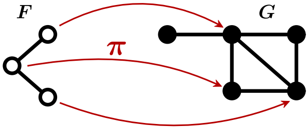
ICML | 2020

Graph Homomorphism Convolution

Universality Results of Graph Homomorphism Densities



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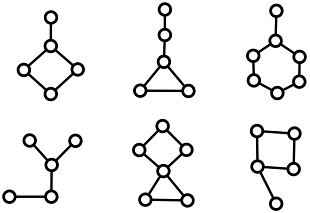
RIKEN Center for Advanced Intelligence Project

July 15, 2020

Outline

Introduction



Graph dataset:
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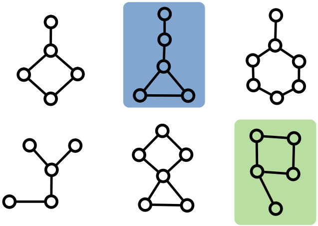
$G_i = (V(G_i), E(G_i))$ is simple.



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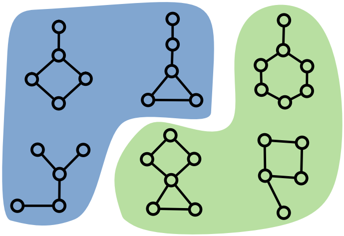

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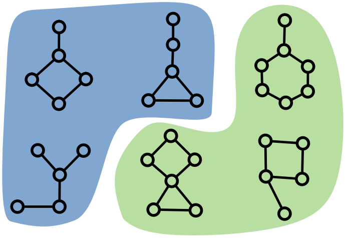

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Applications: Molecule classification, social network classification, point-cloud classification, etc.

! *Common approach*: $\rho : (G, x) \mapsto \rho(G, x) \in \mathbb{R}^d$.

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Kernels (2000s)	**Neural Networks (2010s)**
Based on counting or graph distances	Based on message passing or feature aggregation
Subgraph kernel [GFW03] RW kernel [BOS+05] Tree kernel [CD02, MV09] WL kernel [SSL+11]	GIN [XHLJ19] GraphSAGE [HYL17] SplineCNN [FLWM18] GNT kernel [DHP+19]
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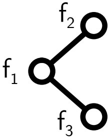
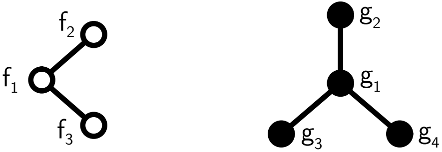
We study *graph homomorphism* count vectors as ρ.

$\boldsymbol{F}$



$$\boldsymbol{F} \longmapsto \boldsymbol{G}$$



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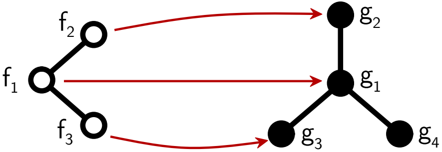
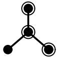


π	f_1	f_2	f_3
	g_1	g_2	g_3

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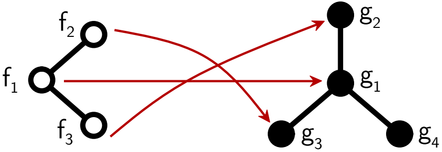

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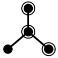	g_1 g_1	g_2 $\cdots$	g_3 $\cdots$	**6**

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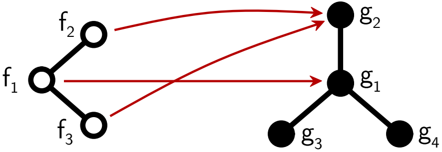

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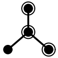
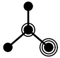
	g_1 g_1	g_2 $\cdots$	g_3 $\cdots$	**6**
	g_1	g_2	g_2	

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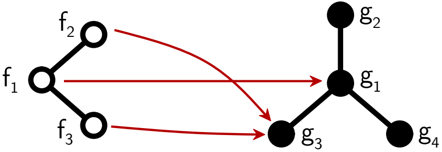

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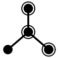
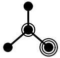
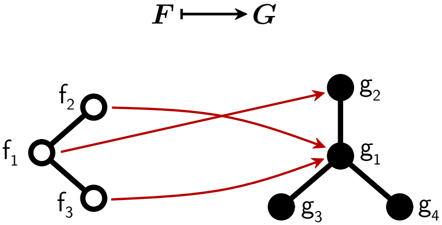
	g_1 g_1	g_2 $\cdots$	g_3 $\cdots$	**6**
	g_1 g_1	g_2 $\cdots$	g_2 $\cdots$	**3**



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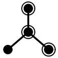
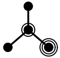
	g_1 g_1	g_2 $\cdots$	g_3 $\cdots$	**6**
	g_1 g_1	g_2 $\cdots$	g_2 $\cdots$	**3**
	g_2	g_1	g_1	

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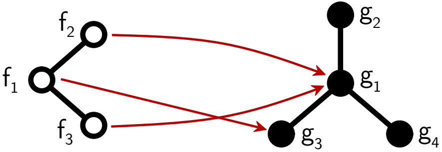

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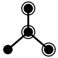
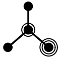
	g_1 g_1	g_2 $\cdots$	g_3 $\cdots$	**6**
	g_1 g_1	g_2 $\cdots$	g_2 $\cdots$	**3**
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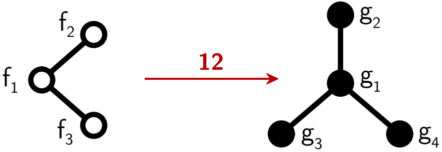

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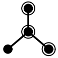
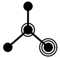
	g_1 g_1	g_2 $\cdots$	g_3 $\cdots$	**6**
	g_1 g_1	g_2 $\cdots$	g_2 $\cdots$	**3**
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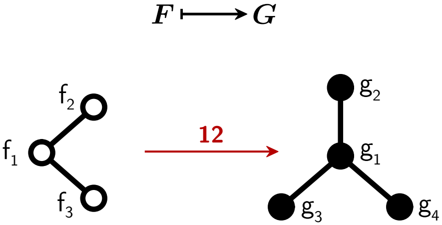

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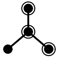
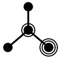
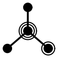
	g_1 g_1	g_2 $\cdots$	g_3 $\cdots$	**6**
	g_1 g_1	g_2 $\cdots$	g_2 $\cdots$	**3**
	g_2 $\cdots$	g_1 g_1	g_1 g_1	**3**

The set of all *connectivity preserving* maps is denoted $\mathrm{Hom}(F, G)$.
Here we have $\mathrm{hom}(F, G) := |\mathrm{Hom}(F, G)| = 12$.

$$\hom(F,G) := \sum_{\pi : V(F) \mapsto V(G)} \prod_{(u,v) \in E(F)} 1[(\pi(u), \pi(v)) \in E(G)]$$

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Graph Homomorphism | Example – Definition

Return 1 for each valid map

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All possible maps

Iverson bracket

For some set of graphs $\mathcal{F}$, the graph *embedding* is given by:

$$G \overset{\mathcal{F}}{\approx} \mathsf{hom}(\mathcal{F}, G) := [\mathsf{hom}(F, G) : F \in \mathcal{F}]$$

Universality Results

Theorem 1 ([Lov67])

Two graphs G_1 and G_2 are isomorphic if and only if hom$(F, G_1) =$ hom(F, G_2) for all simple graphs F. If $|V(G_1)|, |V(G_2)| \leq n$ then we only have to examine F with $|V(F)| \leq n$.

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❗ This hinted that we can build universal approximators for isomorphism-invariant functions on G via hom$(\mathcal{F}, G)$.

❗ Existing universal approximators for graph functions exhibit high dimensionality (high tensor order) [MFSL19, KP19].

Note that homomorphism vector $\hom(\mathcal{F}, G)$ also exhibits high-dimensionality if $\mathcal{F}$ is a set of all simple graphs up to size $|V(G)|$, which is similar to previous research.

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♥ Good news is we have the set $\mathcal{F}$ to "parameterize":

- Some class of $\mathcal{F}$ can be computed efficiently [DST02]
- Restricting $\mathcal{F}$ can lead to different class of universal approximators (this work)

Definition 2 ([BCGR19])

A function $f : \mathcal{G} \mapsto \mathbb{R}$ is $\mathcal{F}$-invariant if $f(G_1) = f(G_2)$ for G_1, G_2 satisfy hom$(\mathcal{F}, G_1) =$ hom$(\mathcal{F}, G_2)$ (termed $\mathcal{F}$-indistinguishable).

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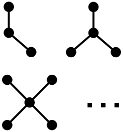
$\mathcal{F}$	$\mathcal{F}$-indistinguishable
	graphs with the same number of vertices
	graphs with the same number of edges
	graphs with the same degree sequence
k-**treewidth**	same results for k-dim WL test [DGR18]

Theorem 3 (Bounded Graphs)

Let f be an $\mathcal{F}$-invariant function. For any positive integer N, there exists a degree N polynomial h_N of $\hom(\mathcal{F}, G)$ such that $f(G) \approx h_N(G)$ for all G with $|V(G)| \leq N$.

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Theorem 4 (Unbounded Graphs)

Let f be a continuous $\mathcal{F}$-invariant function. There exists a degree N polynomial h_N of $\hom(F, G)$ ($F \in \mathcal{F}$) such that $f(G) \approx h_N(G)$ for all G.

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❗ The main idea for our proofs is to unify these theorems under the Stone-Weierstrass Theorem.

Experimental Results

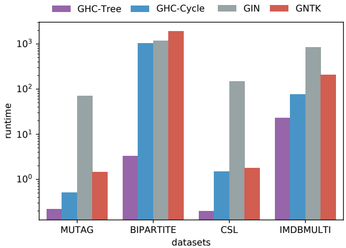
Synthetic graph datasets often used for theoretical studies of graph classification models:

- Circular Skip Links: 150 graphs with 10 isomorphic groups.
- Bipartite: Our synthesized dataset in which random bipartite and random ER graphs are to be distinguished.
- Paulus25: We show the results for strongly regular and co-spectral graphs as a challenge for the future work.

METHODS	CSL	BIPARTITE	PAULUS25
Practical models			
GIN	10.00 ± 0.00	55.75 ± 7.91	7.14 ± 0.00
GNTK	10.00 ± 0.00	58.03 ± 6.84	7.14 ± 0.00
Theory models			
Ring-GNN	$10\sim80 \pm 15.7$	-	-
GHC-Tree	10.00 ± 0.00	52.68 ± 7.15	7.14 ± 0.00
GHC-Cycle	$\mathbf{100.0 \pm 0.00}$	$\mathbf{100.0 \pm 0.00}$	7.14 ± 0.00

We experiment with data from the TU-Dortmund graph kernel benchmark dataset[1].

Methods	MUTAG	IMDB-BIN	IMDB-MUL
Practical models			
GNTK	89.46 ± 7.03	75.61 ± 3.98	51.91 ± 3.56
GIN	89.40 ± 5.60	70.70 ± 1.10	43.20 ± 2.00
PATCHY-SAN	89.92 ± 4.50	71.00 ± 2.20	45.20 ± 2.80
WL kernel	90.40 ± 5.70	73.80 ± 3.90	50.90 ± 3.80
Theory models			
Ring-GNN	-	73.00 ± 5.40	48.20 ± 2.70
GHC-Tree	89.28 ± 8.26	72.10 ± 2.62	48.60 ± 4.40
GHC-Cycles	87.81 ± 7.46	70.93 ± 4.54	47.41 ± 3.67



Since homomorphism vectors are built from $\mathcal{F}$, this method also gives us the ability to look at which sub-structure is important. For these datasets, single vertex, edge, triangle, and star-4 are the top important graphs.

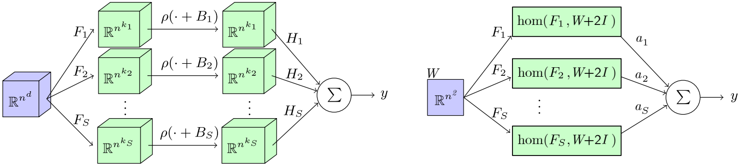
[1] http://graphlearning.io/

Conclusion

Extra Details

In this presentation, few following points are not mentioned:

- Weighted Homomorphism Number: hom$(F, (G, x))$
- Universality results for Weighted Homomorphism
- Invariant/Equivariant Universality results[2]



(a) Tensorized Graph Neural Network (b) Graph Homomorphism Model

[2] `https://arxiv.org/abs/1910.03802`

Remarks and Future Directions

In this work:

- Proposed the study of homomorphism numbers as embeddings for graphs. Our results not only show its general universality, but also the concept of $\mathcal{F}$-invariant universality.
- Proved the universality in unbounded graphs with continuous assumption, and adapted the *graphon* model to prove the universality in general function case.
- Demonstrate the practicality of homomorphism numbers in the graph classification task.

Future:

- To what degree homomorphism vectors generalize other graph kernels?
- Develop learning theory for graphs based on the homomorphism densities.

Thank you for listening!

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