

# Bayesian Deep Learning for Graphs

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# Why ML on Graphs?





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Reproducibility Issues



## DEEP BAYESIAN GRAPH NETS

Bridging Probabilistic  
Modeling with DL4G

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with GMDNs

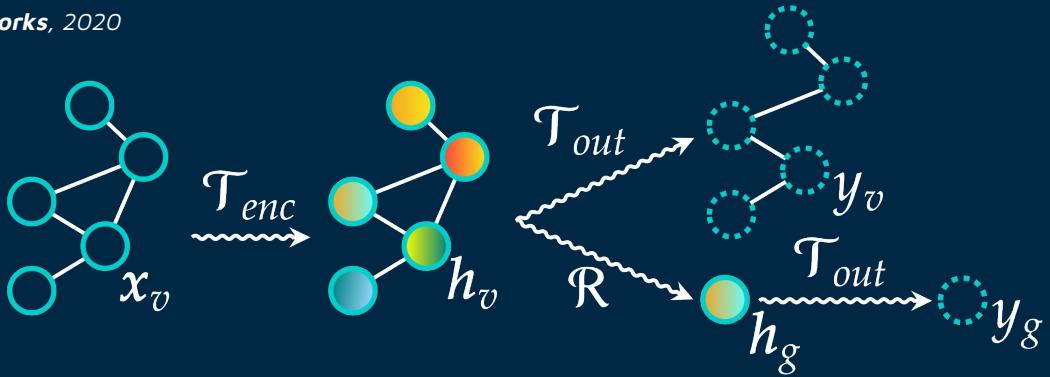


## APPLICATIONS

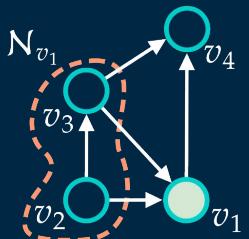
Molecular Biosciences and  
Malware Classification

# The Bigger Picture

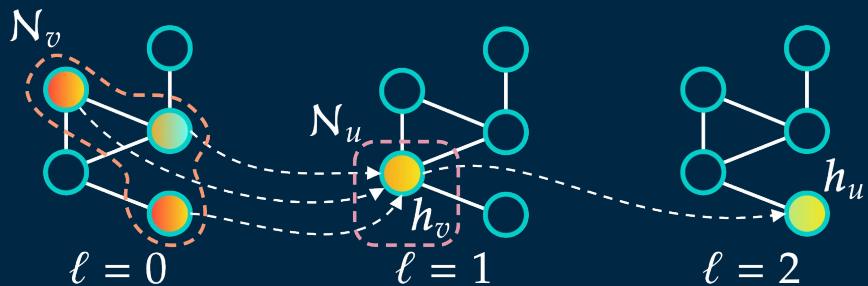
Published in **Neural Networks**, 2020



(1) local



(2) iterative



# Graph Convolutional Layer

Published in **Neural Networks**, 2020

$$\mathbf{h}_v^{\ell+1} = \phi^{\ell+1} \left( \mathbf{h}_v^\ell, \underbrace{\Psi(\{\psi^{\ell+1}(\mathbf{h}_u^\ell) \mid u \in \mathcal{N}_v\})}_{\text{set of } v\text{'s neighboring states}} \right)$$

v's state                          perm. invariant function

Variants/extensions:

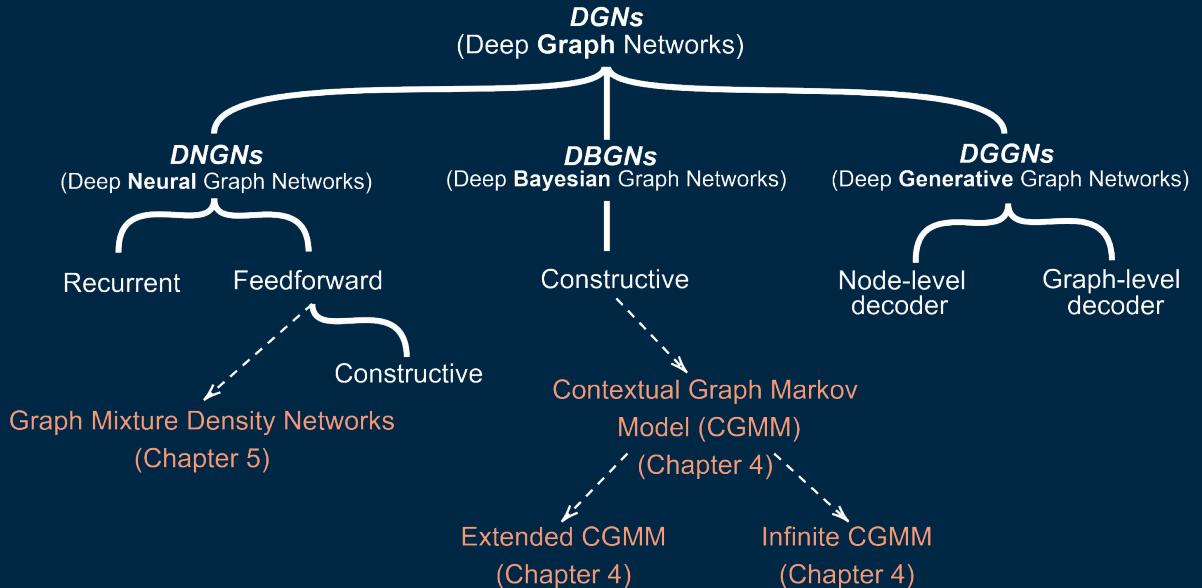
- ◎ Edge-aware convolution
- ◎ Attention over neighbors
- ◎ Laplacian-normalized



Model	Neighborhood Aggregation
NN4G	$\sigma \left( \mathbf{w}^{\ell+1T} \mathbf{x}_v + \sum_{i=0}^{\ell} \sum_{c_k \in \mathcal{C}} \sum_{u \in \mathcal{N}_v^{c_k}} w_{c_k}^i * \mathbf{h}_u^i \right)$
GNN	$\sum_{u \in \mathcal{N}_v} MLP^{\ell+1}(\mathbf{x}_u, \mathbf{x}_v, \mathbf{a}_{uv}, \mathbf{h}_u^\ell)$
GraphESN	$\sigma \left( \mathbf{W}^{\ell+1} \mathbf{x}_u + \hat{\mathbf{W}}^{\ell+1} [\mathbf{h}_{u_1}^\ell, \dots, \mathbf{h}_{u_{\mathcal{N}_v}}^\ell] \right)$
GCN	$\sigma \left( \mathbf{W}^{\ell+1} \sum_{u \in \mathcal{N}(v)} L_{vu} \mathbf{h}_u^\ell \right)$
GAT	$\sigma \left( \sum_{u \in \mathcal{N}_v} \alpha_{uv}^{\ell+1} * \mathbf{W}^{\ell+1} \mathbf{h}_u \right)$
ECC	$\sigma \left( \frac{1}{ \mathcal{N}_v } \sum_{u \in \mathcal{N}_v} MLP^{\ell+1}(\mathbf{a}_{uv})^T \mathbf{h}_u^\ell \right)$
R-GCN	$\sigma \left( \sum_{c_k \in \mathcal{C}} \sum_{u \in \mathcal{N}_v^{c_k}} \frac{1}{ \mathcal{N}_v^{c_k} } \mathbf{W}^{\ell+1} \mathbf{h}_u^\ell + \mathbf{W}^{\ell+1} \mathbf{h}_v^\ell \right)$
GraphSAGE	$\sigma \left( \mathbf{W}^{\ell+1} \left( \frac{1}{ \mathcal{N}_v } [\mathbf{h}_v^\ell, \sum_{u \in \mathcal{N}_v} \mathbf{h}_u^\ell] \right) \right)$
CGMM	$\sum_{i=0}^{\ell} w^i * \left( \sum_{c_k \in \mathcal{C}} w_{c_k}^i * \left( \frac{1}{ \mathcal{N}_v^{c_k} } \sum_{u \in \mathcal{N}_v^{c_k}} \mathbf{h}_u^i \right) \right)$
GIN	$MLP^{\ell+1} \left( (1 + \epsilon^{\ell+1}) \mathbf{h}_v^\ell + \sum_{u \in \mathcal{N}_v} \mathbf{h}_u^\ell \right)$

# A Taxonomy

Published in ***Neural Networks***, 2020



# Analyzing Scholarship Issues

Published in **ICLR**, 2020

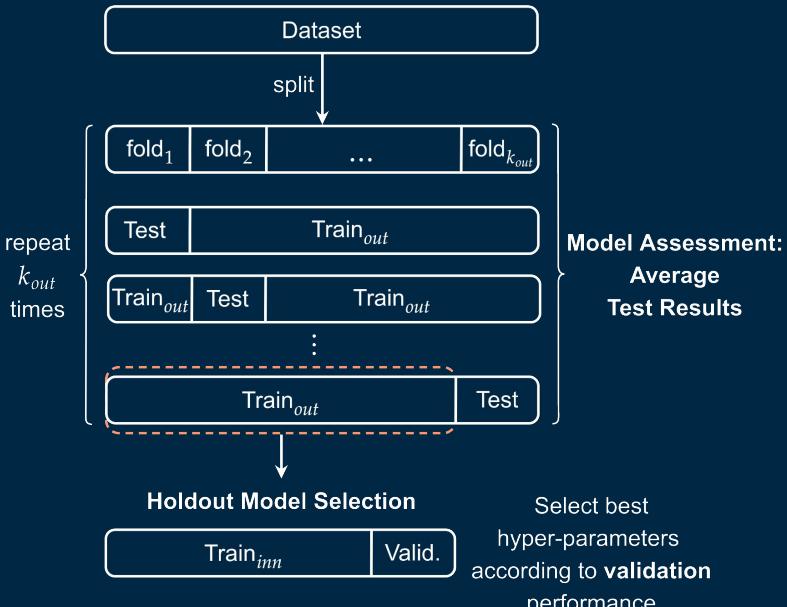
	DGCNN	DiffPool	ECC	GIN
Data preprocessing code	Y	Y	-	Y
Model selection code	N	N	-	N
Model evaluation code	Y	Y	-	Y
Data splits provided	Y	N	N	Y
Label Stratification	Y	N	-	Y
Report accuracy on test	Y	A	A	N
Report standard deviations	Y	N	N	Y

Y → yes

N → no

A → ambiguous

- → not available



A STANDARD & UNIFORM  
EVALUATION SCHEME

# Re-evaluation Results

Published in **ICLR**, 2020

Results on chemical datasets



	D&D	NCI1	PROTEINS	ENZYMES
Baseline	<b><math>78.4 \pm 4.5</math></b>	$69.8 \pm 2.2$	<b><math>75.8 \pm 3.7</math></b>	<b><math>65.2 \pm 6.4</math></b>
DGCNN	$76.6 \pm 4.3$	$76.4 \pm 1.7$	$72.9 \pm 3.5$	$38.9 \pm 5.7$
DiffPool	$75.0 \pm 3.5$	$76.9 \pm 1.9$	$73.7 \pm 3.5$	$59.5 \pm 5.6$
ECC	$72.6 \pm 4.1$	$76.2 \pm 1.4$	$72.3 \pm 3.4$	$29.5 \pm 8.2$
GIN	$75.3 \pm 2.9$	<b><math>80.0 \pm 1.4</math></b>	$73.3 \pm 4.0$	$59.6 \pm 4.5$
GraphSAGE	$72.9 \pm 2.0$	$76.0 \pm 1.8$	$73.0 \pm 4.5$	$58.2 \pm 6.0$

We report the median number of selected layers per model

	IMDB-B		IMDB-M		REDDIT-B		REDDIT-M		COLLAB	
	1	DEG	1	DEG	1	DEG	1	DEG	1	DEG
DGCNN	3	3	3.5	3	4	3	3	2	4	2
DiffPool	1	2	2	1	2	2	2	1	2	1.5
ECC	1	2	1	1	-	-	-	-	-	-
GIN	3	2	4	2	4	4	4	3	4	4
GraphSAGE	4	3	5	4	3	4	3	5	3	5

Results on social datasets



No FEATURES	IMDB-B	IMDB-M	REDDIT-B	REDDIT-5K	COLLAB
Baseline	$50.7 \pm 2.4$	$36.1 \pm 3.0$	$72.1 \pm 7.8$	$35.1 \pm 1.4$	$55.0 \pm 1.9$
DGCNN	$53.3 \pm 5.0$	$38.6 \pm 2.2$	$77.1 \pm 2.9$	$35.7 \pm 1.8$	$57.4 \pm 1.9$
DiffPool	$68.3 \pm 6.1$	$45.1 \pm 3.2$	$76.6 \pm 2.4$	$34.6 \pm 2.0$	$67.7 \pm 1.9$
ECC	$67.8 \pm 4.8$	$44.8 \pm 3.1$	OOR	OOR	OOR
GIN	$66.8 \pm 3.9$	$42.2 \pm 4.6$	<b><math>87.0 \pm 4.4</math></b>	<b><math>53.8 \pm 5.9</math></b>	<b><math>75.9 \pm 1.9</math></b>
GraphSAGE	<b><math>69.9 \pm 4.6</math></b>	<b><math>47.2 \pm 3.6</math></b>	$86.1 \pm 2.0$	$49.9 \pm 1.7$	$71.6 \pm 1.5$



WITH DEGREE	IMDB-B	IMDB-M	REDDIT-B	REDDIT-5K	COLLAB
Baseline	$70.8 \pm 5.0$	<b><math>49.1 \pm 3.5</math></b>	$82.2 \pm 3.0$	$52.2 \pm 1.5$	$70.2 \pm 1.5$
DGCNN	$69.2 \pm 3.0$	$45.6 \pm 3.4$	$87.8 \pm 2.5$	$49.2 \pm 1.2$	$71.2 \pm 1.9$
DiffPool	$68.4 \pm 3.3$	$45.6 \pm 3.4$	$89.1 \pm 1.6$	$53.8 \pm 1.4$	$68.9 \pm 2.0$
ECC	$67.7 \pm 2.8$	$43.5 \pm 3.1$	OOR	OOR	OOR
GIN	<b><math>71.2 \pm 3.9</math></b>	$48.5 \pm 3.3$	<b><math>89.9 \pm 1.9</math></b>	<b><math>56.1 \pm 1.7</math></b>	<b><math>75.6 \pm 2.3</math></b>
GraphSAGE	$68.8 \pm 4.5$	$47.6 \pm 3.5$	$84.3 \pm 1.9$	$50.0 \pm 1.3$	$73.9 \pm 1.7$



Metric: ACCURACY

# Deep Bayesian Graph Nets



# Contextual Graph Markov Model

Published in **ICML**, 2018 & **JMLR**, 2020

Exploit vast amounts of  
raw unlabelled data

**UNSUPERVISED  
EMBEDDINGS**

**PROBABILISTIC**

Relies on simple conditional  
Bayesian networks



Does not suffer from  
vanishing/exploding gradient

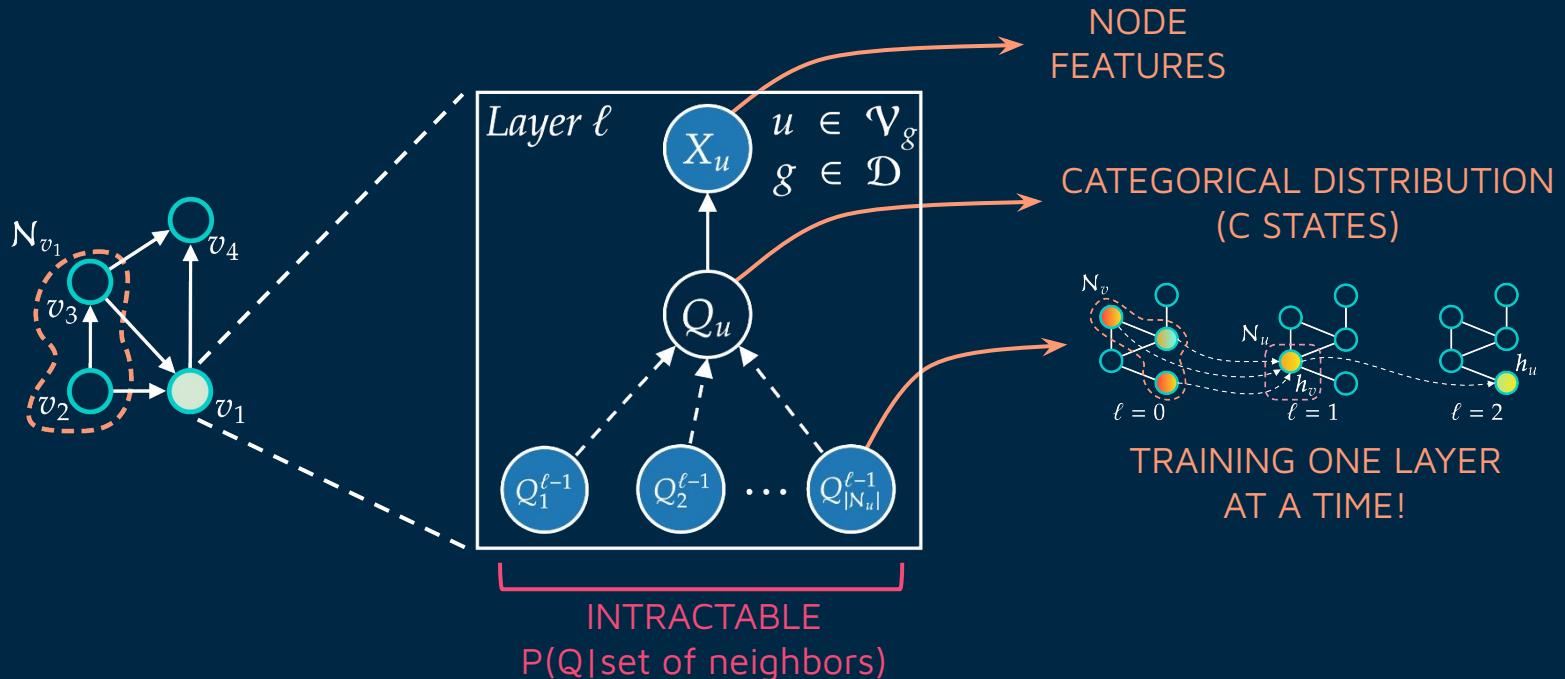
**DEEP**

**EFFICIENT**

Linear (Space/Time) in the  
number of edges

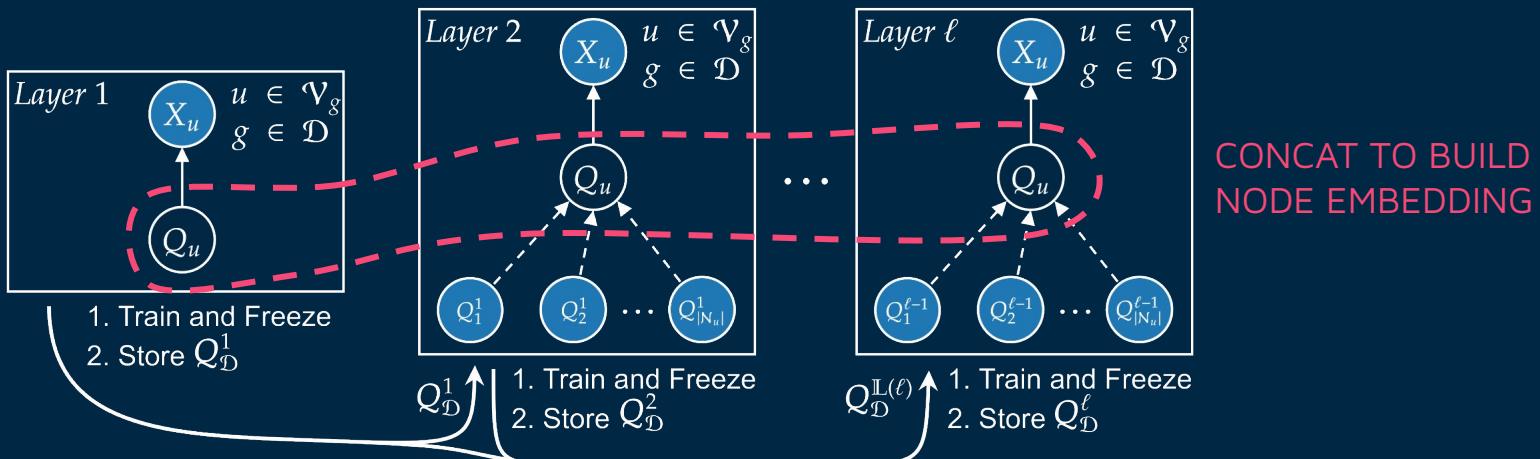
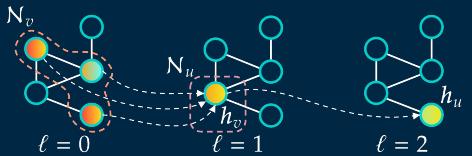
# Contextual Graph Markov Model

Published in **ICML**, 2018 & **JMLR**, 2020



# How-to CGMM

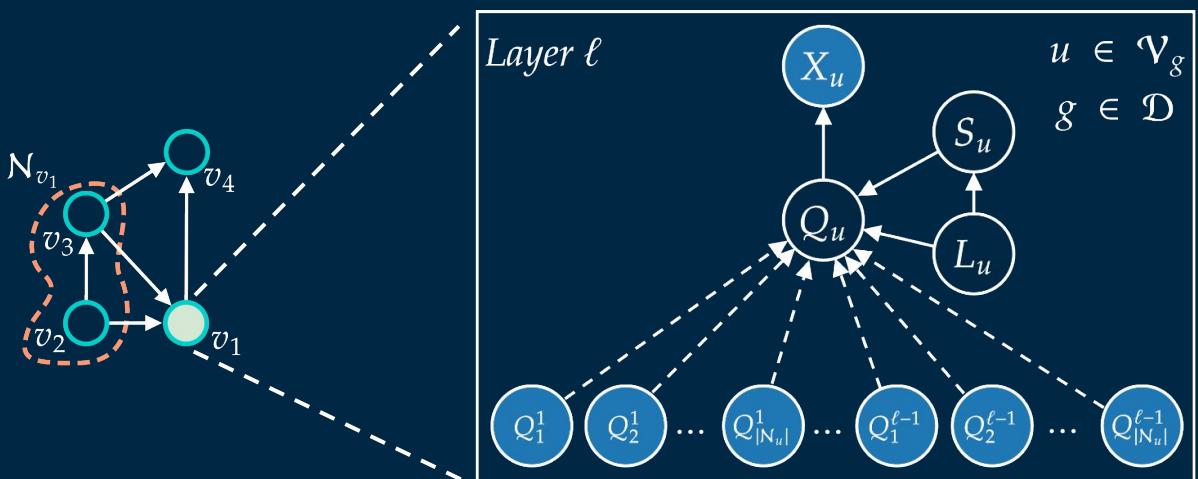
Published in **ICML**, 2018 & **JMLR**, 2020



High-level description of CGMM's incremental construction

# Handling Discrete Edge Features

Published in **ICML**, 2018 & **JMLR**, 2020



INTRODUCE **SWITCHING PARENT** VARIABLES



GROUP FROZEN  
NEIGHBORS BY **EDGE TYPE AND LAYER**



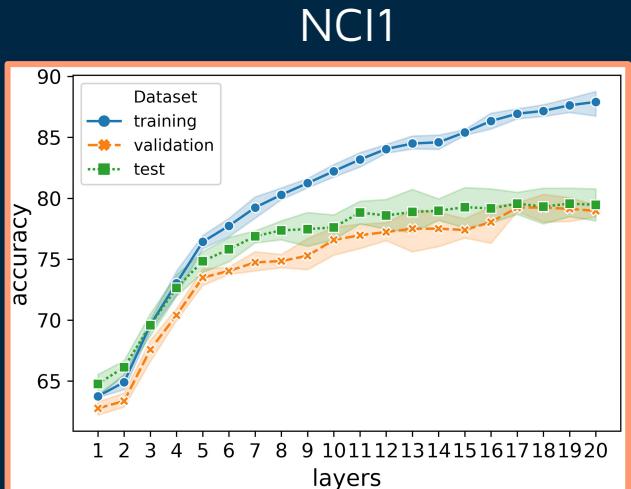
ADDRESS **INTRACTABILITY**  
+ ENHANCED **FLEXIBILITY**

# Graph Classification Results

Published in **ICML**, 2018 & **JMLR**, 2020

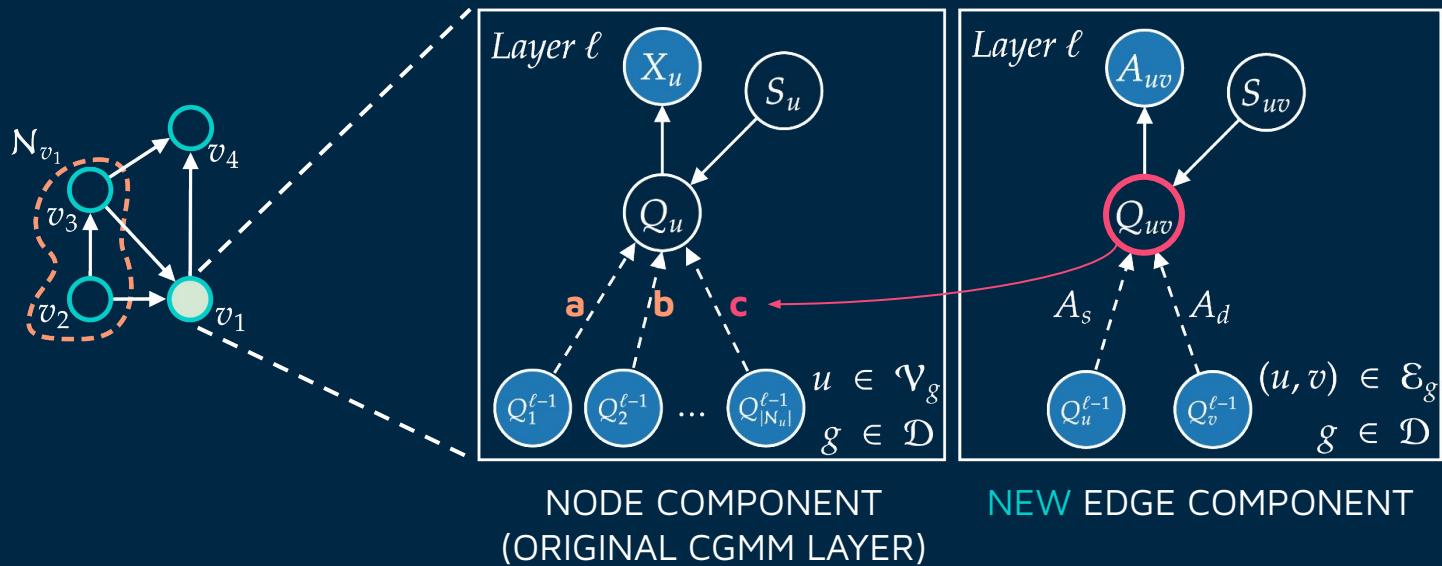
	D&D	NCI1	PROTEINS
BASELINE	<b>78.4 ± 4.5</b>	69.8 ± 2.2	<b>75.8 ± 3.7</b>
DGCNN	76.6 ± 4.3	76.4 ± 1.7	72.9 ± 3.5
DIFFPOOL	75.0 ± 3.5	76.9 ± 1.9	73.7 ± 3.5
ECC	72.6 ± 4.1	76.2 ± 1.4	72.3 ± 3.4
GIN	75.3 ± 2.9	<b>80.0 ± 1.4</b>	73.3 ± 4.0
GRAPH SAGE	72.9 ± 2.0	76.0 ± 1.8	73.0 ± 4.5
CGMM	74.9 ± 3.4	76.2 ± 2.0	74.0 ± 3.9

	IMDB-B	IMDB-M	REDDIT-B	REDDIT-5K	COLLAB
BASELINE	70.8 ± 5.0	<b>49.1 ± 3.5</b>	82.2 ± 3.0	52.2 ± 1.5	70.2 ± 1.5
DGCNN	69.2 ± 3.0	45.6 ± 3.4	87.8 ± 2.5	49.2 ± 1.2	71.2 ± 1.9
DIFFPOOL	68.4 ± 3.3	45.6 ± 3.4	89.1 ± 1.6	53.8 ± 1.4	68.9 ± 2.0
ECC	67.7 ± 2.8	43.5 ± 3.1	-	-	-
GIN	71.2 ± 3.9	48.5 ± 3.3	<b>89.9 ± 1.9</b>	<b>56.1 ± 1.7</b>	75.6 ± 2.3
GRAPH SAGE	68.8 ± 4.5	47.6 ± 3.5	84.3 ± 1.9	50.0 ± 1.3	73.9 ± 1.7
CGMM	<b>72.7 ± 3.6</b>	47.5 ± 3.9	88.1 ± 1.9	52.4 ± 2.2	<b>77.32 ± 2.2</b>



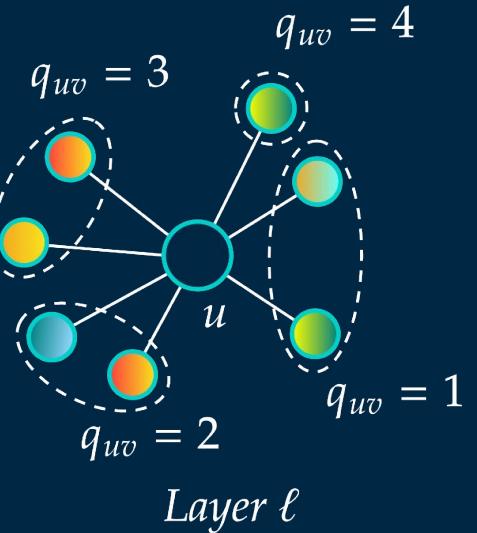
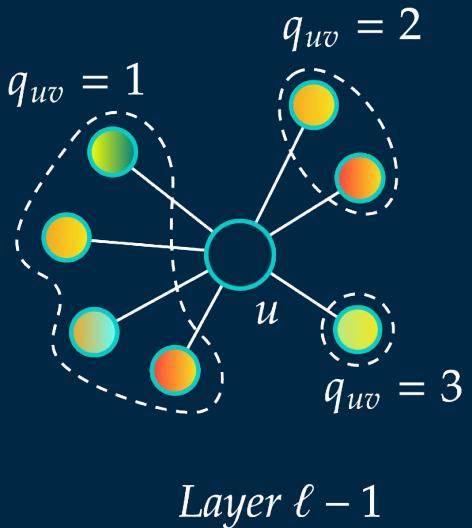
# Extension - Continuous Edge Features

Published in **IJCNN**, 2021



# Dynamic Neighborhood Aggregation

Published in **IJCNN**, 2021



EVEN WHEN EDGE  
FEATURES ARE NOT  
AVAILABLE!

# Graph Class./Regr. Results

Published in **IJCNN**, 2021

## GRAPH CLASSIFICATION

	D&D	NCI1	PROTEINS
BASELINE	<b>78.4 ± 4.5</b>	69.8 ± 2.2	<b>75.8 ± 3.7</b>
DGCNN	76.6 ± 4.3	76.4 ± 1.7	72.9 ± 3.5
DIFFPOOL	75.0 ± 3.5	76.9 ± 1.9	73.7 ± 3.5
ECC	72.6 ± 4.1	76.2 ± 1.4	72.3 ± 3.4
GIN	75.3 ± 2.9	<b>80.0 ± 1.4</b>	73.3 ± 4.0
GRAPHSAGE	72.9 ± 2.0	76.0 ± 1.8	73.0 ± 4.5
CGMM	74.9 ± 3.4	76.2 ± 2.0	74.0 ± 3.9
E-CGMM	73.9 ± 4.1	78.5 ± 1.7	73.3 ± 4.1

## GRAPH REGRESSION on QM7b

	MAE	Relative Improvement
CGMM-no edge attributes	1.52 ± 0.05	19%
CGMM-discretized edges	1.49 ± 0.07	17%
E-CGMM	<b>1.23 ± 0.06</b>	-

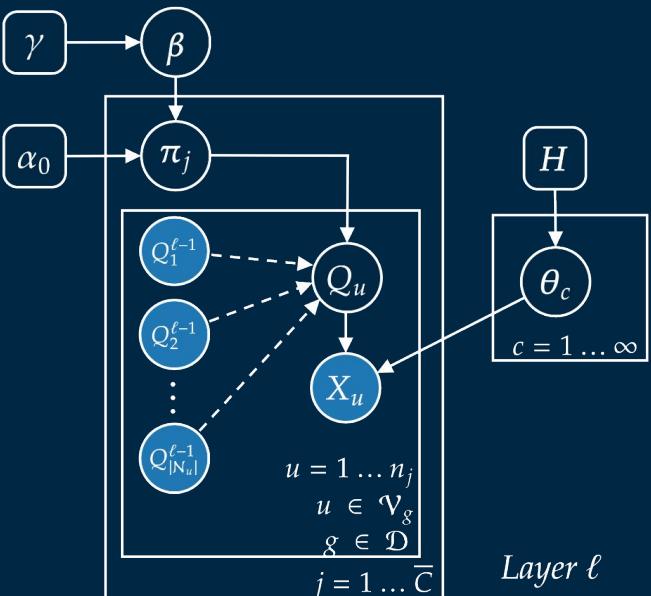
	IMDB-B	IMDB-M	REDDIT-B	REDDIT-5K	COLLAB
BASELINE	70.8 ± 5.0	<b>49.1 ± 3.5</b>	82.2 ± 3.0	52.2 ± 1.5	70.2 ± 1.5
DGCNN	69.2 ± 3.0	45.6 ± 3.4	87.8 ± 2.5	49.2 ± 1.2	71.2 ± 1.9
DIFFPOOL	68.4 ± 3.3	45.6 ± 3.4	89.1 ± 1.6	53.8 ± 1.4	68.9 ± 2.0
ECC	67.7 ± 2.8	43.5 ± 3.1	-	-	-
GIN	71.2 ± 3.9	48.5 ± 3.3	<b>89.9 ± 1.9</b>	<b>56.1 ± 1.7</b>	75.6 ± 2.3
GRAPHSAGE	68.8 ± 4.5	47.6 ± 3.5	84.3 ± 1.9	50.0 ± 1.3	73.9 ± 1.7
CGMM	<b>72.7 ± 3.6</b>	47.5 ± 3.9	88.1 ± 1.9	52.4 ± 2.2	77.32 ± 2.2
E-CGMM	70.7 ± 3.8	48.3 ± 4.1	89.5 ± 1.3	53.7 ± 1.0	<b>(77.45 ± 2.3)</b>

“Can we extend CGMM to  
automatize the choice of its  
hyper-parameters?”

# The Infinite CGMM

*Under Review*

- A Hierarchical Dirichlet Process
  - Automatic choice of # states for  $Q_u$
  - Gibbs sampling inference
  - Can estimate all hyper-parameters with suitable hyper-priors
- Choice of observations' groups determined by neighbors' states
- Batch version for larger datasets



# Graph Classification Results

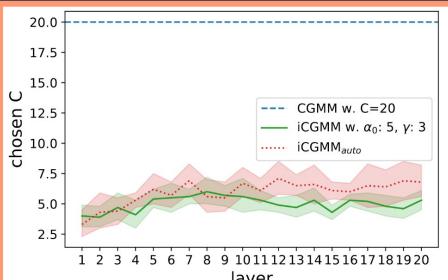
Under Review

## GRAPH CLASSIFICATION

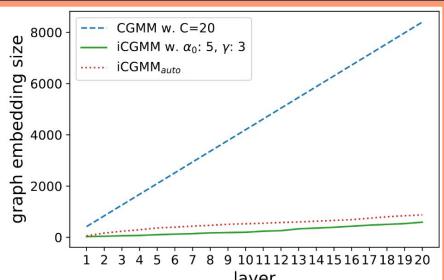
	D&D	NCI1	PROTEINS
BASELINE	$78.4 \pm 4.5$	$69.8 \pm 2.2$	$75.8 \pm 3.7$
DGCNN	$76.6 \pm 4.3$	$76.4 \pm 1.7$	$72.9 \pm 3.5$
DIFFPOOL	$75.0 \pm 3.5$	$76.9 \pm 1.9$	$73.7 \pm 3.5$
ECC	$72.6 \pm 4.1$	$76.2 \pm 1.4$	$72.3 \pm 3.4$
GIN	$75.3 \pm 2.9$	$80.0 \pm 1.4$	$73.3 \pm 4.0$
GRAPHSAGE	$72.9 \pm 2.0$	$76.0 \pm 1.8$	$73.0 \pm 4.5$
CGMM	$74.9 \pm 3.4$	$76.2 \pm 2.0$	$74.0 \pm 3.9$
E-CGMM	$73.9 \pm 4.1$	$78.5 \pm 1.7$	$73.3 \pm 4.1$
ICGMM	$75.6 \pm 4.3$	$76.5 \pm 1.8$	$72.7 \pm 3.4$
ICGMM <sub>f</sub>	$75.0 \pm 5.6$	$76.7 \pm 1.7$	$73.3 \pm 2.9$
ICGMM <sub>auto</sub>	$76.3 \pm 5.6$	$77.6 \pm 1.5$	$73.1 \pm 3.9$
ICGMM <sub>fauto</sub>	$75.1 \pm 3.8$	$76.4 \pm 1.4$	$73.2 \pm 3.9$

	IMDB-B	IMDB-M	REDDIT-B	REDDIT-5K	COLLAB
BASELINE	$70.8 \pm 5.0$	$49.1 \pm 3.5$	$82.2 \pm 3.0$	$52.2 \pm 1.5$	$70.2 \pm 1.5$
DGCNN	$69.2 \pm 3.0$	$45.6 \pm 3.4$	$87.8 \pm 2.5$	$49.2 \pm 1.2$	$71.2 \pm 1.9$
DIFFPOOL	$68.4 \pm 3.3$	$45.6 \pm 3.4$	$89.1 \pm 1.6$	$53.8 \pm 1.4$	$68.9 \pm 2.0$
ECC	$67.7 \pm 2.8$	$43.5 \pm 3.1$	-	-	-
GIN	$71.2 \pm 3.9$	$48.5 \pm 3.3$	$89.9 \pm 1.9$	$56.1 \pm 1.7$	$75.6 \pm 2.3$
GRAPHSAGE	$68.8 \pm 4.5$	$47.6 \pm 3.5$	$84.3 \pm 1.9$	$50.0 \pm 1.3$	$73.9 \pm 1.7$
CGMM	$72.7 \pm 3.6$	$47.5 \pm 3.9$	$88.1 \pm 1.9$	$52.4 \pm 2.2$	$77.32 \pm 2.2$
E-CGMM	$70.7 \pm 3.8$	$48.3 \pm 4.1$	$89.5 \pm 1.3$	$53.7 \pm 1.0$	$77.45 \pm 2.3$
ICGMM <sub>f</sub>	$73.0 \pm 4.3$	$48.6 \pm 3.4$	$91.3 \pm 1.8$	$55.5 \pm 1.9$	$78.6 \pm 2.8$
ICGMM <sub>fauto</sub>	$71.8 \pm 4.4$	$49.0 \pm 3.8$	$91.6 \pm 2.1$	$55.6 \pm 1.7$	$78.9 \pm 1.7$

- =/> performances
- Less waste of states



(a) # states chosen at each layer



(b) Cumulative graph embedding size on NCI1

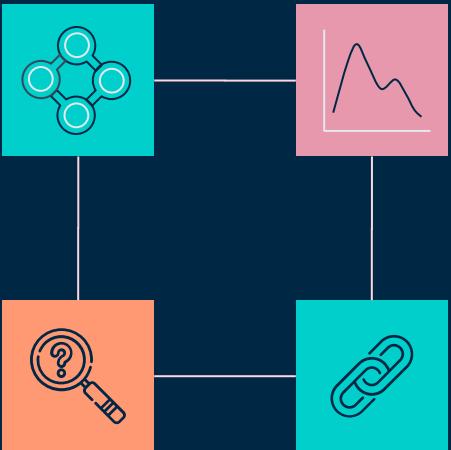
# Graph Mixture Density Nets



# Why GMDNs ?

Published in **ICML**, 2021

**Structure**  
Like Deep Graph Networks



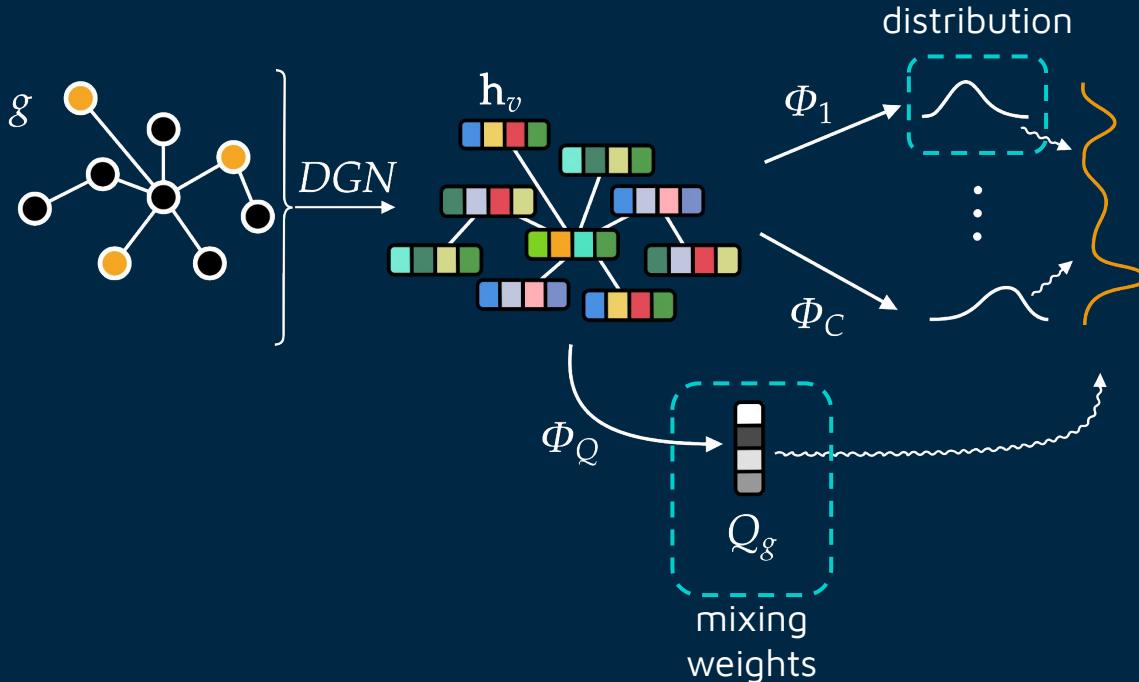
**Multimodality**  
Like Mixture Density Networks

**Uncertainty**  
1) Data Representation  
2) Encoder Expressiveness

**End-to-end**  
Get the best of neural  
and probabilistic worlds

# GMDN in a Nutshell

Published in **ICML**, 2021

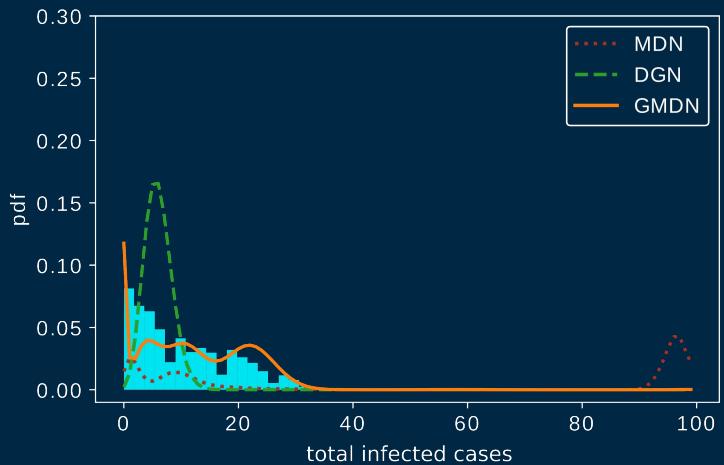


# Results

Published in **ICML**, 2021

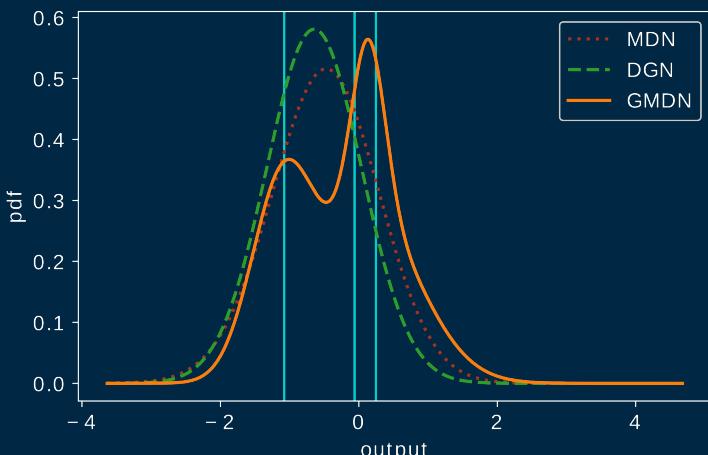
## Synthetic Epidemic Simulations

	BA-100	ER-100	Structure	Multimodal
RAND	-4.60	-4.60	<b>X</b>	<b>X</b>
HIST	-1.16	-2.32	<b>X</b>	<b>✓</b>
MDN	-1.17(.05)	-2.54(.07)	<b>X</b>	<b>✓</b>
DGN	-0.90(.35)	-1.96(.16)	<b>✓</b>	<b>X</b>
GMDN	<b>-0.67(.02)</b>	<b>-1.56(.04)</b>	<b>✓</b>	<b>✓</b>

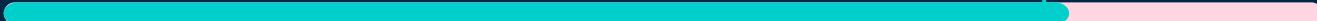
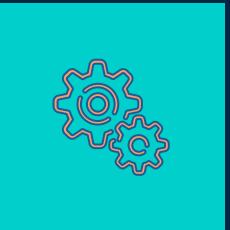


## Chemical Tasks

	alchemy_full		ZINC_full	
	$\log \mathcal{L}$	MAE	$\log \mathcal{L}$	MAE
RAND	-27.12	-	-4.20	-
HIST	-21.91	-	-1.28	-
MDN	-1.36(.90)	0.62(.01)	-1.14(.01)	0.67(.00)
DGN	-7.19(1.3)	0.62(.01)	-0.90(.10)	0.49(.03)
GMDN	<b>-0.57(1.4)</b>	<b>0.61(.02)</b>	<b>-0.75(.10)</b>	<b>0.49(.04)</b>

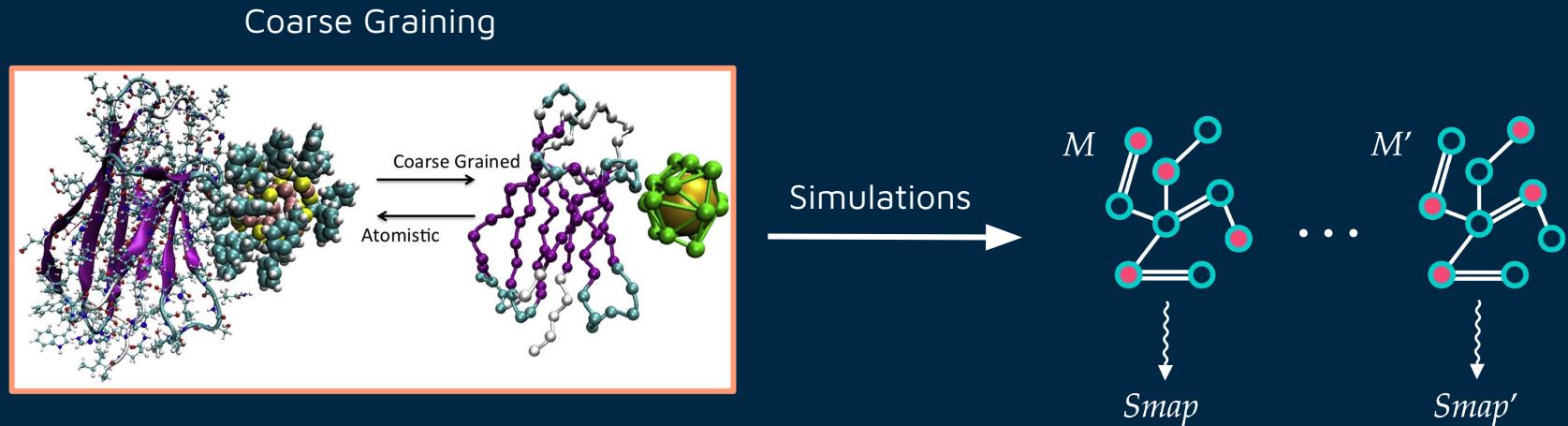


# Applications



# Accelerate Molecular Dynamics

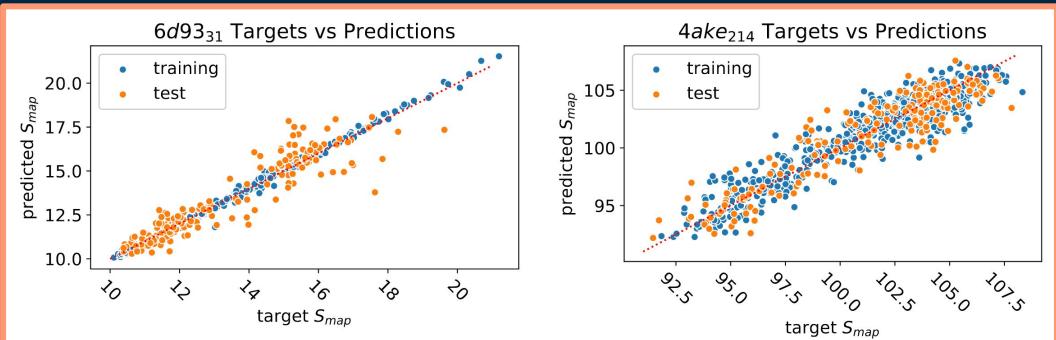
Published in ***Frontiers in Molecular Biosciences***, 2021 (with *Uni Trento*)



find the optimal  
mapping according to → huge cost!  
known criterion

# Results

Published in **Frontiers in Molecular Biosciences**, 2021 (with Uni Trento)



Model / Protein	TR MAE	TR R <sup>2</sup>	VL MAE	VL R <sup>2</sup>	TE MAE	TE R <sup>2</sup>
Baseline / 6d93	0.55	0.86	0.63	0.83	0.65	0.82
DGN / 6d93	0.13	0.99	0.33	0.95	0.33	0.96
Baseline / 4ake	1.78	0.70	1.75	0.65	1.86	0.69
DGN / 4ake	0.91	0.92	1.2	0.85	1.35	0.84

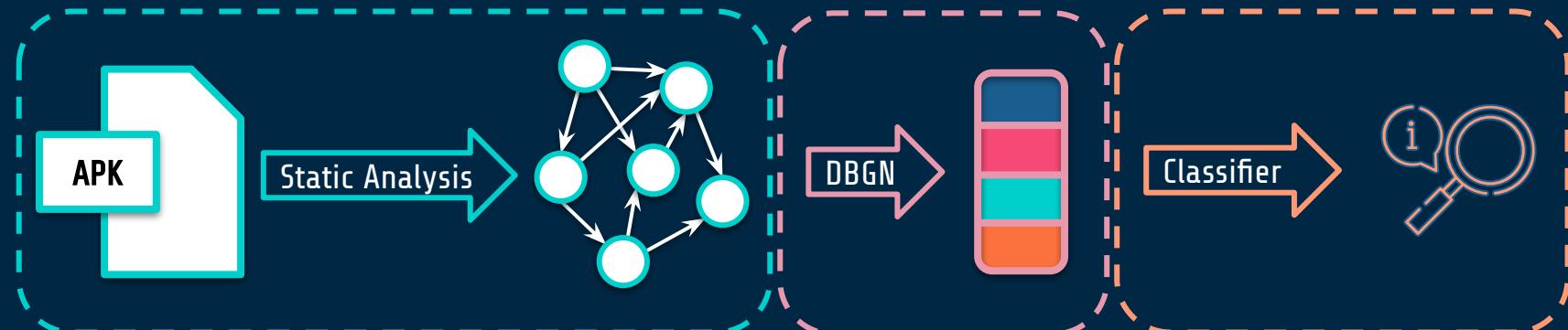
Protein	Single measure	Inference GPU (CPU)	Improvement GPU (CPU)
6d93	$\simeq 2.1$ mins	$\simeq 0.9(98.7)$ ms	$\simeq 140000 \times (1276 \times)$
4ake	$\simeq 8.0$ mins	$\simeq 4.8(1103.2)$ ms	$\simeq 100000 \times (435 \times)$

Accurate

Fast  
Prediction

# Robust Malware Classification

Published in **ESANN**, 2021 (with **IIT CNR**)



1. Create a **Call Graph** dataset
2. **Do not consider** node features, use node out-degrees
3. Build **unsupervised** graph embeddings
4. **Robust** structural malware classification

	TR Loss	TR Acc.	VL Loss	VL Acc.	TE Loss	TE Acc.
BASELINE	$1.2 \pm 0.05$	$55.6 \pm 0.5$	$1.1 \pm 0.01$	$60.6 \pm 0.9$	$1.1 \pm 0.03$	$56.7 \pm 0.5$
CGMM	$0.01 \pm 0.01$	$99.8 \pm 0.4$	$0.16 \pm 0.01$	$97.9 \pm 0.2$	$0.13 \pm 0.01$	$96.4 \pm 0.6$
E-CGMM	$0.03 \pm 0.02$	$99.4 \pm 0.6$	$0.59 \pm 0.003$	$98.4 \pm 0.3$	$0.19 \pm 0.02$	$97.3 \pm 0.4$
iCGMM <sub>f</sub>	$0.05 \pm 0.01$	$98.7 \pm 0.5$	$0.27 \pm 0.04$	$94.8 \pm 0.5$	$0.35 \pm 0.03$	$93.6 \pm 0.6$
iCGMM <sub>f<sub>auto</sub></sub>	$0.07 \pm 0.03$	$97.93 \pm 0.9$	$0.25 \pm 0.02$	$95.8 \pm 0.5$	$0.42 \pm 0.1$	$92.7 \pm 0.5$

# Conclusions

- **Introductory** contributions
  - Mathematical systematization of DL4G literature
  - Addressing empirical reproducibility issues
- **Methodological** contributions
  - Basic architecture (CGMM)
  - Extensions (E-CGMM, iCGMM)
  - Modeling multimodality with graphs (GMDN)
- **Practical** contributions
  - Molecular dynamics
  - Malware classification

# Future Directions

- **Uncertainty** Modeling
  - Epistemic / Aleatoric via sampling from learned distributions
  - Useful in physics engine simulators
- Handling **missing features**
- **Temporal** graphs
- **Interpretability** analyses
  - Variations in likelihood / multimodal distribution w.r.t. changes in the graph

# THANK YOU!



Davide  
Bacci



Alessio  
Micheli



Daniele  
Castellana



Marco  
Podda

Internal Committee: Roberto Grossi (UniPi), Luca Oneto (UniGe)

International Reviewers: Mark Coates (McGill), Shirui Pan (Monash)

# List of Publications

- ★ Bacciu D., **Errica F.**, Micheli A., "Contextual Graph Markov Model: A Deep and Generative Approach to Graph Processing", ***ICML*** 2018
- ★ **Errica F.**, Podda M., Bacciu D., Micheli A., "A Fair Comparison of Graph Neural Networks for Graph Classification", ***ICLR*** 2020
- ★ Bacciu D., **Errica F.**, Micheli A., Podda M., "A Gentle Introduction to Deep Learning for Graphs", ***Neural Networks*** 2020
- ★ Bacciu D., **Errica F.**, Micheli A., "Probabilistic Learning on Graphs via Contextual Architecture", ***JMLR***, 2020
- ★ **Errica F.**, Bacciu D., Micheli A., "Theoretically Expressive and Edge-aware Graph Learning", ***ESANN*** 2020
- ★ **Errica F.**, Giulini M., Bacciu D., Menichetti R., Micheli A., Potestio R., "A deep graph network-enhanced sampling approach to efficiently explore the space of reduced representations of proteins", ***Frontiers in Molecular Biosciences*** 2021
- ★ Atzeni D., **Errica F.**, Bacciu D., Micheli A., "Modeling Edge Features with Deep Bayesian Graph Networks", ***IJCNN*** 2021
- ★ **Errica F.**, Edizel B., Denoyer L., Petroni F., Plachouras V., Silvestri F., Riedel S., "Context Matching for Low-Resource Classification", ***IJCNN*** 2021
- ★ **Errica F.**, Bacciu D., Micheli A., "Graph Mixture Density Networks", ***ICML*** 2021
- ★ **Errica F.**, Iadarola G., Martinelli F., Mercaldo F., Micheli A., "Robust Malware Classification via Deep Graph Networks on Call Graph Topologies", ***ESANN*** 2021
- ★ Carta A., Cossu A., **Errica F.**, Bacciu D., "Catastrophic Forgetting in Deep Graph Networks: an Introductory Benchmark for Graph Classification", Workshop on Graph Learning Benchmarks, ***WWW*** 2021 - **spotlight**

Questions?

THANKS

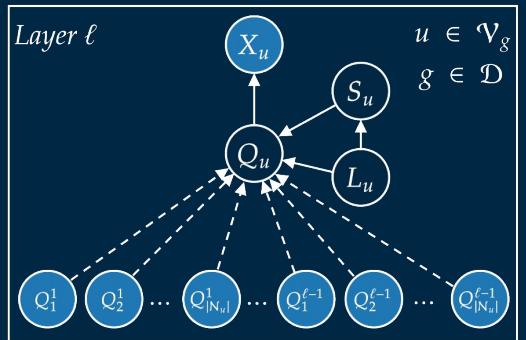


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# CGMM Formulation

To summarize, the likelihood of a graph under the extended formulation of CGMM can be therefore written as

$$\begin{aligned}
 \mathcal{L}(\boldsymbol{\theta} \mid g) &= \prod_{u \in \mathcal{V}_g} \sum_{i=1}^C P_{\boldsymbol{\theta}}(X_u = x_u \mid Q_u = i) P(Q_u = i \mid \mathbf{Q}_{\mathcal{N}_u}^{\mathbb{L}(\ell)}) \approx \\
 &\approx \prod_{u \in \mathcal{V}_g} \sum_{i=1}^C \underbrace{P_{\boldsymbol{\theta}}(X_u = x_u \mid Q_u = i)}_{emission} \sum_{\ell' \in \mathbb{L}(\ell)} \underbrace{P_{\boldsymbol{\theta}}(L_u = \ell')}_{SP\ layer} \sum_{a=1}^{|\mathcal{A}_g|} \underbrace{P_{\boldsymbol{\theta}}^{\ell'}(S_u = a)}_{SP\ edge} \times \\
 &\quad \times \frac{1}{|\mathcal{N}_u^a|} \sum_j^C \underbrace{P_{\boldsymbol{\theta}}^{\ell',a}(Q_u = i \mid Q_*^{\ell',a} = j)}_{SP\text{-}aware\ transition} \sum_{v \in \mathcal{N}_u^a} q_v^{\ell'}(j). \tag{4.4}
 \end{aligned}$$



**Complexity:** Linear in # of edges

# iCGMM Formulation

Overall, the generative process of a single iCGMM layer can be formalized as follows:

$$\begin{aligned}
 \boldsymbol{\beta} | \gamma &\sim \text{Stick}(\gamma) & j_u | \mathbf{Q}_{\mathcal{N}_u}^{\ell-1} &= \psi(\mathbf{Q}_{\mathcal{N}_u}^{\ell-1}) \\
 \boldsymbol{\pi}_j | \boldsymbol{\beta}, \alpha_0 &\sim \text{DP}(\alpha_0, \boldsymbol{\beta}) & q_u | j_u, (\boldsymbol{\pi}_j)_{j=1}^{\bar{C}} &\sim \boldsymbol{\pi}_{j_u} \\
 \boldsymbol{\theta} | \mathbf{H} &\sim \mathbf{H} & x_u | q_u, (\boldsymbol{\theta})_{c=1}^{\infty} &\sim F(\boldsymbol{\theta}_{q_u}),
 \end{aligned} \tag{4.7}$$

