A Simple Latent Variable Model for Graph Learning and Inference

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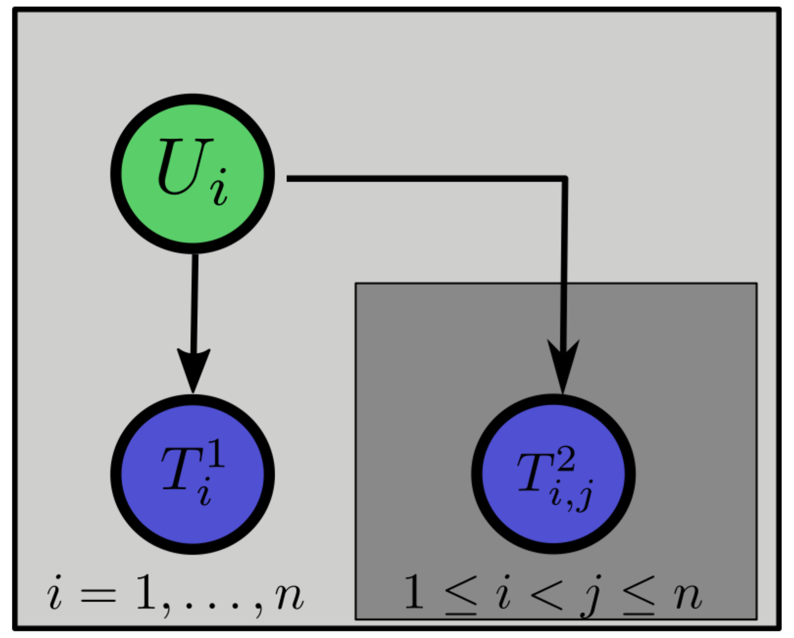
The Naive Histogram AHK Model

The AHK Model

Generating a random graph with n nodes, node attributes $A_0, \ldots, A_{a-1}$ and edge relations $E_0, \ldots, E_{e-1}$:



- U_i: latent variable for node i; uniformly distributed in $[0, 1]$
- T_i^1: random variable defining the attribute vector of i, conditional on U_i
- $T_{i,j}^2$: random variable defining the edge connections between i and j, conditional on U_i, U_j.

Projectivity: probability of an induced sub-graph of $m < n$ nodes does not depend on n.

Naive Histogram AHK

The conditional distributions for $T_i^1, T_{i,j}^2$ are defined

- piecewise constant on a partition of $[0, 1]$ ("histogram")
- attributes, edges independent given U_i ("naive")
- permutation invariant

Special case of AHK model: *Graphon*; special case of NH-AHK: *Stochastic block model*

Inference and Learning

Inference requires summation over unobserved bin memberships of the U_i:

NP-hard in n (reduction of 3-coloring problem)

Importance sampling: for observed graph ω, bins $b_0, \ldots, b_{n-1}$ sampled according to a proposal distribution Q that approximates

$$Q(b_0, \ldots, b_{n-1}) \approx P(\omega | b_0, \ldots, b_{n-1})$$

(also used for approximate gradient computation).

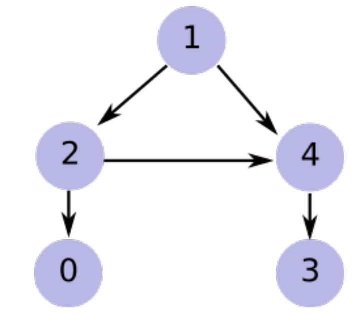
- \- sample generation cubic in n
- \+ in practice very good approximation of target distribution $P(b_0, \ldots, b_{n-1} | \omega)$
- \+ no extra cost for handling incomplete data
- \+ *projectivity* of AHK $\Rightarrow$ can query or learn (approximately) from smaller induced sub-graphs.

Learning and Querying: DAGs

Training data: 100 directed acyclic graphs with 3 to 7 nodes.
Learned model: granularity 2, 6 parameters.

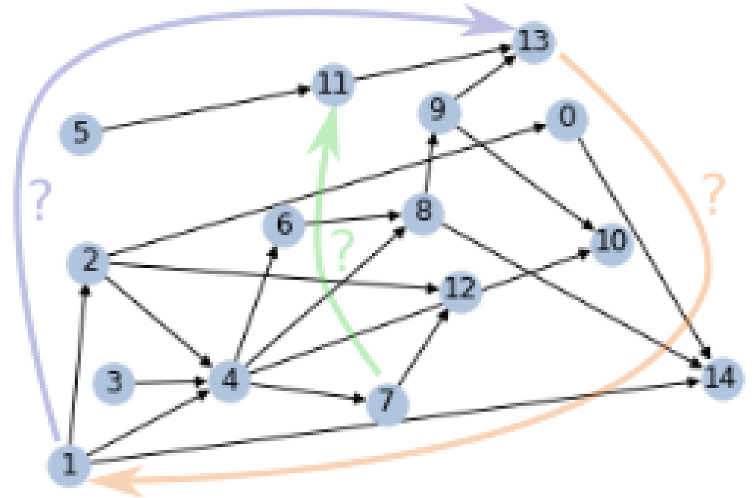
Task: Infer probabilities of (combinations of) edges.

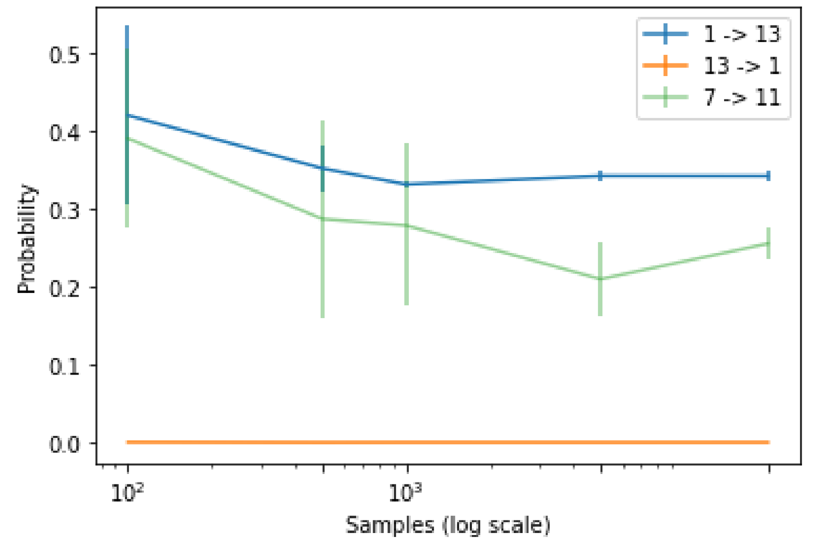
Query graph: all edges that are not drawn are assumed *unknown*



Query edge(s)	Probability (exact)
$1 \rightarrow 0$	0.43
$0 \rightarrow 3$	0.29
$3 \rightarrow 0$	0.16
$3 \rightarrow 2$	0.005
$1 \rightarrow 0 \& 0 \rightarrow 3$	0.134
$0 \rightarrow 3 \& 3 \rightarrow 0$	0.0017

Sampling inference for larger query graph (5 runs; 100 to 20.000 samples):

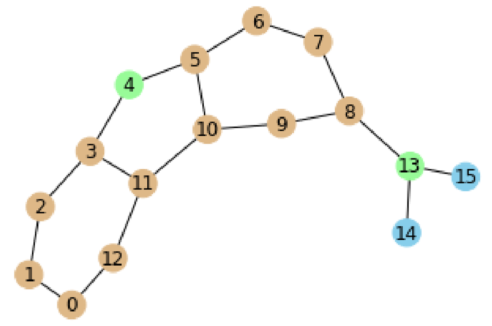




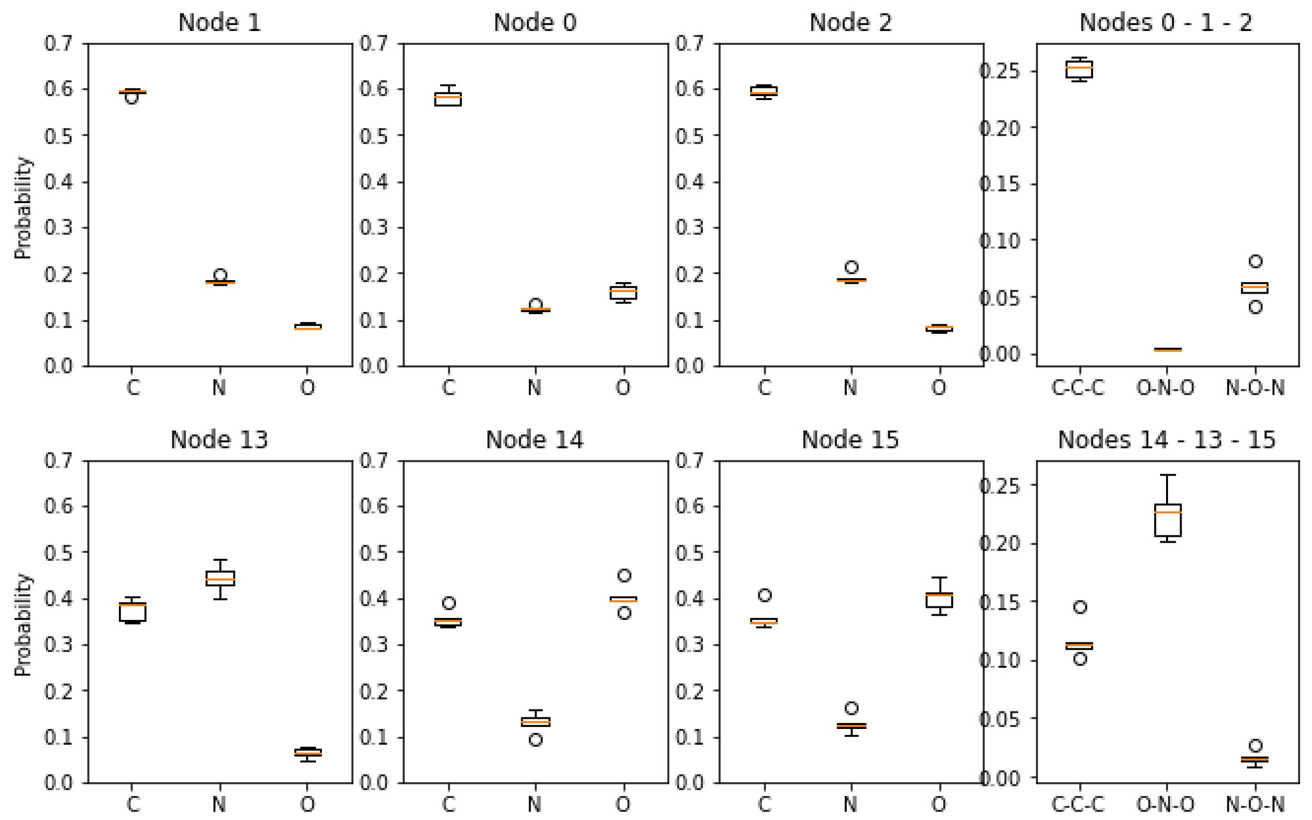
Learning and Querying: Molecules

Training data: MUTAG molecules (187 out of 188)
Learned model: granularity 10, 125 parameters.

Query molecule (last out of 188):



Task: predict elements of atom groups 0,1,2 and 13,14,15, given elements of remaining atoms.



Graph Generation

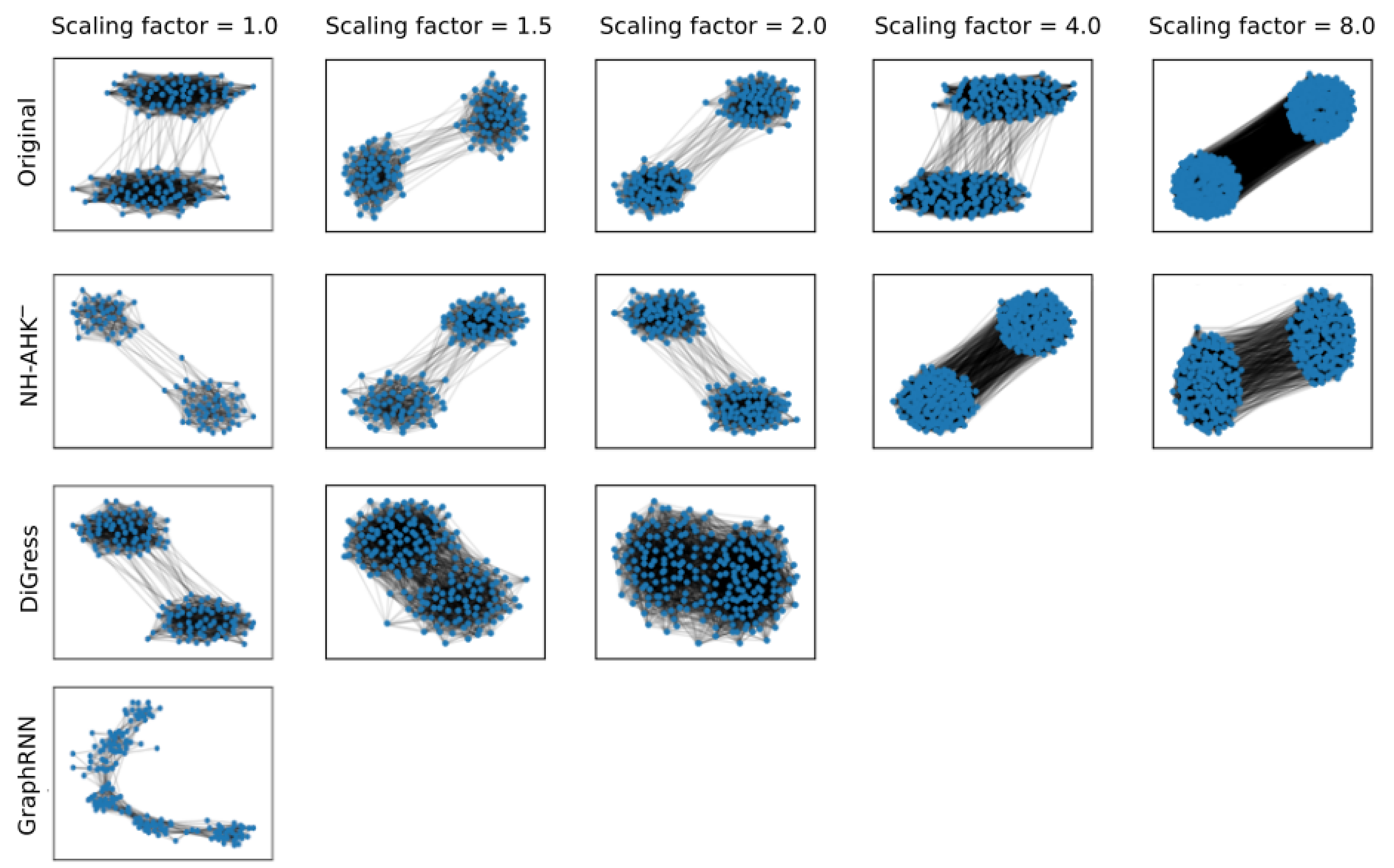
Training data: • *Community*: 500 two-community graphs.
• *EGO*: 816 2-hop ego networks from the Citeseer network.

Learned models: • (*Community*) granularity 2, 3 parameters.
• (*EGO*) granularity 2, 6 parameters.

Task: generate new graphs; also bigger than training examples.

Results: EMD between number of communities, modularity, diameter and radius of generated and test networks.

Method	Stat. (*Community*)	1	1.5	2	4	8	Stat. (*EGO*)	1	1.5	2	4	8
		Scaling factor						Scaling factor				
NH-AHK⁻	nb of com.	0.02	**0.00**	**0.00**	**0.00**	**0.00**	dia.	0.47	**0.75**	1.00	1.15	1.73
DiGress		**0.00**	0.20	0.53	-	-		**0.32**	0.78	**0.33**	**0.35**	**0.40**
GraphRNN		1.05	-	-	-	-		2.08	-	-	-	-
ER		2.42	2.07	1.90	1.25	1.23		0.40	2.03	1.48	0.96	2.05
NH-AHK⁻	mod.	0.03	**0.03**	**0.02**	**0.02**	**0.02**	rad.	0.39	**0.13**	**0.03**	**0.10**	**0.05**
DiGress		**0.00**	0.08	0.14	-	-		**0.08**	0.29	0.05	0.85	1.05
GraphRNN		0.06	-	-	-	-		1.11	-	-	-	-
ER		0.29	0.34	0.36	0.40	0.43		0.39	1.13	1.29	1.77	1.94



Summary

NH-AHK ...
- lightweight model (few parameters)
- support for general inference tasks
- graph generation for arbitrary target sizes

Paper & Code: `https://github.com/manfred-jaeger-aalborg/AHK`

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