUM is a C++ library for graphical models. It is designed for easily building applications using graphical models such as Bayesian networks, influence diagrams, decision trees, GAI networks or Markov decision processes.

aGrUM is written to provide the basic building blocks to perform the following tasks :

- designing graphical models,
- learning graphical models,
- elicitation of graphical models,
- inference within graphical models,
- planification.

The probabilistic graphical models currently present in the library are the following:

- Bayesian networks (first and main target),
- Influence Diagrams,
- Markov networks,
- Credal networks,
- O3PRM (Probabilistic Relational Models).

pyAgrum

pyAgrum is a Python wrapper for the C++ aGrUM library (using SWIG interface generator). It provides a high-level interface to the part of aGrUM allowing to create, model, learn, use, calculate with and embed Bayesian Networks and other graphical models. Some specific (python and C++) codes are added in order to simplify and extend the aGrUM API.

Several topics have been added to pyAgrum (as pure python modules using pyAgrum) :

- Scikit-learn-compliant probabilistic classifiers based on Bayesian networks,
- Probabilistic causality (causal networks, do-calculus),
- dynamic Bayesian network,
- tools for explainability in Bayesian networks.

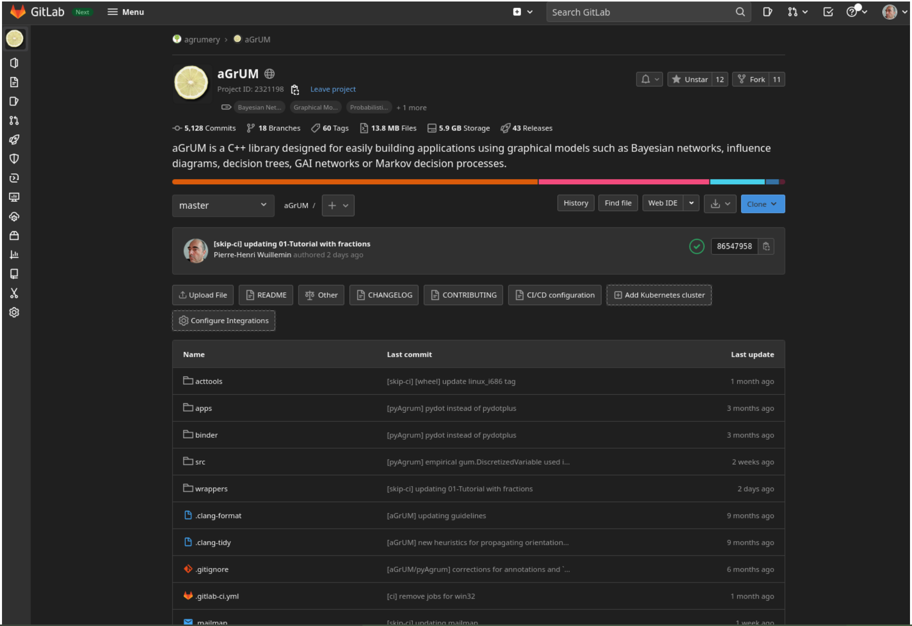
See the tutorials as jupyter notebooks for more details.

Installation : here

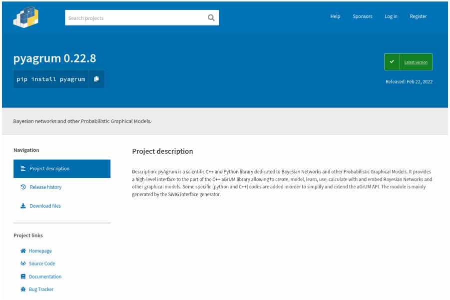
Licence

aGrUM/pyAgrum is released under the Gnu Lesser General Public License (LGPL v3.0), which means it can be freely copied and distributed, and costs nothing. Especially, aGrUM can be used and linked into both free software and proprietary software, provided that the code used under the LGPL is re-licensed under the LGPL (the other parts of the software are permitted have other licenses.). If you wish to integrate the aGrUM library into your product without being affected by the LGPL v.3, please contact us.

aGrUM/pyAgrum on gitlab.com



pyAgrum on pipy/anaconda/binder/readthedocs



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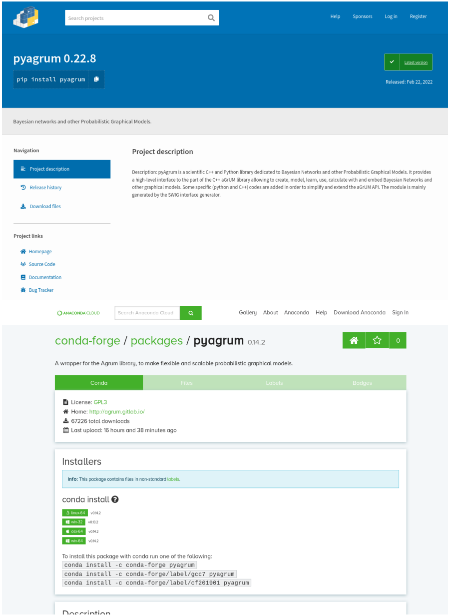

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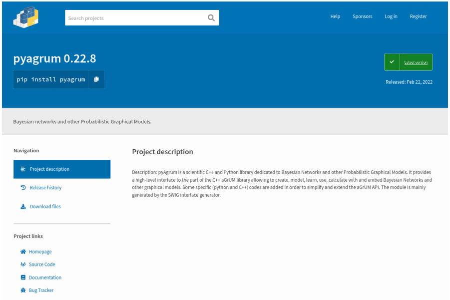

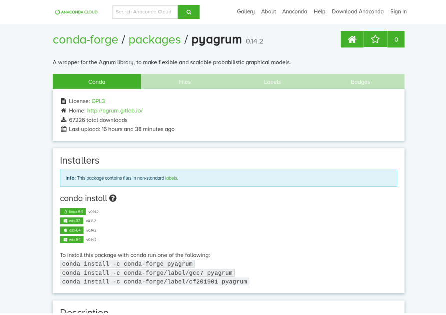

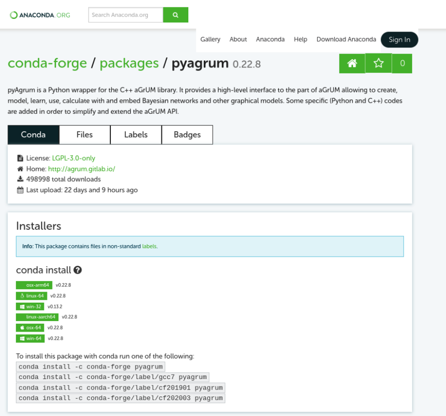

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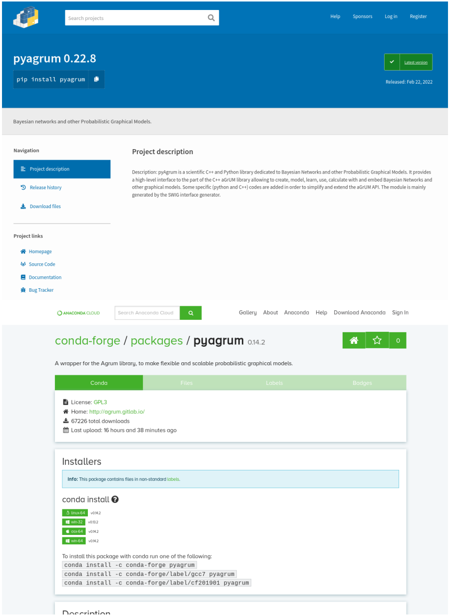
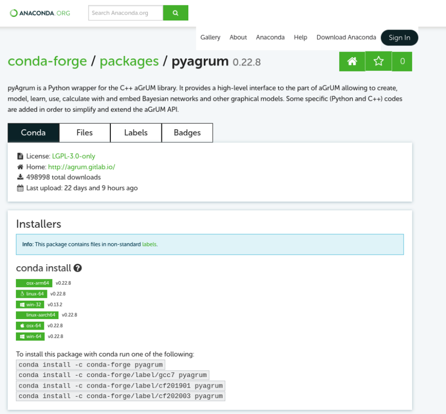
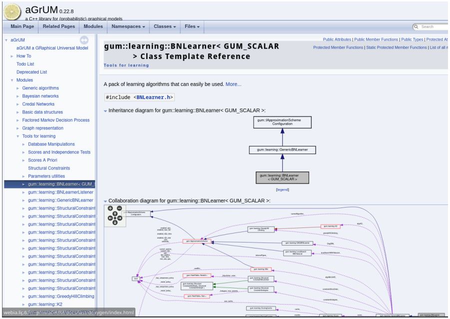




Code quality in aGrUM/pyAgrum : documentation



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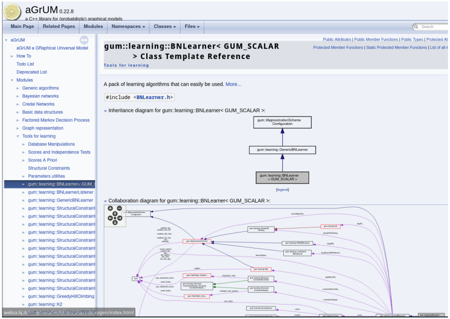

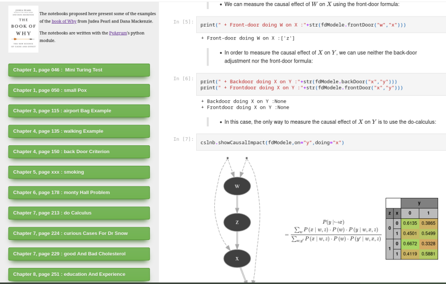

$$P(y \mid \hookrightarrow x) = \frac{\sum_w P(x \mid w,z) \cdot P(w) \cdot P(y \mid w,x,z)}{\sum_{w,y'} P(x \mid w,z) \cdot P(w) \cdot P(y' \mid w,x,z)}$$

z	x	y = 0	y = 1
0	0	0.6135	0.3865
0	1	0.4501	0.5499
1	0	0.6672	0.3328
1	1	0.4119	0.5881

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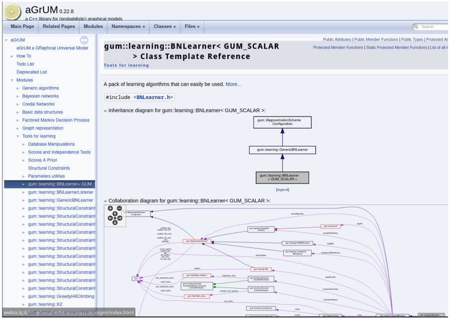

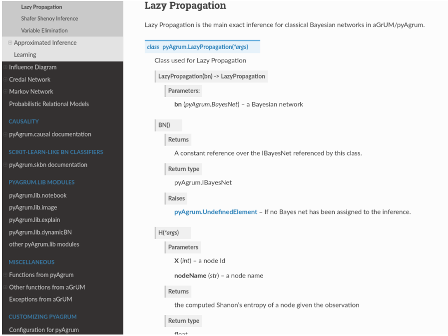

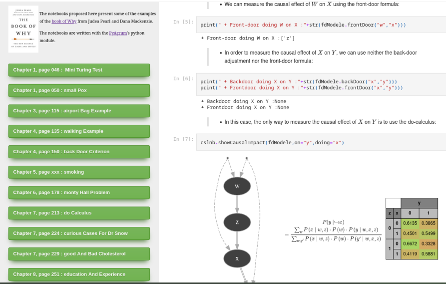

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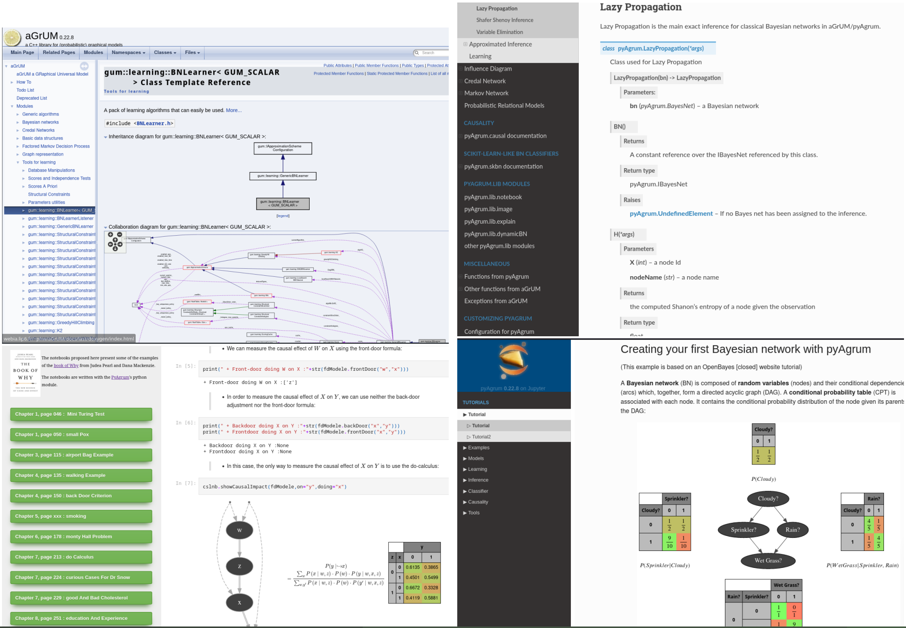
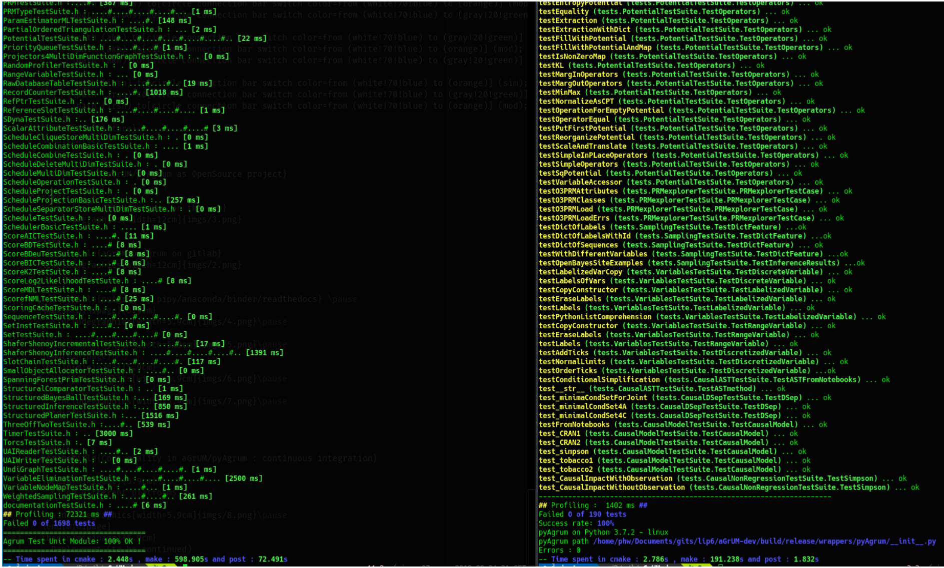
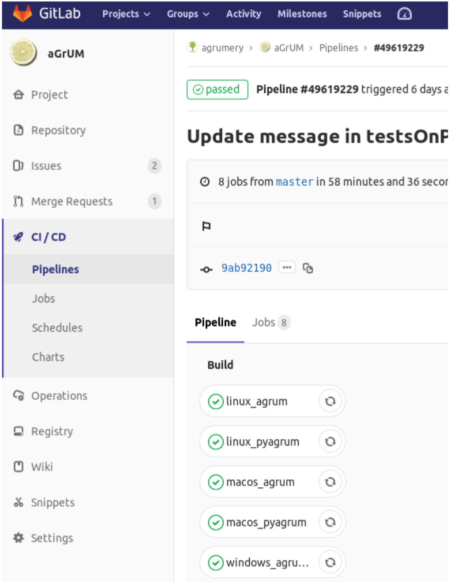


Code quality in aGrUM/pyAgrum : tests

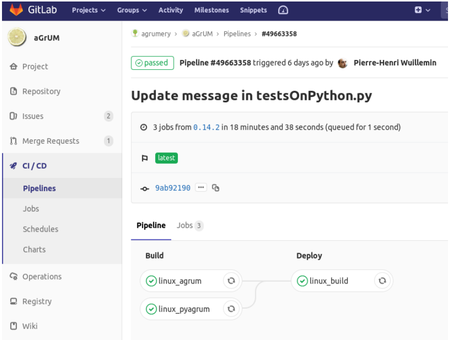


Code quality in aGrUM/pyAgrum : continuous integration

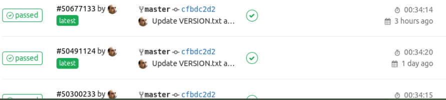
CI on different platforms



Deployment (to be continued)



Nightly build (and tests)



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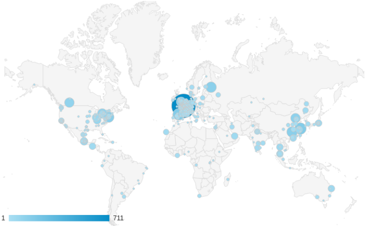

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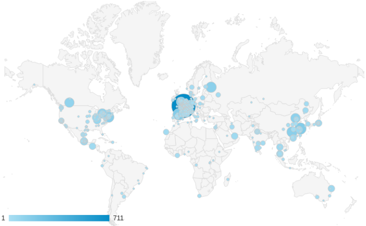

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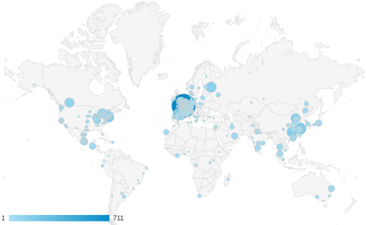

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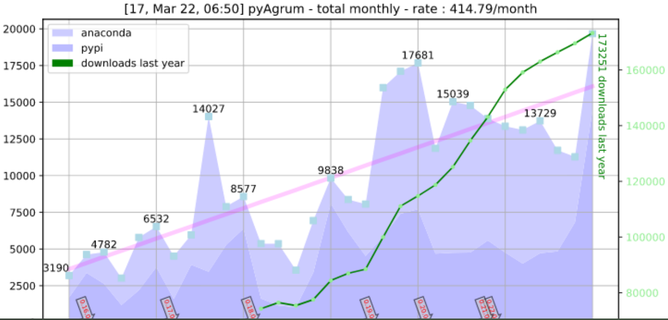

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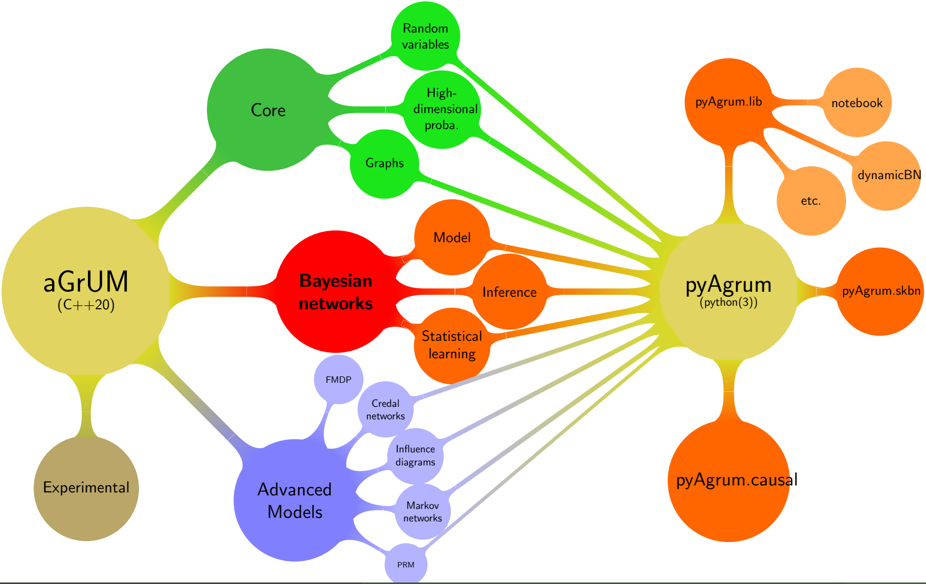
    - weaknesses, strengths
    - missing features
    - Ragrum, JSagrum
    - Steering committee
    - ?

Introspection : focus on 3 elementary components



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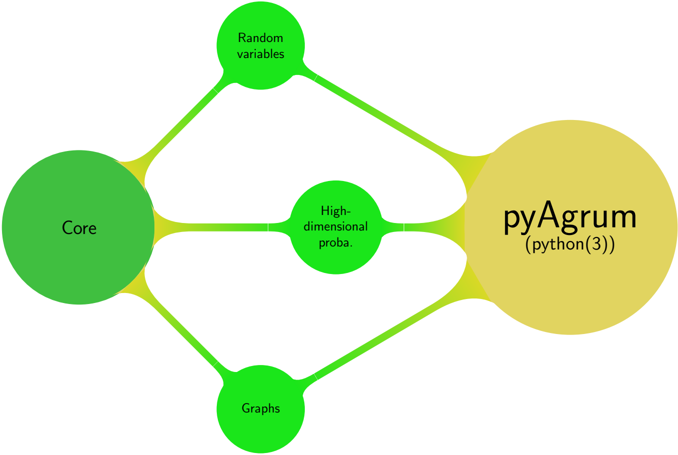

Representation of Discrete Variable

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Data structure : `DiscreteVariable`

goal : map a finite domain $[0, \cdots, \mathit{domainSize}]$ on a list of labels.

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For a `DiscreteVariable` `X` that can take the values a, e, i, o, u, y, `X` is represented by an array :

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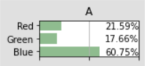
gum.LabelizedVariable

`A{Red|Green|Blue}`

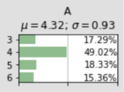
A		
Red	Green	Blue
0.2159	0.1766	0.6075



gum.RangeVariable

`A[3,6]`

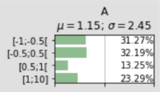
A			
3	4	5	6
0.1729	0.4902	0.1833	0.1536



gum.DiscretizedVariable

`A[-1,-0.5,0.5,1,10]`

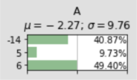
A			
[-1;-0.5[	[-0.5;0.5[	[0.5;1[	[1;10]
0.3127	0.3219	0.1325	0.2329



gum.IntegerVariable

`A{-14|5|6}`

A		
-14	5	6
0.4087	0.0973	0.4940



```python
def aff(name,fastStx):
    bn=gum.fastBN(fastStx)
    return (f"<h2>{name}</h2>",
            f"<tt>{fastStx}</tt>",
            gnb.getPotential(bn.cpt(0)),
            gnb.getPosterior(bn,target=0,evs={}))

gnb.sideBySide(*aff("gum.LabelizedVariable","A{Red|Green|Blue}"),
               *aff("gum.RangeVariable","A[3,6]"),
               *aff("gum.DiscretizedVariable","A[-1,-0.5,0.5,1,10]"),
               *aff("gum.IntegerVariable","A{-14|5|6}"),
              ncols=4)
```

gum.LabelizedVariable

`A{Red|Green|Blue}`

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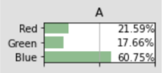
Red	Green	Blue
0.2159	0.1766	0.6075



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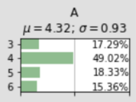

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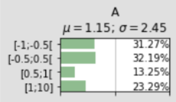

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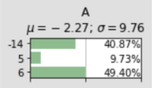

A shared and simple API for all Discrete Variables

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```python
def apiDiscreteVar(variable,value,position):
    print(f"{variable} : {value=}, {position=}")
    print(f" + {variable.domainSize()=}")
    print(f" + {variable[value]=}")
    print(f" + {variable.index(value)=}")
    print(f" + {variable.label(position)=}")

apiDiscreteVar(bn.variable("A"),"Green",0)
apiDiscreteVar(bn.variable("B"),"5",0)
apiDiscreteVar(bn.variable("C"),"0.75",0)
apiDiscreteVar(bn.variable("D"),"5",0)
```

```
A:Labelized(<Red,Green,Blue>) : value='Green', position=0
 + variable.domainSize()=3
 + variable[value]=1
 + variable.index(value)=1
 + variable.label(position)='Red'
B:Range([3,6]) : value='5', position=0
 + variable.domainSize()=4
 + variable[value]=2
 + variable.index(value)=2
 + variable.label(position)='3'
C:Discretized(<[-1;-0.5[,[-0.5;0.5[,[0.5;1[,[1;10]>) : value='0.75', position=0
 + variable.domainSize()=4
 + variable[value]=2
 + variable.index(value)=2
 + variable.label(position)='[-1;-0.5['
D:Integer(<-14,5,6>) : value='5', position=0
 + variable.domainSize()=3
 + variable[value]=1
 + variable.index(value)=1
 + variable.label(position)='-14'
```

Representation of graphs

Data structure : `Directed|Mixed|UnorientedGraph`

goal : represent a list of `Arc` (a, b) and `Edge` $\{b, a\}$ between positive integers.

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Several type of graphs :

- `DiGraph`
  - `DAG (Directed Acyclic Graph)`
- `UndiGraph` (and `CliqueGraph`)
- `MixedGraph`

API for graphs

- node : `addNode`, `addNodeWithId(a)`, `addNodes(nbr)` , `eraseNode(a)`

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- arcs, edges : `addEdge`, `eraseEdge`, etc.

API for graphs

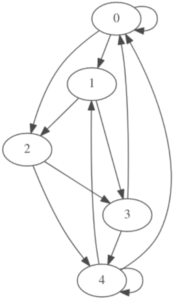
- node : addNode, addNodeWithId(a), addNodes(nbr) , eraseNode(a)
- arcs, edges : addEdge, eraseEdge, etc.
- accessors : parents,children,neighbour, etc.
- algorithms : topologicalOrder, moralGraph, connectedComponents, etc.
- visualisation : toDot() (used by pyAgrum.lib.notebook for instance)

Digraph

```
g=gum.DiGraph()
g.addNodes(5) # returns the generated nodeId
```

```
{0, 1, 2, 3, 4}
```

```
for i in range(5):
    g.addArc(i,(i+1)%5)
    g.addArc(i,(i+2)%5)
g.addArc(0,0)
g.addArc(4,4)
g
```



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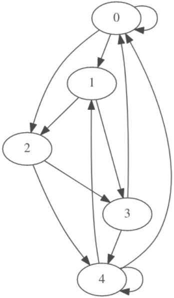
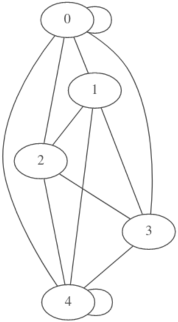


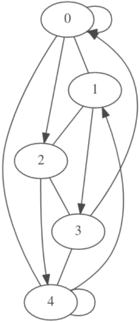
UndiGraph

```python
g=gum.UndiGraph()
g.addNodes(5)
for i in range(5):
    g.addEdge(i,(i+1)%5)
    g.addEdge(i,(i+2)%5)
g.addEdge(0,0)
g.addEdge(4,4)
g
```



Mixed Graph

```python
g=gum.MixedGraph()
g.addNodes(5)
for i in range(5):
    g.addEdge(i,(i+1)%5)
    g.addArc(i,(i+2)%5)
g.addArc(0,0)
g.addEdge(4,4)
g
```



Representation of multi-dimensionnal arrays

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goal : representation of multi-dimensional arrays (of float) without ambiguity on dimensions.

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Implementing tensor algebra

$$f(a, b, c) = g(b, a, c) + h(b, c)$$

		A	
C	**B**	**0**	**1**
0	**0**	1.0000	2.0000
	1	3.0000	4.0000
1	**0**	5.0000	6.0000
	1	7.0000	8.0000

$g(a, b, c)$

	B	
C	**0**	**1**
0	1.0000	3.0000
1	5.0000	7.0000

$h(b, c)$

		B	
A	**C**	**0**	**1**
0	**0**	2.0000	6.0000
	1	10.0000	14.0000
1	**0**	3.0000	7.0000
	1	11.0000	15.0000

$f(a, b, c) = g(a, b, c) + h(b, c)$

API for Potential

Quite complex API.

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Creation and operations on Potential

API for Potential

Quite complex API.

Creation and operations on Potential

```
a=gum.LabelizedVariable("A","descr of A",2)
b=gum.LabelizedVariable("B","descr of B",2)
c=gum.LabelizedVariable("C","descr of C",2)

g=gum.Potential().add(b).add(a).add(c).fillWith([1,2,3,4,5,6,7,8])
h=gum.Potential().add(b).add(c).fillWith([1,3,5,7])

f=g+h
```

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Methods on Potential

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b=gum.LabelizedVariable("B","descr of B",2)
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g=gum.Potential().add(b).add(a).add(c).fillWith([1,2,3,4,5,6,7,8])
h=gum.Potential().add(b).add(c).fillWith([1,3,5,7])

f=g+h
```

Methods on Potential

```
gnb.sideBySide(f,f.sum(),f.margSumOut("B"),
              captions=['$$f(a,b,c)$$','$$\sum_{a,b,c} f(a,b,c)$$','$$\sum_{b} f(a,b,c)$$'])
```

		B	
A	C	0	1
0	0	2.0000	5.0000
	1	10.0000	13.0000
1	0	4.0000	7.0000
	1	12.0000	15.0000

$f(a,b,c)$

68.0

$\sum_{a,b,c} f(a,b,c)$

	C	
A	0	1
0	7.0000	23.0000
1	11.0000	27.0000

$\sum_{b} f(a,b,c)$

API for Potential

Quite complex API.

Creation and operations on Potential

```
a=gum.LabelizedVariable("A","descr of A",2)
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c=gum.LabelizedVariable("C","descr of C",2)

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gnb.sideBySide(f,f.sum(),f.margSumOut("B"),
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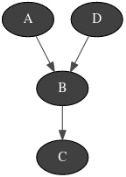
Potential for probabilities

Potential for probabilities

```
bn=gum.fastBN("A->B->C;D->B")
gnb.sideBySide(bn,bn.cpt("A"),bn.cpt("B"),bn.cpt("C"),bn.cpt("D"))
```



A	
0	1
0.1495	0.8505

		B	
D	A	0	1
0	0	0.6356	0.3644
	1	0.6883	0.3117
1	0	0.2372	0.7628
	1	0.3500	0.6500

	C	
B	0	1
0	0.5294	0.4706
1	0.3654	0.6346

D	
0	1
0.7158	0.2842

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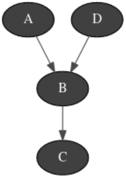

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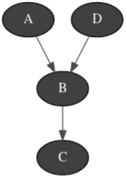

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```
pABCD=bn.cpt("A")*bn.cpt("B")*bn.cpt("C")*bn.cpt("D")
pABCD
```

A	C	B	D: 0	D: 1
0	0	0	0.0360	0.0053
0	0	1	0.0143	0.0118
0	1	0	0.0320	0.0047
0	1	1	0.0247	0.0206
1	0	0	0.2218	0.0448
1	0	1	0.0693	0.0574
1	1	0	0.1972	0.0398
1	1	1	0.1204	0.0997

Potential for probabilities

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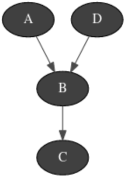
```



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```
pABCD.margSumOut(["A","B"])/pABCD.margSumIn("C")
```

	C	
D	0	1
0	0.7409	0.6943
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Using these components to build new model in pyAgrum

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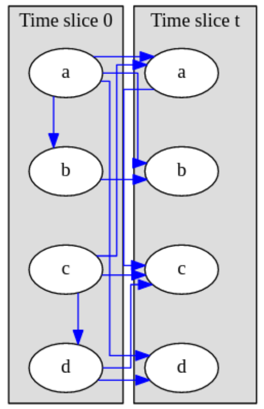
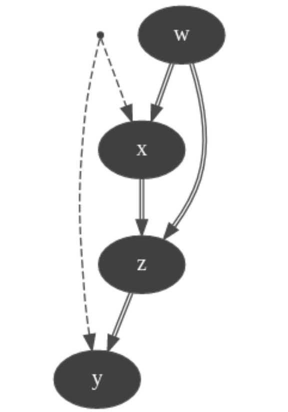
Two models exist only in pyAgrum and has been developped mainly from those components :

dynamic Bayesian Network



Causal model



dynamic Bayesian Networks

dBN (dynamic BN)

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dynamic Bayesian Networks

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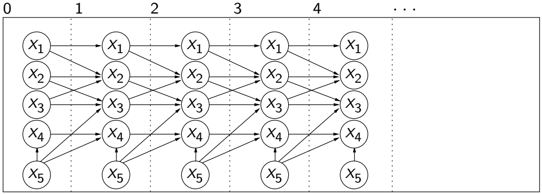

dynamic Bayesian networks : 2-TBN

2-TBN

A dynamic Bayesian network is defined by

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2-TBN

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- initial distributions ($P(X^{(0)})$),

dynamic Bayesian networks : 2-TBN

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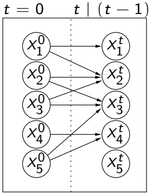

$P(x_1^{(t)}, \ldots, x_5^{(t)} \mid x_1^{(t-1)}, \ldots, x_5^{(t-1)})$

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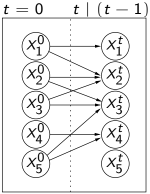

$$P(x_1^{(t)}, \dots, x_5^{(t)} \mid x_1^{(t-1)}, \dots, x_5^{(t-1)}) \quad = P(x_1^{(t)} \mid x^{(t-1)})$$

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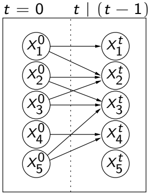

$$P(x_1^{(t)},\ldots,x_5^{(t)} \mid x_1^{(t-1)},\ldots,x_5^{(t-1)}) \quad = P(x_1^{(t)} \mid x^{(t-1)})\, P(x_2^{(t)} \mid x_1^{(t-1)}, x_2^{(t-1)}, x_3^{(t-1)})$$

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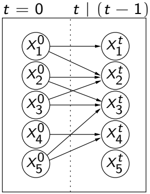

$$
\begin{aligned}
P(x_1^{(t)}, \dots, x_5^{(t)} \mid x_1^{(t-1)}, \dots, x_5^{(t-1)}) \quad &= P(x_1^{(t)} \mid x^{(t-1)}) \\
&P(x_2^{(t)} \mid x_1^{(t-1)}, x_2^{(t-1)}, x_3^{(t-1)}) \\
&P(x_3^{(t)} \mid x_2^{(t-1)}, x_3^{(t-1)}, x_4^{(t-1)}) \\
&P(x_4^{(t)} \mid x_4^{(t-1)}, x_5^{(t-1)})
\end{aligned}
$$

1024 versus 4+16+16+8+2=46 ! !

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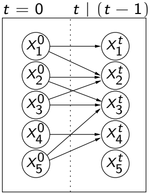

$$P(x_1^{(t)},\ldots,x_5^{(t)} \mid x_1^{(t-1)},\ldots,x_5^{(t-1)}) \quad = P(x_1^{(t)} \mid x^{(t-1)})\, P(x_2^{(t)} \mid x_1^{(t-1)}, x_2^{(t-1)}, x_3^{(t-1)})\, P(x_3^{(t)} \mid x_2^{(t-1)}, x_3^{(t-1)}, x_4^{(t-1)})\, P(x_4^{(t)} \mid x_4^{(t-1)}, x_5^{(t-1)})\, P(x_5^{(t)})$$

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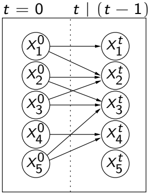

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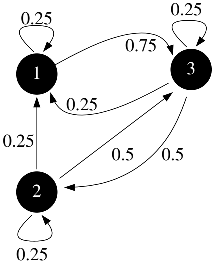
The representation a.k.a 2TBN (2 timeslices BN) allow the modelisation of a virtually infinite Bayesian network which is the unrolled model from time 0.

Markov Chain and dynamic Bayesian network



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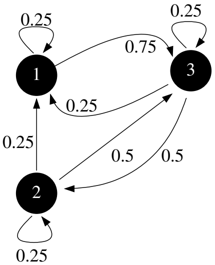

$$P(X^n \mid X^{n-1}) = \begin{pmatrix} 0.25 & 0 & 0.75 \\ 0.25 & 0.25 & 0.5 \\ 0.25 & 0.5 & 0.25 \end{pmatrix}$$

Markov chain

- a discrete variable (X^n) (at time n).
- Parameters for this model :
  - Initial condition : $P(X^O)$
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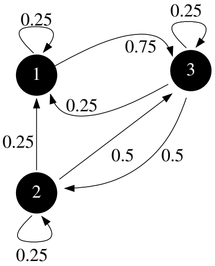
Equivalent dynamic Bayesian network :

Markov Chain and dynamic Bayesian network



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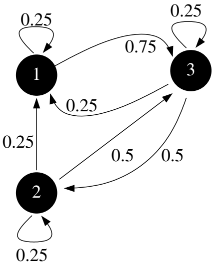
dBN : $X^0 \longrightarrow X^1 \longrightarrow X^2 \longrightarrow X^3 \longrightarrow \cdots$

2TBN : $\boxed{X^0} \longrightarrow \boxed{X^n}$

Markov Chain and dynamic Bayesian network



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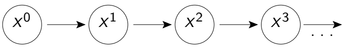
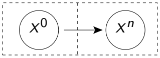
dBN : 

2TBN : 

Could we do the same with continuous time ?

Continuous-Time Markov Process

Dynamic processus dynamique verifying :

- a discrete variable

Continuous-Time Markov Process

Dynamic processus dynamique verifying :

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- a transition from a state to another can happen any time,

$$\underbrace{0 \qquad\qquad}_{X(0)} t_1 \underbrace{\qquad\qquad\qquad\qquad\qquad}_{X(t_1)} t_2 \underbrace{\qquad}_{X(t_2)} t_3 \cdots$$

Continuous-Time Markov Process

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$$\forall s > r, \forall t > 0, P(X(s+t)|X(s)), X(r)) = P(X(s+t)|X(s)))$$

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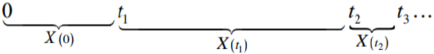

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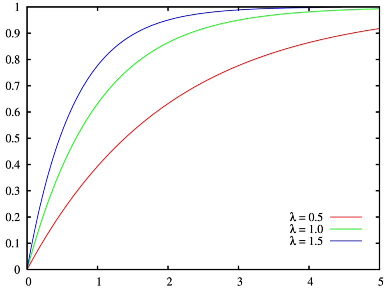
Exponential distribution

$$D \sim Exp(\lambda)$$

- Cumulative distribution function
  $\forall d > 0, F(d) = 1 - e^{-\lambda d}$
- $\mathbb{E}(D) = \lambda^{-1}$
- $\sigma(D) = \lambda^{-1}$



Continuous Time Markov Chain (CTMC)

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Continuous Time Markov Chain

$(X_t \in x_1, \cdots, x_n)_{t \geq 0}$ CdMTC is defined by

Continuous Time Markov Chain (CTMC)

A CTMC is a continuous stochastic process in which, for each state, the process will change state according to an exponential random variable and then move to a different state as specified by the probabilities of a stochastic matrix.

Minimum of independent exponential distributions

$$X \sim Exp(\lambda), Y \sim Exp(\mu), X \perp\!\!\!\perp Y \Rightarrow min(X, Y) \sim Exp(\lambda + \mu)$$

Continuous Time Markov Chain

$(X_t \in x_1, \cdots, x_n)_{t \geq 0}$ CdMTC is defined by

- $P(X_0)$
- $\forall i, j \geq n, q_{i,j}$ tels que
    1. $q_{i,i} \in \mathbb{R}^-$
    2. $\forall i \neq j, q_{i,j} \in \mathbb{R}^+$
    3. $\forall i, \sum_j q_{i,j} = 0$

$$Q_X = \begin{pmatrix} -0.21 & 0.20 & 0.01 \\ 0.05 & -0.10 & 0.05 \\ 0.01 & 0.20 & -0.21 \end{pmatrix}$$

intensity matrix

$q_{i,j}$ is the parameter of the exponential distribution controlling the transition from state i to state j
$-q_{i,i}$ is the paramter of the exponential distribution controlling a transition from state i.

Properties

$(X_t \in x_1, \cdots, x_n)_{t \geq 0}$ CTMC :

- $P(X_0)$
- $Q_X = (q_{i,j})_{i \leq n, j \leq n}$ intensity matrix

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$$\text{draw}(exp(-q_{i,i})) \text{ puis draw}((p_{i,j}, j \neq i)).$$

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Convergence

With some good conditions (ergodicity), $P(X_t) \underset{t \to \infty}{\longrightarrow} P(X^*)$

- Forward sampling :

  draw($exp(-q_{i,i})$) puis draw($(p_{i,j}, j \neq i)$).
- Convergence of $P(X_t) = P(X_0) exp(Q_X t) \underset{t \to \infty}{\longrightarrow} P^*$

factorized CTMC : CTBN

CTBN

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Q_X is a CIM $\iff \forall <pa_X>, Q_{X|<pa_X>}$ intensity matrix.

factorized CTMC : CTBN

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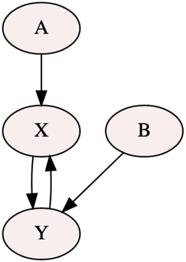
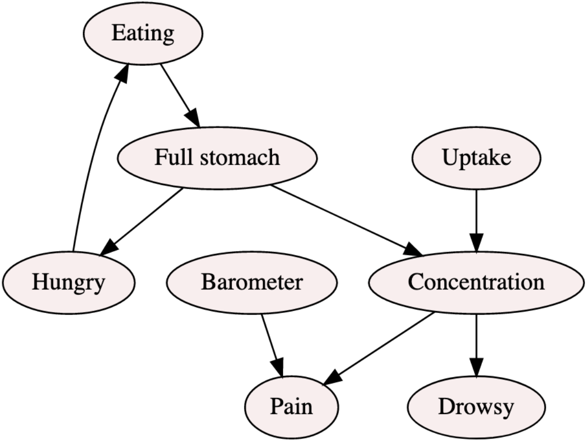


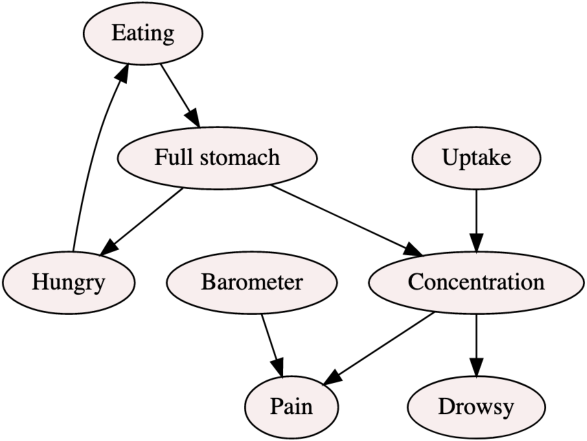
	A#j	
A#i	**a0**	**a1**
a0	-1.0000	1.0000
a1	2.0000	-2.0000

			X#j	
Y	**A**	**X#i**	**x0**	**x1**
y0	**a0**	**x0**	-1.0000	1.0000
		x1	2.0000	-2.0000
	a1	**x0**	-10.0000	10.0000
		x1	20.0000	-20.0000
y1	**a0**	**x0**	-5.0000	5.0000
		x1	6.0000	-6.0000
	a1	**x0**	-50.0000	50.0000
		x1	60.0000	-60.0000

CTBN - properties

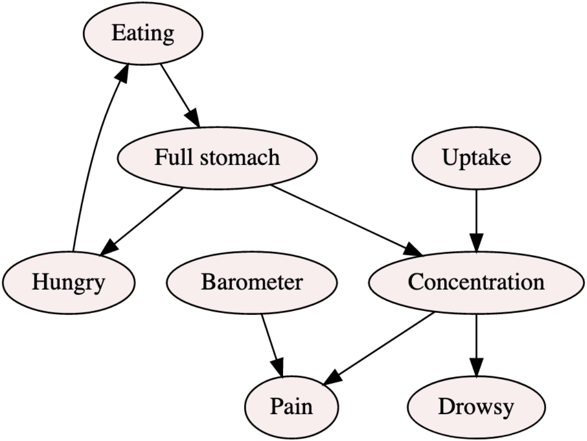


CTBN - properties



- Arc always temporal (which allows 'cycle') :
  $A \to B \iff P(B_{t+\delta_t} \mid A_t, \cdots) = \cdots$

CTBN - properties



- Arc always temporal (which allows 'cycle') :
  $A \rightarrow B \iff P(B_{t+\delta_t} \mid A_t, \cdots) = \cdots$
- **A Continuous-Time Bayseian network is a joint continuous-time Markov process.**

From a CTBN to the Markov process : amalgamation

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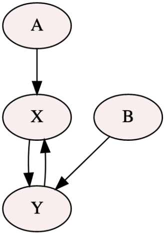
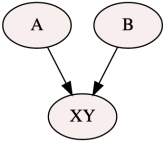
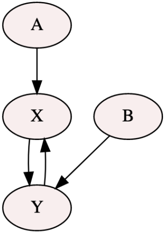
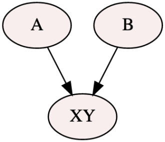




From a CTBN to the Markov process : amalgamation





$$\mathbf{Q}_{X|a_0,y_0} = \begin{array}{c c} & \begin{array}{cc} x_0 & x_1 \end{array} \\ \begin{array}{c} x_0 \\ x_1 \end{array} & \begin{pmatrix} -1 & 1 \\ 2 & -2 \end{pmatrix} \end{array} \quad \mathbf{Q}_{Y|b_1,x_0} = \begin{array}{c c} & \begin{array}{cc} y_0 & y_1 \end{array} \\ \begin{array}{c} y_0 \\ y_1 \end{array} & \begin{pmatrix} -3 & 3 \\ 4 & -4 \end{pmatrix} \end{array}$$

$$\mathbf{Q}_{X|a_0,y_1} = \begin{array}{c c} & \begin{array}{cc} x_0 & x_1 \end{array} \\ \begin{array}{c} x_0 \\ x_1 \end{array} & \begin{pmatrix} -5 & 5 \\ 6 & -6 \end{pmatrix} \end{array} \quad \mathbf{Q}_{Y|b_1,x_1} = \begin{array}{c c} & \begin{array}{cc} y_0 & y_1 \end{array} \\ \begin{array}{c} y_0 \\ y_1 \end{array} & \begin{pmatrix} -7 & 7 \\ 8 & -8 \end{pmatrix} \end{array}$$

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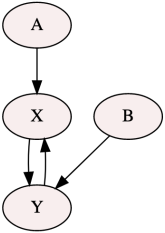

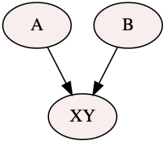

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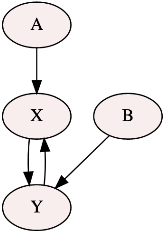
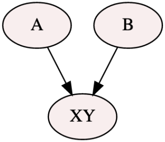
$$\mathbf{Q}_{XY|a_0,b_1} = \begin{array}{c c} & \begin{array}{cccc} (x_0,y_0) & (x_0,y_1) & (x_1,y_0) & (x_1,y_1) \end{array} \\ \begin{array}{c} (x_0,y_0) \\ (x_0,y_1) \\ (x_1,y_0) \\ (x_1,y_1) \end{array} & \begin{pmatrix} -4 & 3 & 1 & 0 \\ 4 & -9 & 0 & 5 \\ 2 & 0 & -9 & 7 \\ 0 & 6 & 8 & -14 \end{pmatrix} \end{array}$$

From a CTBN to the Markov process : amalgamation





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The amalgamation of all the CIMs of a CTBN produces the intensity matrix of the joint Markov process.

Forward sampling dans un CTBN

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CTBN Forward sampling

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1. $(X_{t+1}, D_t) = (argmin, min)_{X \in CTBN} Draw(Q_X)$

Forward sampling dans un CTBN

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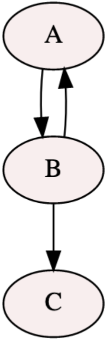

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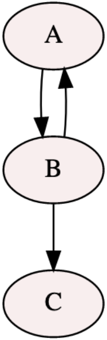
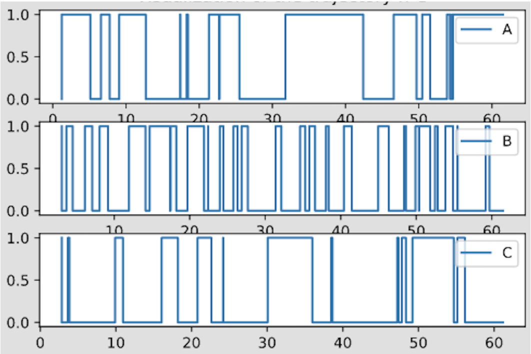




Implémentation (rapide)

Goal1 : way to define a CTBN

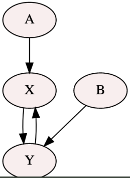
Goal1 : way to define a CTBN

```python
ctbn = Ctbn()
ctbn.add(gum.LabelizedVariable("A", "A", ["a0", "a1"]))
ctbn.add(gum.LabelizedVariable("B", "B", ["b0", "b1"]))
ctbn.add(gum.LabelizedVariable("X", "X", ["x0", "x1"]))
ctbn.add(gum.LabelizedVariable("Y", "Y", ["y0", "y1"]))

ctbn.addArc("A", "X")
ctbn.addArc("Y", "X")
ctbn.addArc("B", "Y")
ctbn.addArc("X", "Y")

ctbn.CIM("A")[:] = [[-1, 1],
                    [2, -2]]
ctbn.CIM("B")[:] = [[-3, 3],
                    [2, -2]]
ctbn.CIM("X")[{"A": "a0", "Y": "y0"}] = [[-1, 1],
                                         [2, -2]]
ctbn.CIM("X")[{"A": "a1", "Y": "y0"}] = [[-1, 1],
                                         [3, -3]]
ctbn.CIM("X")[{"A": "a0", "Y": "y1"}] = [[-5, 5],
                                         [6, -6]]
ctbn.CIM("X")[{"A": "a1", "Y": "y1"}] = [[-5, 5],
                                         [4, -4]]
ctbn.CIM("Y")[{"B": "b0", "X": "x0"}] = [[-2, 2],
                                         [5, -5]]
ctbn.CIM("Y")[{"B": "b1", "X": "x0"}] = [[-3, 3],
                                         [4, -4]]
ctbn.CIM("Y")[{"B": "b0", "X": "x1"}] = [[-3, 3],
                                         [5, -5]]
ctbn.CIM("Y")[{"B": "b1", "X": "x1"}] = [[-7, 7],
                                         [8, -8]]

gnb.sideBySide(ctbn,ctbn.CIM("A")._pot,ctbn.CIM("X")._pot)
```



	A#j	
A#i	a0	a1
a0	-1.0000	1.0000
a1	2.0000	-2.0000

			X#j	
Y	A	X#i	x0	x1
y0	a0	x0	-1.0000	1.0000
		x1	2.0000	-2.0000
	a1	x0	-1.0000	1.0000
		x1	3.0000	-3.0000
y1	a0	x0	-5.0000	5.0000
		x1	6.0000	-6.0000
	a1	x0	-5.0000	5.0000
		[illegible]	[illegible]	[illegible]

Goal2 : implement amalgamation

Goal2 : implement amalgamation

```python
im=CIM()
for x in ctbn.names():
    im*=ctbn.CIM(x)
im.to_matrix()
```

```
array([[ -7.,   1.,   3.,   0.,   1.,   0.,   0.,   0.,   2.,   0.,   0.,
          0.,   0.,   0.,   0.,   0.],
       [  2.,  -8.,   0.,   3.,   0.,   1.,   0.,   0.,   0.,   2.,   0.,
          0.,   0.,   0.,   0.,   0.],
       [  2.,   0.,  -7.,   1.,   0.,   0.,   1.,   0.,   0.,   0.,   3.,
          0.,   0.,   0.,   0.,   0.],
       [  0.,   2.,   2.,  -8.,   0.,   0.,   0.,   1.,   0.,   0.,   0.,
          3.,   0.,   0.,   0.,   0.],
       [  2.,   0.,   0.,   0.,  -9.,   1.,   3.,   0.,   0.,   0.,   0.,
          0.,   3.,   0.,   0.,   0.],
       [  0.,   3.,   0.,   0.,   2., -11.,   0.,   3.,   0.,   0.,   0.,
          0.,   0.,   3.,   0.,   0.],
       [  0.,   0.,   2.,   0.,   2.,   0., -12.,   1.,   0.,   0.,   0.,
          0.,   0.,   0.,   7.,   0.],
       [  0.,   0.,   0.,   3.,   0.,   2.,   2., -14.,   0.,   0.,   0.,
          0.,   0.,   0.,   0.,   7.],
       [  5.,   0.,   0.,   0.,   0.,   0.,   0.,   0., -14.,   1.,   3.,
          0.,   5.,   0.,   0.,   0.],
       [  0.,   5.,   0.,   0.,   0.,   0.,   0.,   0.,   2., -15.,   0.,
          3.,   0.,   5.,   0.,   0.],
       [  0.,   0.,   4.,   0.,   0.,   0.,   0.,   0.,   2.,   0., -12.,
          1.,   0.,   0.,   5.,   0.],
       [  0.,   0.,   0.,   4.,   0.,   0.,   0.,   0.,   0.,   2.,   2.,
        -13.,   0.,   0.,   0.,   5.],
       [  0.,   0.,   0.,   0.,   5.,   0.,   0.,   0.,   6.,   0.,   0.,
          0., -15.,   1.,   3.,   0.],
       [  0.,   0.,   0.,   0.,   0.,   5.,   0.,   0.,   0.,   4.,   0.,
          0.,   2., -14.,   0.,   3.],
```

Goal3 : implement the 2 'inference'

Goal3 : implement the 2 'inference'

```
ie=SimpleCtbnInference(ctbn)
ie.makeInference()
gnb.sideBySide(ie.posterior("A"),ie.posterior("B"),ie.posterior("Y"),ie.posterior("X"))
```

A	
a0	a1
0.6667	0.3333

B	
b0	b1
0.4000	0.6000

Y	
y0	y1
0.6100	0.3900

X	
x0	x1
0.6065	0.3935

```
ie=ForwardSampleCtbnInference(ctbn)
ie.makeInference()
gnb.sideBySide(ie.posterior("A"),ie.posterior("B"),ie.posterior("Y"),ie.posterior("X"))
```

A	
a0	a1
0.6651	0.3349

B	
b0	b1
0.3968	0.6032

Y	
y0	y1
0.6081	0.3919

X	
x0	x1
0.6060	0.3940

Goal3 : implement the 2 'inference'

```
ie=SimpleCtbnInference(ctbn)
ie.makeInference()
gnb.sideBySide(ie.posterior("A"),ie.posterior("B"),ie.posterior("Y"),ie.posterior("X"))
```

A	
a0	a1
0.6667	0.3333

B	
b0	b1
0.4000	0.6000

Y	
y0	y1
0.6100	0.3900

X	
x0	x1
0.6065	0.3935

```
ie=ForwardSampleCtbnInference(ctbn)
ie.makeInference()
gnb.sideBySide(ie.posterior("A"),ie.posterior("B"),ie.posterior("Y"),ie.posterior("X"))
```

A	
a0	a1
0.6651	0.3349

B	
b0	b1
0.3968	0.6032

Y	
y0	y1
0.6081	0.3919

X	
x0	x1
0.6060	0.3940

Classes to code

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- CIM

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- CIM from `(gum.Potential)`

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- CTBN,

Classes to code

- CIM from `(gum.Potential)`
- CTBN, `(gum.DiGraph,gum.DiscreteVariable,CIM)`

Classes to code

- CIM from `(gum.Potential)`
- CTBN, `(gum.DiGraph,gum.DiscreteVariable,CIM)`
- Convergence
  - 'Exact' method ($exp(IM)$)
  - Sampling (Forward Sampling)

CIM

CIM

CIM : wrapper de Potential

```python
def __init__(self, pot=None):
  if pot is None:
    self._pot = gum.Potential()
  else:
    self._pot = gum.Potential(pot)
  self._recordVars()

def add(self, v) -> "CIM":
  self._pot.add(v)
  self._recordVars()
  return self

def nbrDim(self) -> int:
  return self._pot.nbrDim()

def extract(self, ctxt) -> "CIM":
  return CIM(self._pot.extract(ctxt))

@property
def var_names(self):
  return self._pot.var_names

def __getitem__(self, i):
  return self._pot[i]

def __setitem__(self, i, v):
  self._pot[i] = v
```

CIM : Amalgamation

CIM : Amalgamation

Algorithm 2.2 Amalgamate two nodes of a CTBN.

Amalgamate(X, Y)

$\mathbf{Q}_{XY|\mathbf{Pa}(XY)} \leftarrow \emptyset$
for each $\langle pa_{Y \setminus X} \rangle \in \mathbf{pa}_{X \setminus Y}$ **and** $\langle pa_{X \setminus Y} \rangle \in \mathbf{pa}_{Y \setminus X}$
  $\mathbf{Q}^{XY} \leftarrow \mathbf{0}$
  for $i, j = 1, \ldots, |X|$ **and** $l, k = 1, \ldots, |Y|$
    $\mathbf{Q}^{X} \leftarrow \mathbf{Q}_{X|\langle pa_{X \setminus Y} \rangle, x_i}$
    $\mathbf{Q}^{Y} \leftarrow \mathbf{Q}_{Y|\langle pa_{Y \setminus X} \rangle, y_k}$
    if $i = j \wedge k = l$
      $q^{XY}_{(i,j),(k,l)} \leftarrow q^{X}_{i,j} + q^{Y}_{k,l}$
    else if $i = j \wedge k \neq l$
      $q^{XY}_{(i,j),(k,l)} \leftarrow q^{Y}_{k,l}$
    else if $i \neq j \wedge k = l$
      $q^{XY}_{(i,j),(k,l)} \leftarrow q^{X}_{i,j}$
    end if
  end for
  $\mathbf{Q}_{XY|\langle pa_{XY} \rangle} \leftarrow \mathbf{Q}^{XY}$
  $\mathbf{Q}_{XY|\mathbf{Pa}(XY)} \leftarrow \mathbf{Q}_{XY|\mathbf{Pa}(XY)} \cup \{\mathbf{Q}_{XY|\langle pa_{XY} \rangle}\}$
end for
return $\mathbf{Q}_{XY|\mathbf{Pa}(XY)}$

CIM : Amalgamation

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$\mathbf{Q}_{XY|\mathbf{Pa}(XY)} \leftarrow \emptyset$
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  $\mathbf{Q}^{XY} \leftarrow \mathbf{0}$
  for $i, j = 1, \ldots, |X|$ **and** $l, k = 1, \ldots, |Y|$
    $\mathbf{Q}^{X} \leftarrow \mathbf{Q}_{X|\langle pa_{X\setminus Y}\rangle, x_i}$
    $\mathbf{Q}^{Y} \leftarrow \mathbf{Q}_{Y|\langle pa_{Y\setminus X}\rangle, y_k}$
    if $i = j \wedge k = l$
      $q^{XY}_{(i,j),(k,l)} \leftarrow q^{X}_{i,j} + q^{Y}_{k,l}$
    else if $i = j \wedge k \neq l$
      $q^{XY}_{(i,j),(k,l)} \leftarrow q^{Y}_{k,l}$
    else if $i \neq j \wedge k = l$
      $q^{XY}_{(i,j),(k,l)} \leftarrow q^{X}_{i,j}$
    end if
  end for
  $\mathbf{Q}_{XY|\langle pa_{XY}\rangle} \leftarrow \mathbf{Q}^{XY}$
  $\mathbf{Q}_{XY|\mathbf{Pa}(XY)} \leftarrow \mathbf{Q}_{XY|\mathbf{Pa}(XY)} \cup \{\mathbf{Q}_{XY|\langle pa_{XY}\rangle}\}$
end for
return $\mathbf{Q}_{XY|\mathbf{Pa}(XY)}$

```python
    i = amal.instantiation()
    iX = cimX.instantiation()
    iY = cimY.instantiation()
    i.setFirst()
    while not i.end():
      iX.setVals(i)
      iY.setVals(i)
      for v in pXinY:
        iY.chgVal(v, iX[CIM.var_i(v.name())])
      for v in pYinX:
        iX.chgVal(v, iY[CIM.var_i(v.name())])
      dX = True
      for v in sX:
        if iX[CIM.var_i(v)] != iX[CIM.var_j(v)]:
          dX = False
          break
      dY = True
      for v in sY:
        if iY[CIM.var_i(v)] != iY[CIM.var_j(v)]:
          dY = False
          break
      if dX and dY:
        amal[i] = cimX[iX] + cimY[iY]
      elif dY:
        amal[i] = cimX[iX]
      elif dX:
        amal[i] = cimY[iY]
      else:
        amal[i] = 0

      i.inc()

    return amal
```

Implementations

- CIM : 210 lines
- CTBN
- Inférence
  - Simple
  - Sampling

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CTBN

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- oriented graph (`gum.DiGraph`),
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- `CIMs` in a dictionnary.

CTBN

Mainly : synchronization of 3 very differents objects :

- oriented graph (`gum.DiGraph`),
- Discrete random variables in a dictionnary (`gum.DiscreteVariable`)
- `CIM`s in a dictionnary.

```python
def __init__(self):
    self.graph = gum.DiGraph()
    self.cim = {}
    self.id2var = {}
    self.name2id = {}

def add(self, var: gum.DiscreteVariable) -> NodeId:
    n = NodeId(self.graph.addNode())
    self.id2var[n] = var
    self.name2id[var.name()] = n

    self.bn0.add(var)

    v_i = var.clone()
    v_i.setName(CIM.var_i(var.name()))

    v_j = var.clone()
    v_j.setName(CIM.var_j(var.name()))

    self.cim[n] = CIM().add(v_j).add(v_i)

    return n

def addArc(self, val1: NameOrId, val2: NameOrId) -> Tuple[NodeId, Node
    n1 = self._nameOrId(val1)
    n2 = self._nameOrId(val2)

    self.graph.addArc(n1, n2)

    self.cim[n2].add(self.id2var[n1])

    return (n1, n2)
```

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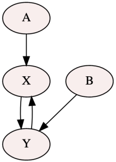
```
ctbn = Ctbn()
ctbn.add(gum.LabelizedVariable("A", "A", ["a0", "a1"]))
ctbn.add(gum.LabelizedVariable("B", "B", ["b0", "b1"]))
ctbn.add(gum.LabelizedVariable("X", "X", ["x0", "x1"]))
ctbn.add(gum.LabelizedVariable("Y", "Y", ["y0", "y1"]))

ctbn.addArc("A", "X")
ctbn.addArc("Y", "X")
ctbn.addArc("B", "Y")
ctbn.addArc("X", "Y")

ctbn.CIM("A")[:] = [[-1, 1],
                    [2, -2]]
ctbn.CIM("B")[:] = [[-3, 3],
                    [2, -2]]
ctbn.CIM("X")[{"A": "a0", "Y": "y0"}] = [[-1, 1],
                                         [2, -2]]
ctbn.CIM("X")[{"A": "a1", "Y": "y0"}] = [[-1, 1],
                                         [3, -3]]
ctbn.CIM("X")[{"A": "a0", "Y": "y1"}] = [[-5, 5],
                                         [6, -6]]
ctbn.CIM("X")[{"A": "a1", "Y": "y1"}] = [[-5, 5],
                                         [4, -4]]
ctbn.CIM("Y")[{"B": "b0", "X": "x0"}] = [[-2, 2],
                                         [5, -5]]
ctbn.CIM("Y")[{"B": "b1", "X": "x0"}] = [[-3, 3],
                                         [4, -4]]
ctbn.CIM("Y")[{"B": "b0", "X": "x1"}] = [[-3, 3],
                                         [5, -5]]
ctbn.CIM("Y")[{"B": "b1", "X": "x1"}] = [[-7, 7],
                                         [8, -8]]

gnb.sideBySide(ctbn,ctbn.CIM("A")._pot,ctbn.CIM("X")._pot)
```



	A#j	
A#i	a0	a1
a0	-1.0000	1.0000
a1	2.0000	-2.0000

			X#j	
Y	A	X#i	x0	x1
y0	a0	x0	-1.0000	1.0000
		x1	2.0000	-2.0000
	a1	x0	-1.0000	1.0000
		x1	3.0000	-3.0000
y1	a0	x0	-5.0000	5.0000
		x1	6.0000	-6.0000
	a1	x0	-5.0000	5.0000
		x1	4.0000	-4.0000

Inférence simple

Inférence simple

```python
class SimpleCtbnInference(CtbnInference):
    '''
    Exact inference using amalgamation to compute the Intensity Matrix corresponding to the ctbn
    (very bad for large models)
    '''

    def __init__(self, cim: Ctbn):
        super().__init__(cim)
        self._joint = None

    def makeInference(self):
        q = CIM()
        for nod in self._model.nodes():
            q = q.amalgamate(self._model.CIM(nod))

        q.from_matrix(expm(5000 * q.to_matrix()))

        t0 = gum.Potential()
        for n in q.var_names:
            if n[-1] == "i":
                t0.add(q._pot.variable(n))
        t0.fillWith(1).normalize()

        self._joint = (t0 * q._pot).margSumOut(t0.var_names)

    def posterior(self, name: str) -> gum.Potential:
        vj = CIM.var_j(name)
        return gum.Potential().add(self._model.variable(name)).fillWith(self._joint.margSumIn(vj), [vj])
```

Implémentations

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Forward Sampling

Forward Sampling

Algorithm 2.1 Forward sample CTBN.

ForwardSample($\mathcal{N}$)

for each $X \in \mathcal{N}$
    choose $X(0)$ by sampling from $\mathcal{B}$
end for
$t \leftarrow 0$, $\sigma \leftarrow \emptyset$
repeat until termination
    $\mathit{Append}(\sigma, \langle X, t \rangle)$
    for each $X \in \mathcal{N}$
        if $\mathit{time}(X) \neq \mathit{null}$ **then** continue **end for**
        $\mathbf{A}_X \leftarrow \mathbf{A}_{X|\mathbf{Pa}(X)}$
        $i \leftarrow X(t)$
        $\Delta t \sim \text{Exponential}(a_{i,i})$
        $\mathit{time}(X) \leftarrow t + \Delta t$
    end for
    $X' \leftarrow \text{argmin}_{X \in \mathcal{N}} (\mathit{time}(X))$
    $t \leftarrow \mathit{time}(X')$
    $X(t) \sim \text{Multinomial}(\mathbf{A}_{X'}, X(t))$
    $\mathit{time}(X') = \mathit{null}$
    for each $Y \in \mathbf{Ch}(X')$
        $\mathit{time}(Y) = \mathit{null}$
    end for
end repeat
return σ

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    end for
end repeat
return σ

Conclusion

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Code based on the result of a student project (L2).

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goals reached !

- model CTBN : compact representation of continuous-time Markov processes with a very large state space .
- pyAgrum : toolbox for the implementation of new graphical models.

And now ?

- aGrUM/pyAgrum still a lab/academic tool. We will not stop maintaining & developing !
- Many users imply many responsabilities
  - Interaction
    gitlab issues, discord, gitter, linkedin, researchGate, what else ?
  - Structuration
    communauty (?), consortium (?)
  - Scientific orientation ?
    - models
    - algorithms
    - scientific committee
    - ?
  - Development orientation ?
    - weaknesses, strengths
    - missing features
    - Ragrum, JSagrum
    - Steering committee
    - ?