The *Primula* System: user's guide
Version 3.0
Example: `Generalized inference: model-level explainer with MAP inference`

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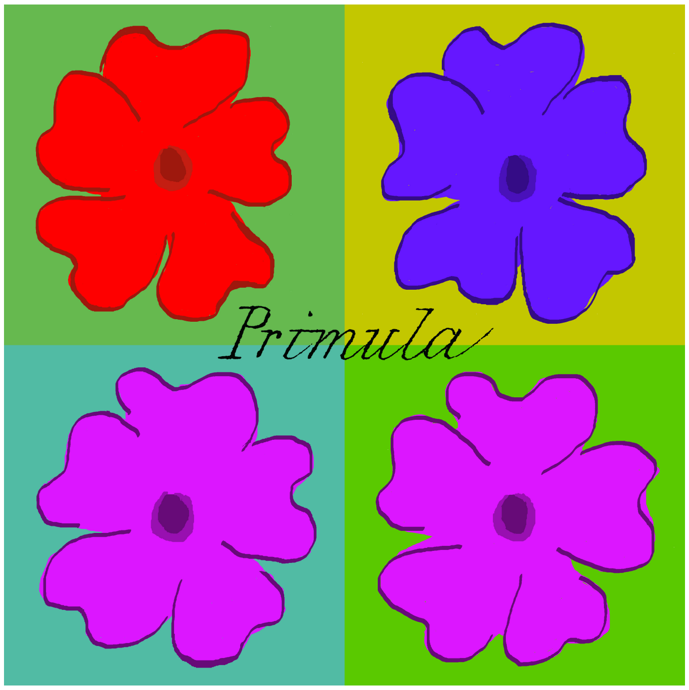
September 8, 2023



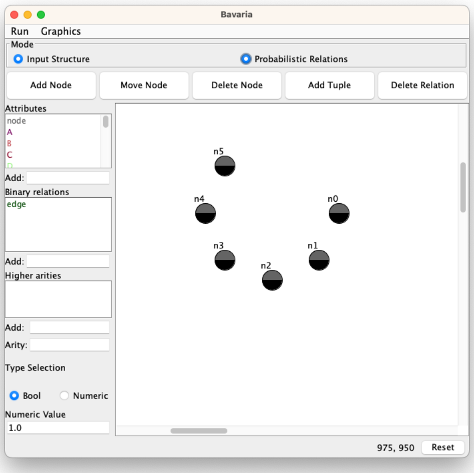
Generalized inference: model-level explainer

In this example we show how it is possible to work with GNNs and RBNs. The *.rbn file is a Relational Bayesian Network that is computationally equivalent to a Graph Neural Network, in particular the architecture used is an ACR-GNN from the The Logical Expressiveness of Graph Neural Networks paper. This RBN contains the weights of a trained ACR-GNN model on a synthetic dataset. This dataset is composed by random graphs, where each node can have 7 different types [A, B, C, D, E, F, G]. Positive graphs have inside two specific motifs: one with a node A connected to two node B *(B - A - B)*, and the other is one node C connected to two nodes D *(C - D - C)*. We trained a ACR-GNN to classify the two classes obtaining high accuracy (0.9904), and we export the trained model into a computationally equivalent RBN. Edges in the dataset are not directed, and in the RBN definition direction do not have any importance or meaning for the final results. With this trained GNN written into an RBN we can have much more inference power. In this example we will show how this RBN-GNN combination can be used as a model-level explainer able to reproduce the most probable graph for a given class.

MAP inference

Load the model file `rbn_acr_synth.rbn` and the one of the data file `*.rdef` from the folder.

Select in the *Primula* console Modules:Bavaria to open the graphical data editor. In *Bavaria* press the toggle Probabilistic Relations to view also the attributes of nodes, there will be two color: grey for the ”node” attribute, while the black for the constraints. You will see something like this:



About the constraints: With RBNs we can impose some constraint for the graph generation during the MAP inference, those constraints in this case are useful to assign an high probability to having assigned only one attribute of the 7 different types for each node. In this case it will very hard to have graphs with multiple or zero types assigned.

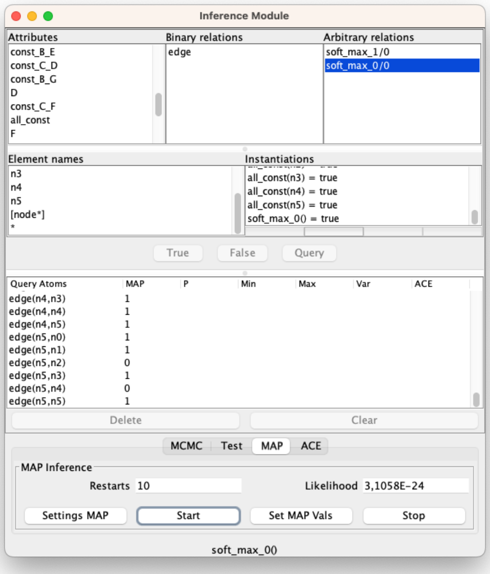
Setting Queries. Open the Modules:Inference Module and click the 'Query' button to activate the query mode:

Nodes: select the blue attribute from the 'Attributes' list and click on the `[node*]` to select all the nodes. In the synthetic example, each node has 7 possible attributes [A, B, C, D, E, F, G].
In order to do this, click on one attribute (e.g. C) and click on the `[node*]` element in the Element names list. This assigns the selected Attributes to all nodes. Repeat this process for all 7 attributes (Note: the Query button can only be clicked on the first time).

Edges: Assign all possible edge combinations to the nodes by selecting the edge attribute in the Binary relations list, and double-clicking again on the `[node*]` element (this require to be in the "query mode", click on the Query button to enter in this mode).

Class: Set the class for which you want to compute the most probable graph. In the compiled RBN, all positive classes are assigned to the Arbitrary relation `soft_max_0/0`, negative to `soft_max_1/0`. Click the True button and then click on the `soft_max_0/0` relation to assign it as the true value.

Computing MAP. Start the MAP computation by clicking the MAP button and then clicking the Settings MAP button. A new window will open, allowing you to set the number of restarts you want (-1 to stop manually or another value, e.g., 10). Click the Start button in the Inference Module and wait for the restarts to complete or manually stop the computation. When the computation finishes, press the 'Set MAP Vals' button to apply the computed values to the graph.



Attributes: const_B_E, const_C_D, const_B_G, D, const_C_F, all_const, F

Binary relations: edge

Arbitrary relations: soft_max_1/0, soft_max_0/0

Element names: n3, n4, n5, [node*], *

Instantiations:
all_const(n3) = true
all_const(n4) = true
all_const(n5) = true
soft_max_0() = true

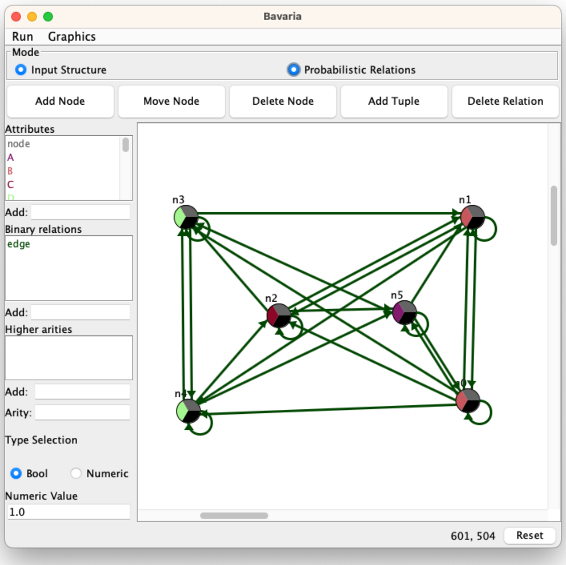
Query Atoms	MAP	P	Min	Max	Var	ACE
edge(n4,n3)	1					
edge(n4,n4)	1					
edge(n4,n5)	1					
edge(n5,n0)	1					
edge(n5,n1)	1					
edge(n5,n2)	0					
edge(n5,n3)	1					
edge(n5,n4)	0					
edge(n5,n5)	1					

Restarts 10

Likelihood 3,1058E-24

soft_max_0()

Visualizing the results. View the computed values from Bavaria. Save these results in an .rdef file by clicking on the *Primula* main interface's Save Data option under the Run menu.



Mode: [✓ Input Structure] [✓ Probabilistic Relations]

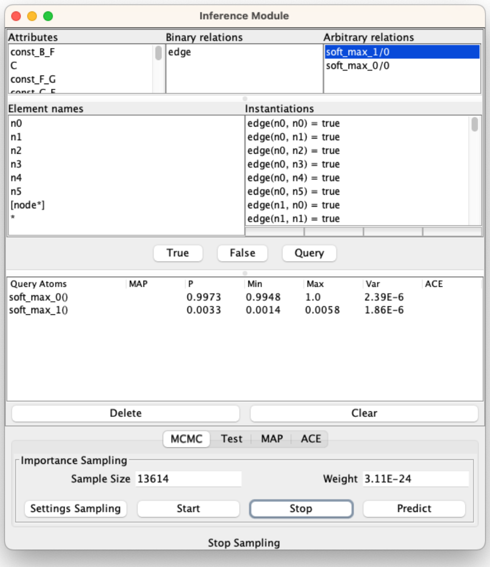
Type Selection: [✓ Bool] Numeric

Numeric Value: 1.0

Extra: additional analysis

It is possible to compute the probability that this generated graph for the model directly on the *Primula* interface. The .rbn file represent the model and we can use the MCMC inference module to estimate the probability that the generated graph has on the GNN model with few decimals of error.

Open the saved .rdef file computed with the MAP inference with a text editor. This file is an XML-like file with all the attributes specified for the graph. In the `<ProbabilisticRelsCase>` there are written all the assignments for the elements in the graph. Look for for the relation `<d rel="soft_max_0" args="()" val="true"/>` and delete that from the .rdef file. In this way we are not assign the class to the graph and it will be possible to compute the true probability (otherwise it will be as 1.0 for the assignment).
Load the modified .rdef file computed with the MAP inference into *Primula* with the same .rbn of the computation of before. Open the Inference Module and click on the MCMC button. Click on the Query button to query which class we want to select and click to the texttsoft_max_0/0 class in the Arbitrary relations (it is possible also to click on both the classes to have also the probability of the other class). Click on the Start button and wait some seconds, the Sample Size will increase and in the Query Atoms it will be possible to see the computed probability under the P column.



```
Attributes        Binary relations   Arbitrary relations
const_B_F         edge               soft_max_1/0
C                                    soft_max_0/0
const_F_G
```

```
Element names     Instantiations
n0                edge(n0, n0) = true
n1                edge(n0, n1) = true
n2                edge(n0, n2) = true
n3                edge(n0, n3) = true
n4                edge(n0, n4) = true
n5                edge(n0, n5) = true
[node*]           edge(n1, n0) = true
*                 edge(n1, n1) = true
```

Query Atoms	MAP	P	Min	Max	Var	ACE
soft_max_0()		0.9973	0.9948	1.0	2.39E-6	
soft_max_1()		0.0033	0.0014	0.0058	1.86E-6	

Sample Size 13614 Weight 3.11E-24