Scalable and Interpretable Graph Modeling with Graph Grammars

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Satyaki Sikdar

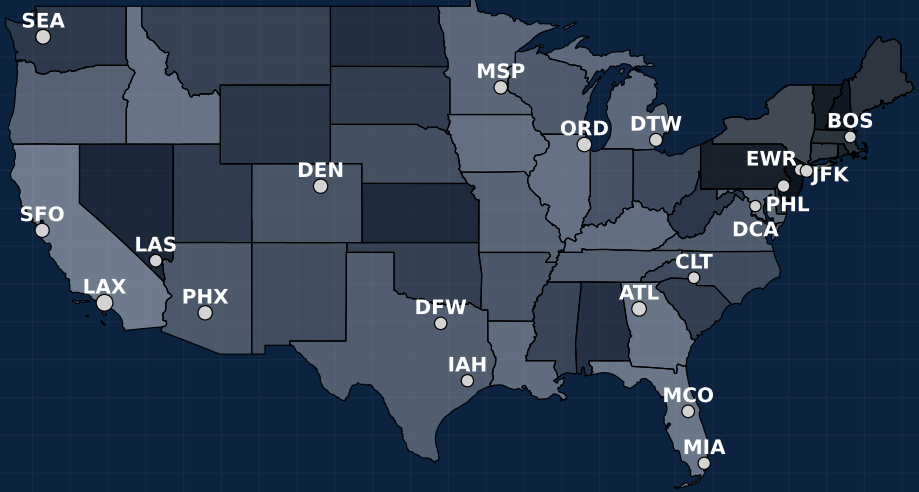
Ph.D. Defense

Committee: Dr. Tim Weninger, Chair

Dr. David Chiang · Dr. Peter Kogge · Dr. Danai Koutra

Introduction

US Flights Network in 2011



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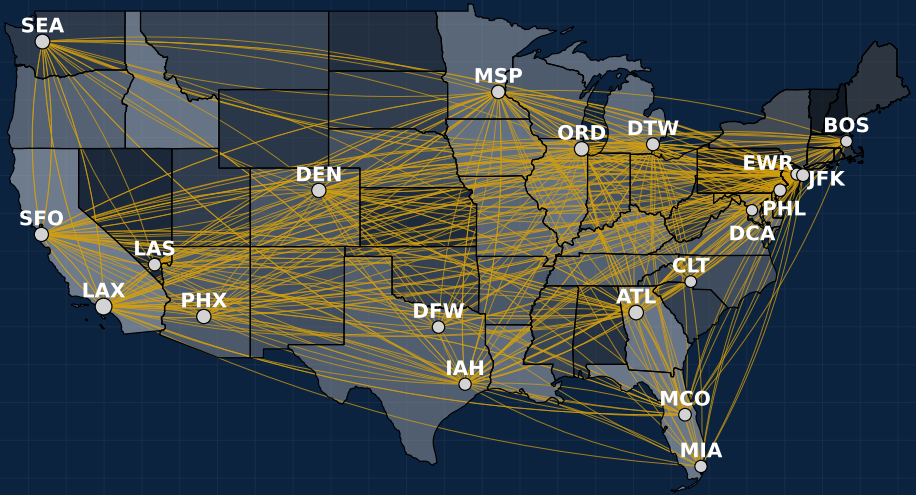

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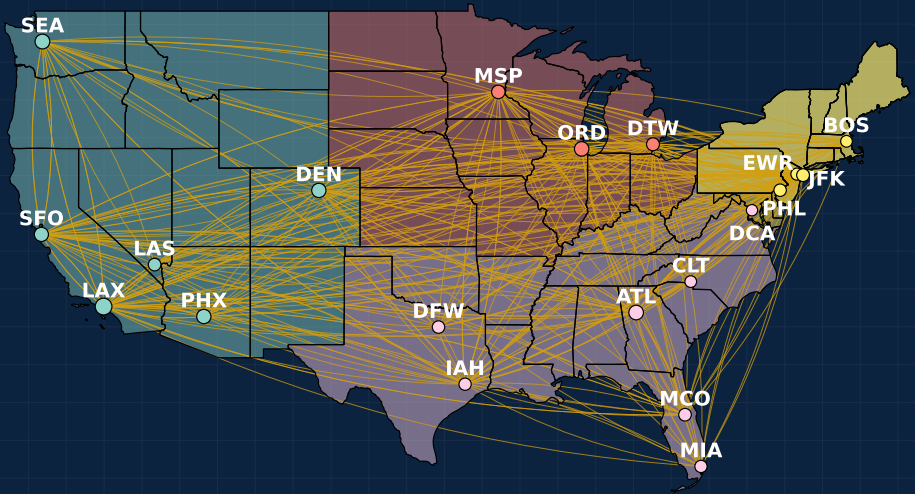

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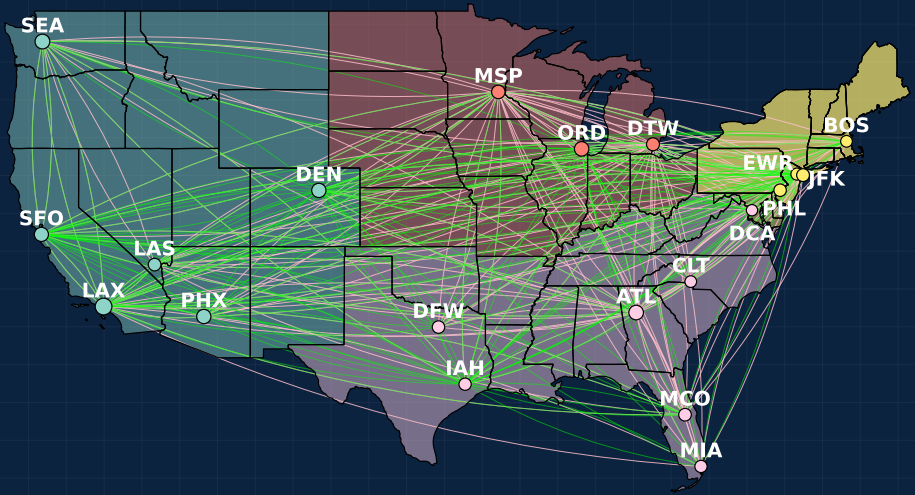

How to Study Graphs?

Subgraph Mining

- Extract *statistically significant* patterns

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Subgraph Mining

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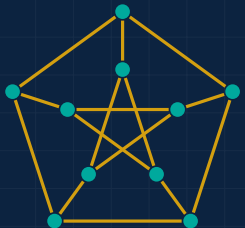
Graph Representation Learning

- Learn low-dimensional *embedding* of nodes

Graph Generative Models



Original Graph H

Scalable and Interpretable Graph Modeling with Graph Grammars

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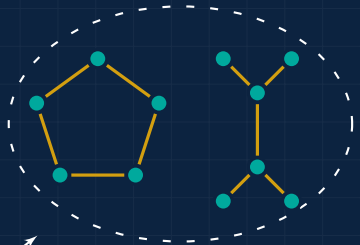
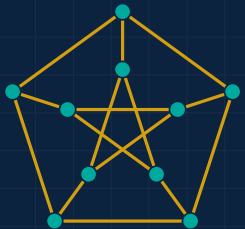


Extracted Features Θ



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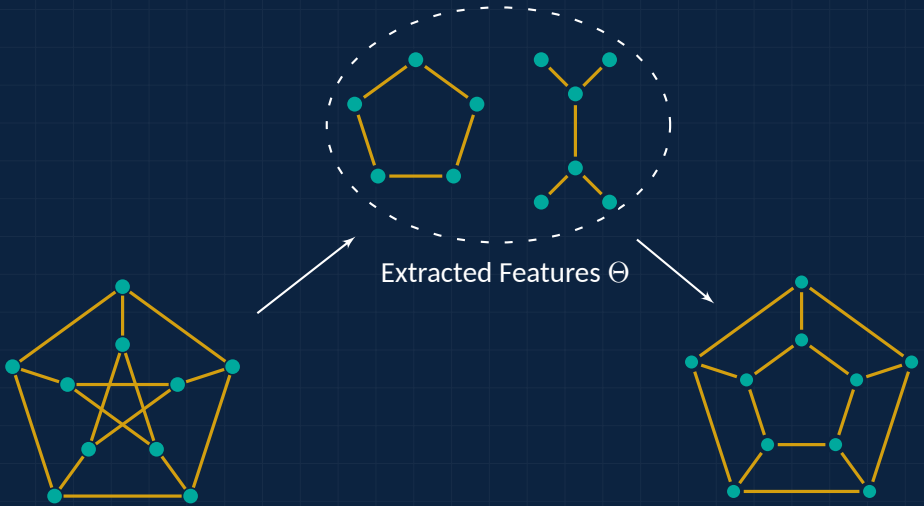

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A Brief History of Recent Graph Models

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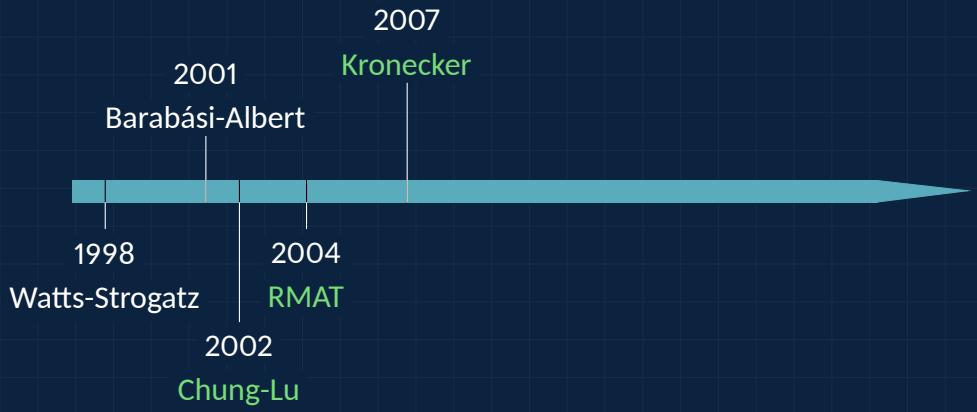

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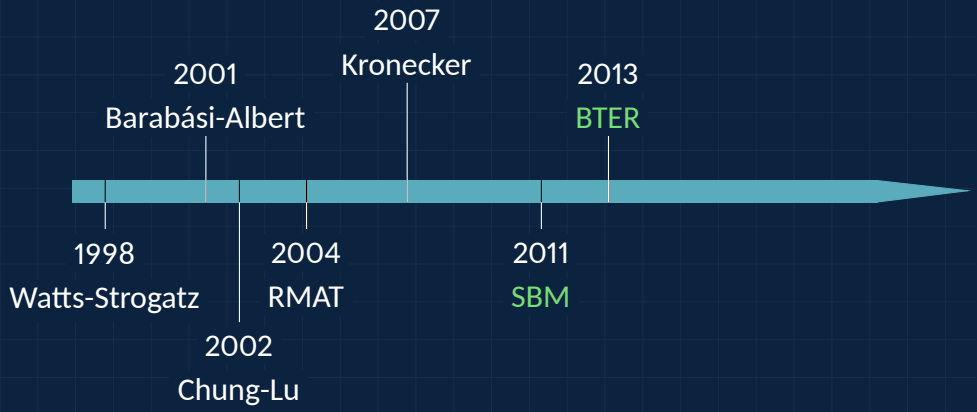

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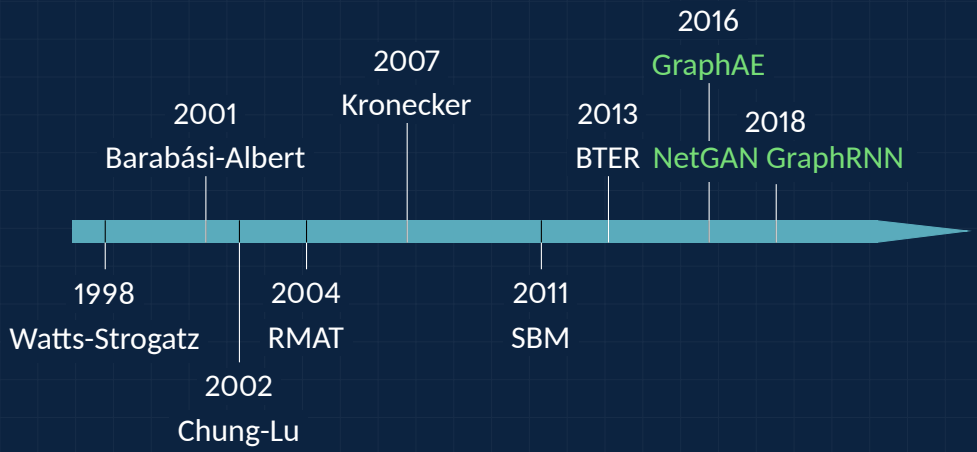

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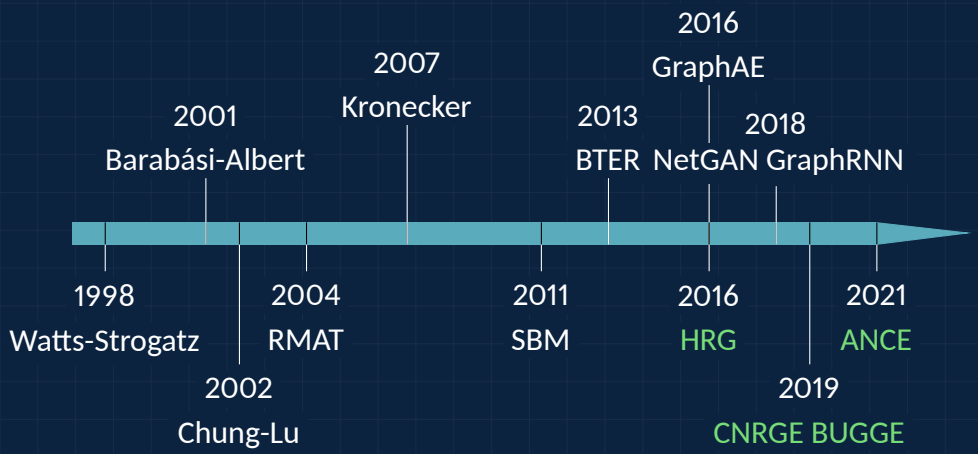

A Fork in the Road

Thesis Statement

Scalably and methodically extracting graph grammar rules provide a unique insight into understanding the inner workings of real-world graphs. Furthermore, these rules can generate accurate copies of the input, allowing for highly interpretable models.

Analyzing the performance of graph models undergoing a stress test reveals and amplifies the latent biases and sheds new light on their inner workings.

A Fork in the Road

List of Publications

ICGT 18	*Synchronous Hyperedge Replacement Graph Grammars*
ICDM 19	*Modeling Graphs with Vertex Replacement Grammars*
BigData 19	*Towards Interpretable Graph Modeling with Vertex Replacement Grammars*
WSDM 21	*Joint Subgraph-to-Subgraph Transitions: Generalizing Triadic Closure for Powerful and Interpretable Graph Modeling*
TKDE 21	*The Infinity Mirror Test for Graph Models*
WSDM 22+	*Attributed Vertex Replacement Graph Grammars*

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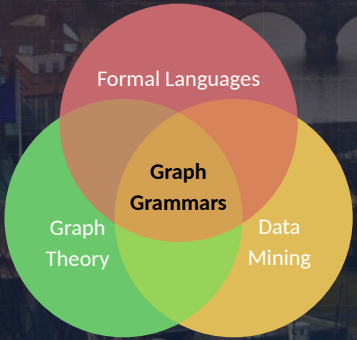

ICDM 19 *Modeling Graphs with Vertex Replacement Grammars*

WSDM 22∗ *Attributed Vertex Replacement Graph Grammars*

The Big Picture

Studying Complex Systems

- Discovering the *building blocks*
- Figuring how the pieces *fit* together

Formalism

- String grammars for natural *language* processing
- Graph grammars for *graph* mining

String Grammars

CFG Production Rules

- S → NP VP
- NP → the N
- VP → V NP
- N → cat | song
- V → sings | eats

String Grammars

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- S → NP VP
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S

S

String Grammars

CFG Production Rules

- S → NP VP
- NP → the N
- VP → V NP
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S

S

String Grammars

CFG Production Rules

- S $\rightarrow$ NP VP
- NP $\rightarrow$ the N
- VP $\rightarrow$ V NP
- N $\rightarrow$ cat | song
- V $\rightarrow$ sings | eats

$S \Rightarrow NP\ VP$

String Grammars

CFG Production Rules

- S → NP VP
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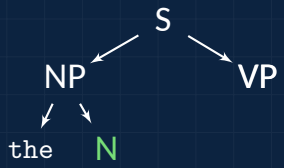

S ⇒ NP VP ⇒ the N VP

String Grammars

CFG Production Rules

- S → NP VP
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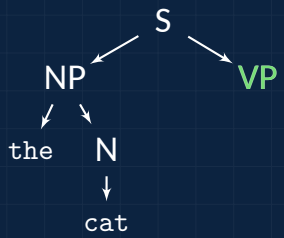

S ⇒ NP VP ⇒ the N VP ⇒ the cat VP

String Grammars

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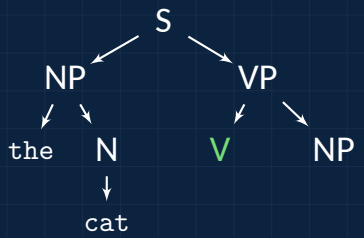

S ⇒ NP VP ⇒ the N VP ⇒ the cat VP ⇒ the cat V NP

String Grammars

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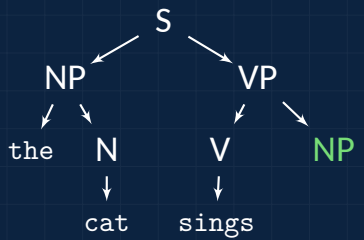
- V → sings | eats



S ⇒ NP VP ⇒ the N VP ⇒ the cat VP ⇒ the cat V NP
⇒ the cat sings NP

String Grammars

CFG Production Rules

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- NP → the N
- VP → V NP
- N → cat | song
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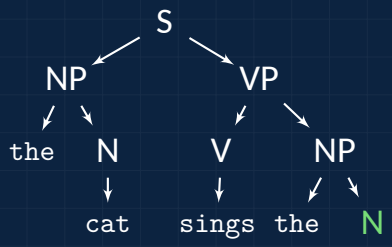

S ⇒ NP VP ⇒ the N VP ⇒ the cat VP ⇒ the cat V NP
⇒ the cat sings NP ⇒ the cat sings the N

String Grammars

CFG Production Rules

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- NP → the N
- VP → V NP
- N → cat | song
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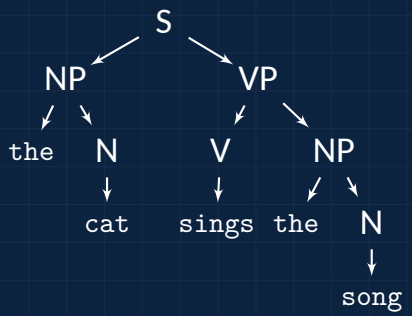
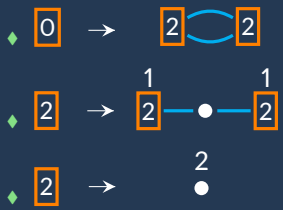


$$S \Rightarrow NP\ VP \Rightarrow \text{the}\ N\ VP \Rightarrow \text{the cat}\ VP \Rightarrow \text{the cat}\ V\ NP$$
$$\Rightarrow \text{the cat sings}\ NP \Rightarrow \text{the cat sings the}\ N$$
$$\Rightarrow \text{the cat sings the song}$$

Context Free Graph Grammars

NCE Production Rules



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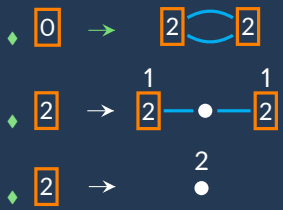

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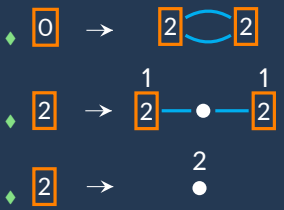

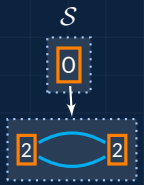

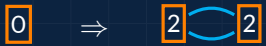

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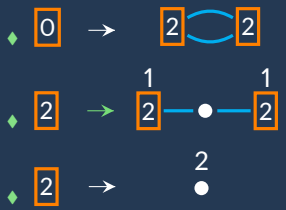

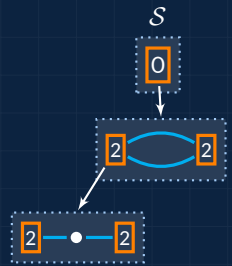

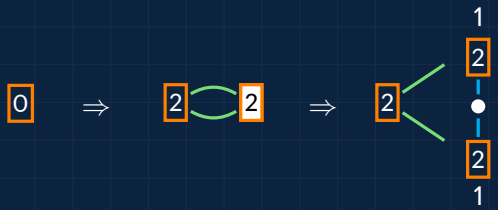

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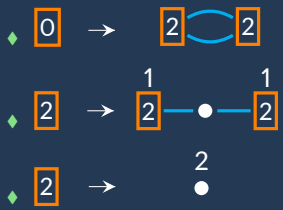

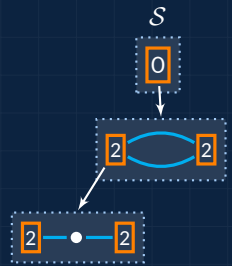

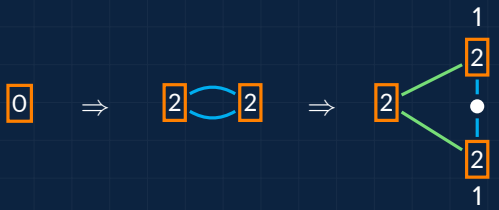

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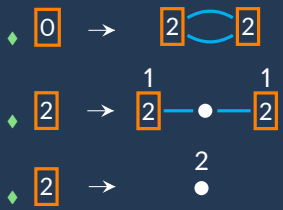

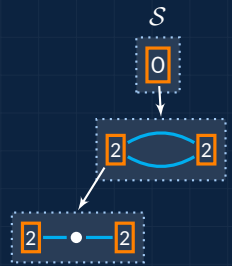

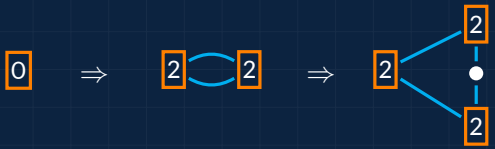

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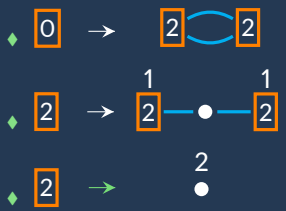

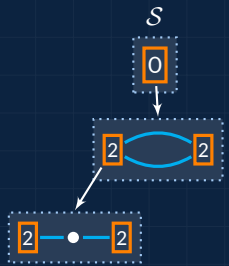

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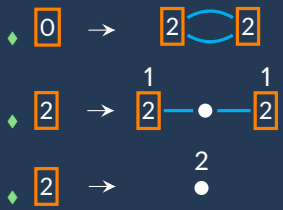

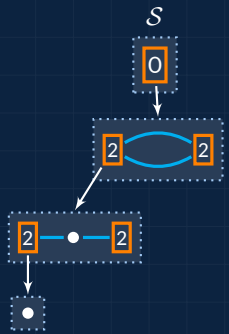

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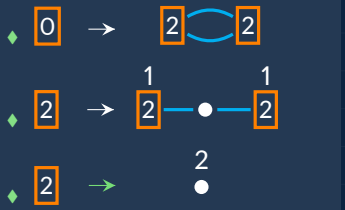

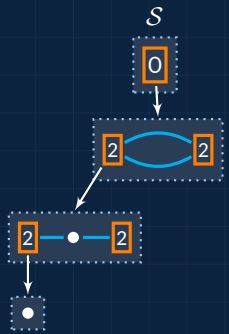

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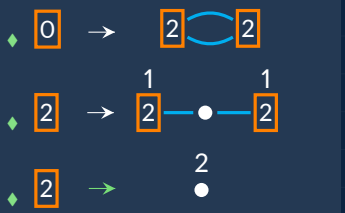

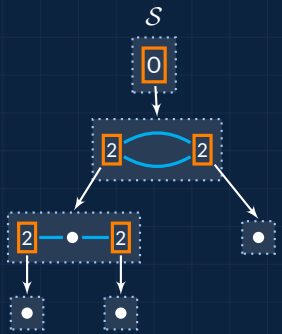

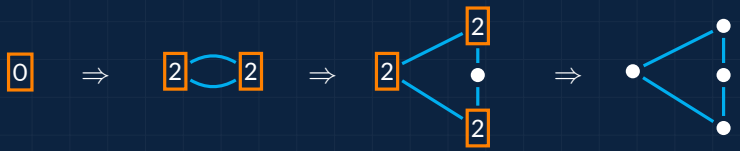

Graph Grammar Pipeline

Input Graph H

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Graph Grammar Pipeline

Input Graph H

Bottom-up, Clustering-based

Graph Grammar Pipeline

Input Graph *H*

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Graph Grammar Pipeline

Input Graph *H*

Grammar Extractor

Graph Generator

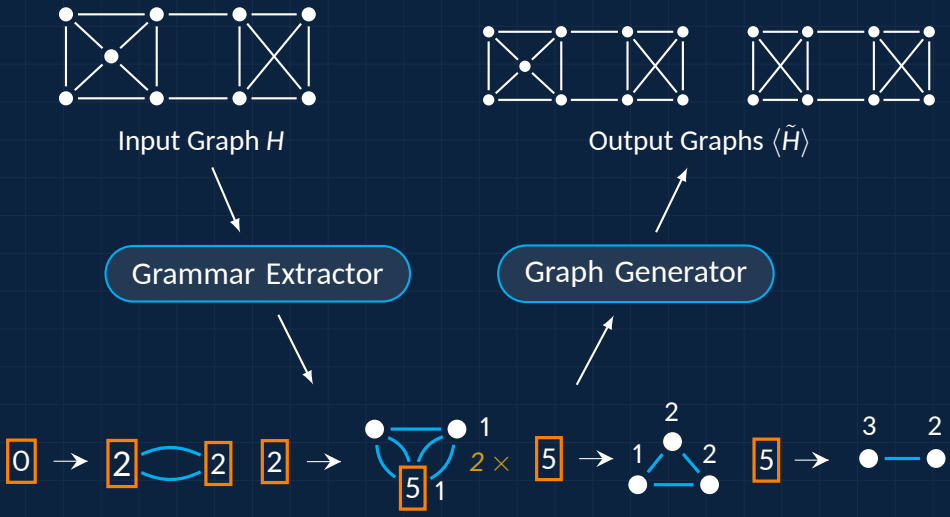
Graph Grammar Pipeline

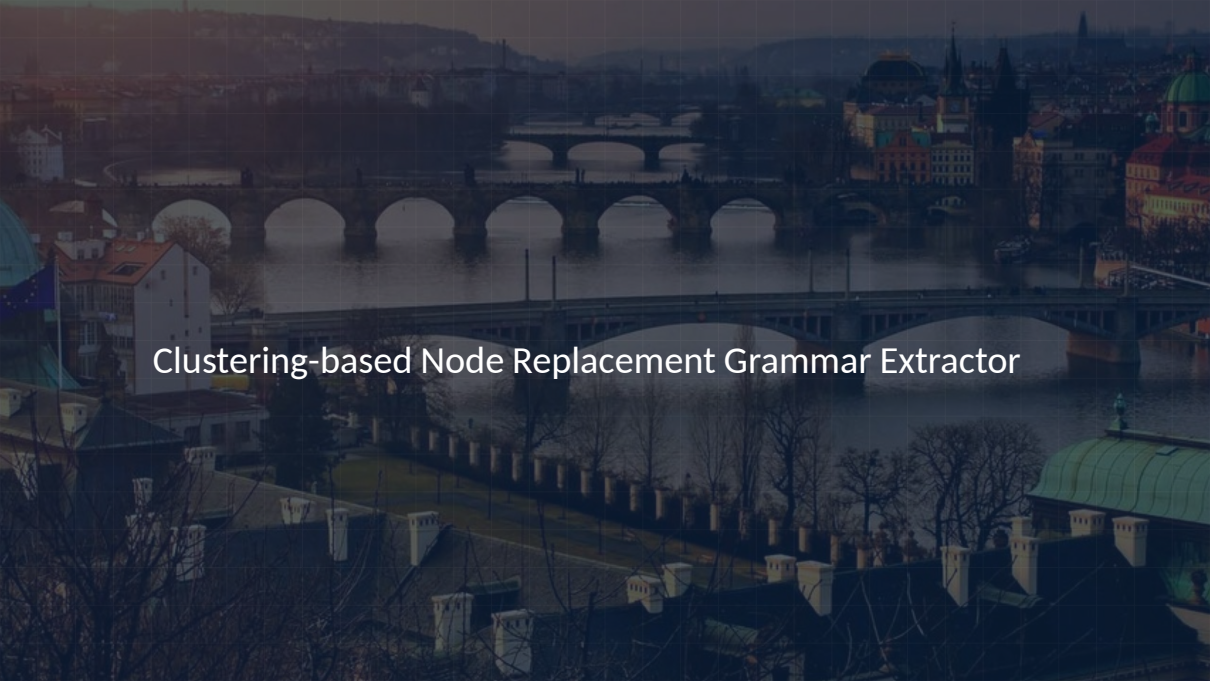
Input Graph *H*

Grammar Extractor

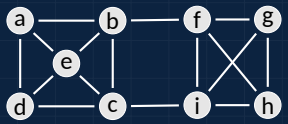
Random, Attribute-aware

Graph Grammar Pipeline




Clustering-based Node Replacement Grammar Extractor

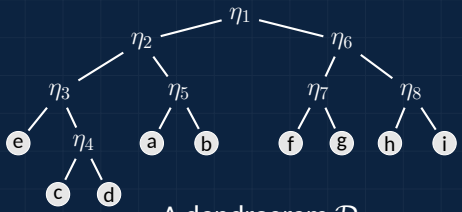
Hierarchical Graph Clustering



Graph H

Leiden
Louvain

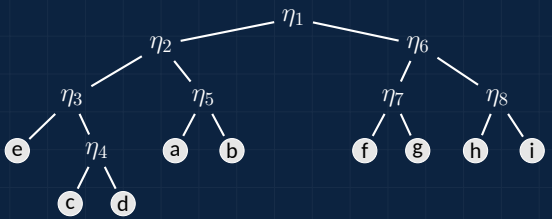
Spectral
MinCut



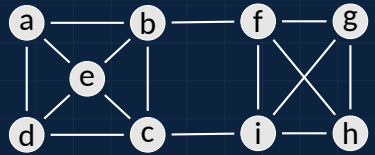
A dendrogram $\mathcal{D}$

Extracting NCE Rules I

($\mu = 3$)



Current Dendrogram $\mathcal{D}$



Current Graph H

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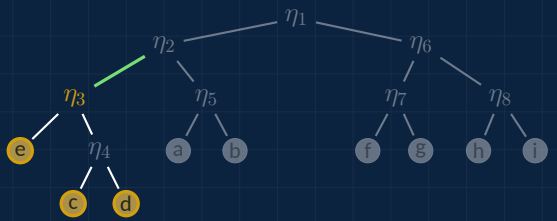
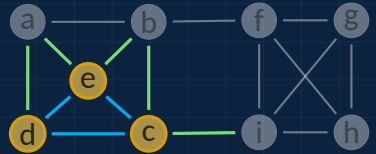
($\mu = 3$)



Current Dendrogram $\mathcal{D}$



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Extracted NCE Rule

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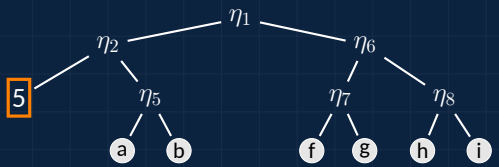
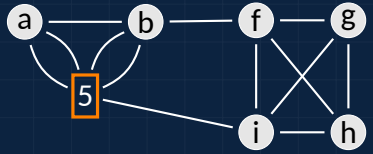
Extracting NCE Rules I ($\mu = 3$)



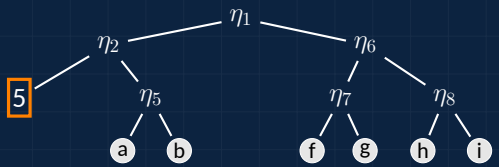
Updated Dendrogram $\mathcal{D}'$



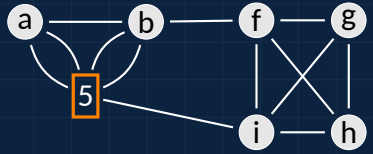
Updated Graph H'

Extracting NCE Rules II

($\mu = 3$)



Current Dendrogram $\mathcal{D}$



Current Graph H

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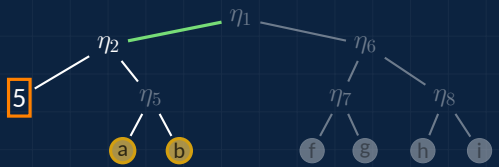
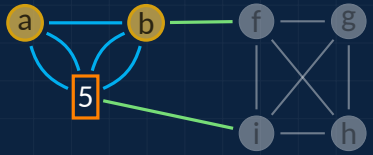
Extracting NCE Rules II

($\mu = 3$)



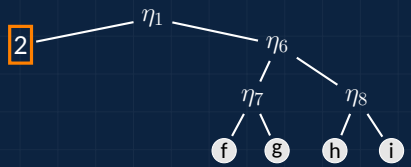
Current Dendrogram $\mathcal{D}$



Current Graph H

Extracted NCE Rule

Extracting NCE Rules II ($\mu = 3$)



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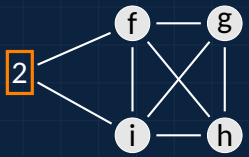

Updated Graph H'

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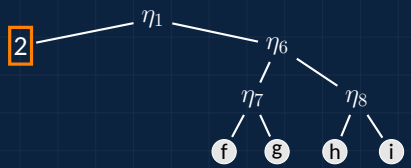
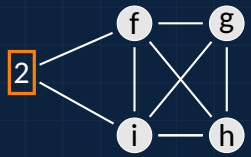
Extracting NCE Rules III ($\mu = 3$)



Current Dendrogram $\mathcal{D}$



Current Graph H

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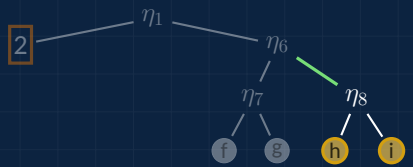
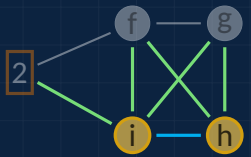
Extracting NCE Rules III

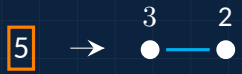
($\mu = 3$)



Current Dendrogram $\mathcal{D}$



Current Graph H



Extracted NCE Rule

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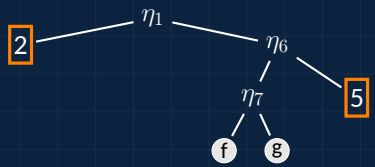
($\mu = 3$)

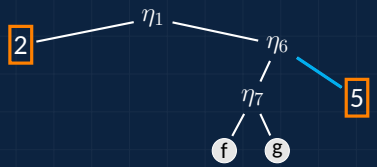


Updated Dendrogram $\mathcal{D}'$

Updated Graph H'

Extracting NCE Rules IV

($\mu = 3$)



Current Dendrogram $\mathcal{D}$

Current Graph *H*

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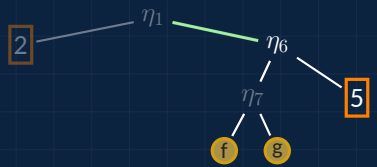
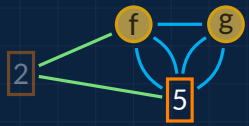
Extracting NCE Rules IV ($\mu = 3$)



Current Dendrogram $\mathcal{D}$



Current Graph H

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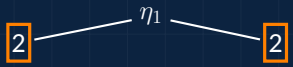
Extracting NCE Rules IV ($\mu = 3$)



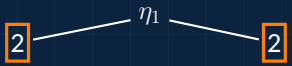
Updated Dendrogram $\mathcal{D}'$

Updated Graph H'

Extracted NCE Rule

Extracting NCE Rules V

($\mu = 3$)

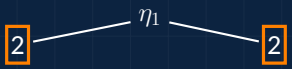


Current Dendrogram $\mathcal{D}$

Current Graph H

Extracting NCE Rules V

($\mu = 3$)



Current Dendrogram $\mathcal{D}$

Current Graph H

Extracted NCE Rule

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Extracting NCE Rules V

($\mu = 3$)

Updated Dendrogram $\mathcal{D}$

Updated Graph H

Extracting NCE Rules V

($\mu = 3$)

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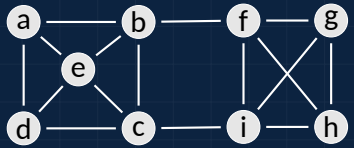
0

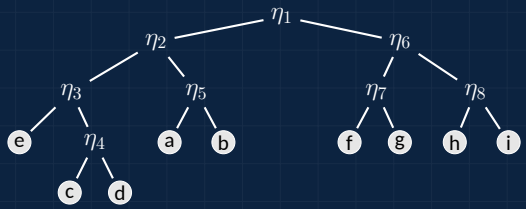
Updated Dendrogram $\mathcal{D}$

Updated Graph H

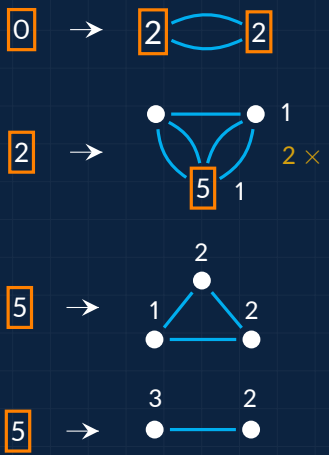
Extracted NCE Grammar



Graph H



Dendrogram $\mathcal{D}$



Extracted NCE rules

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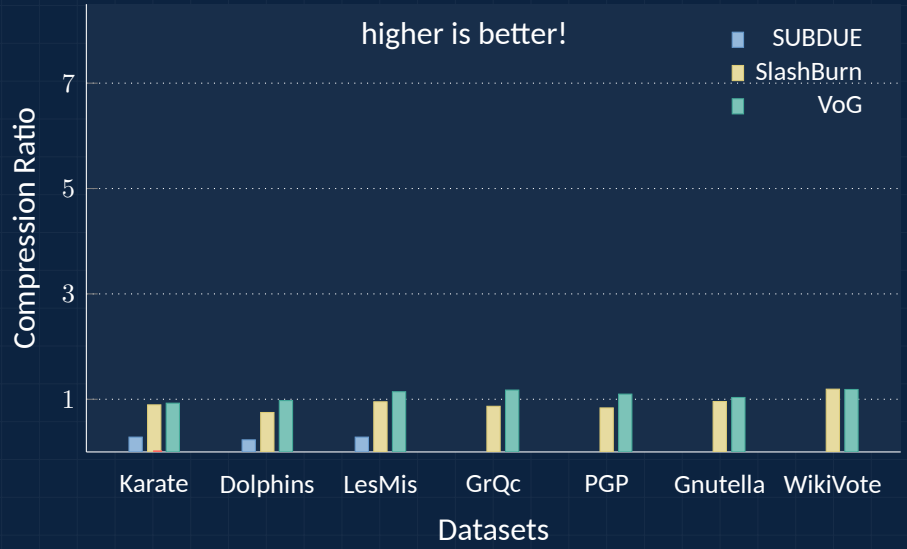
Model Size Comparison



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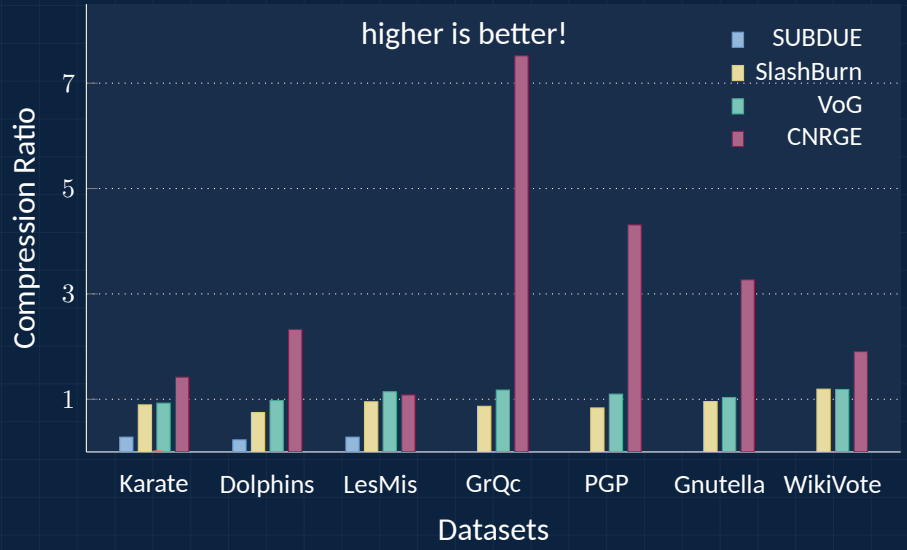
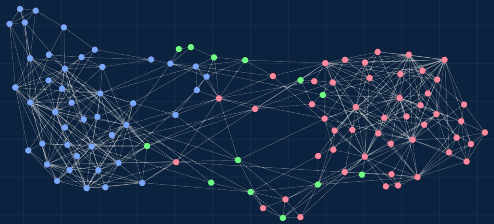


Attributed Graphs



Homophily in PolBooks graph

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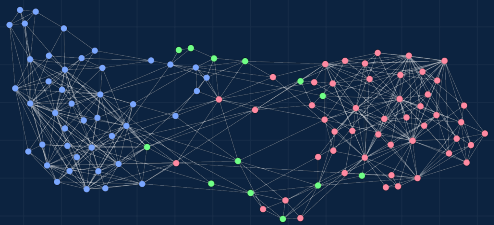
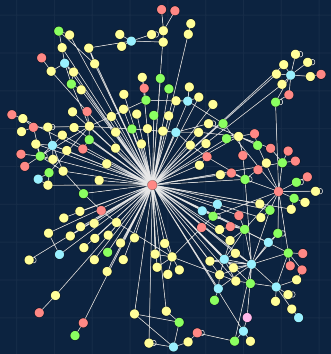


Homophily in PolBooks graph



Heterophily in Texas CS website

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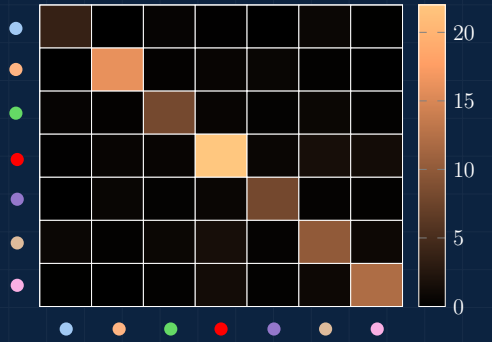
Real-world Grammars: Cora

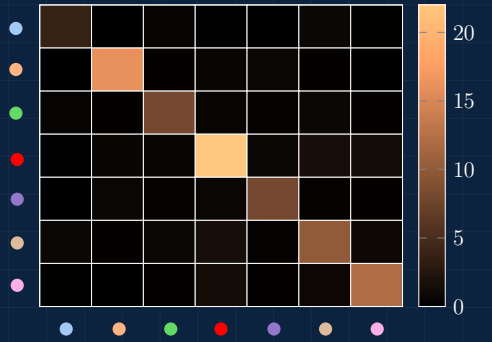
Node Distribution



Edge Mixing Matrix

Real-world Grammars: Cora

Node Distribution



Edge Mixing Matrix

6 Most-frequent Rule RHSs

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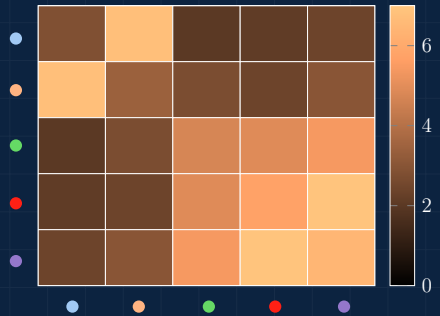
Real-world Grammars: Chameleon

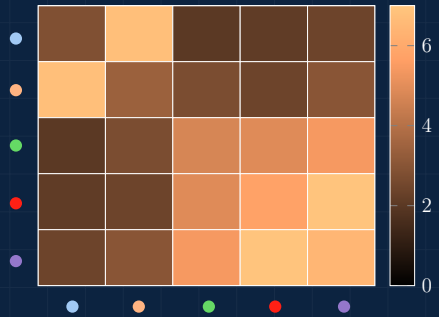
Node Distribution



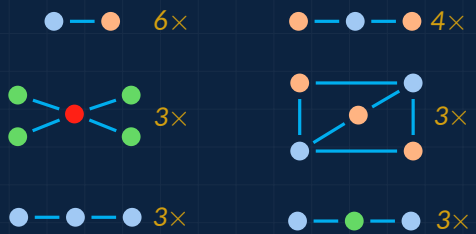
Edge Mixing Matrix

Real-world Grammars: Chameleon

Node Distribution

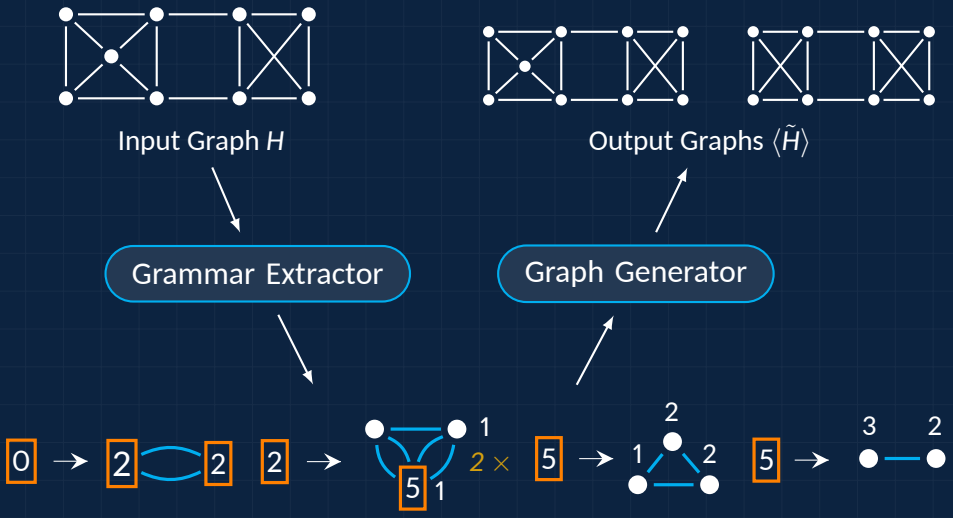


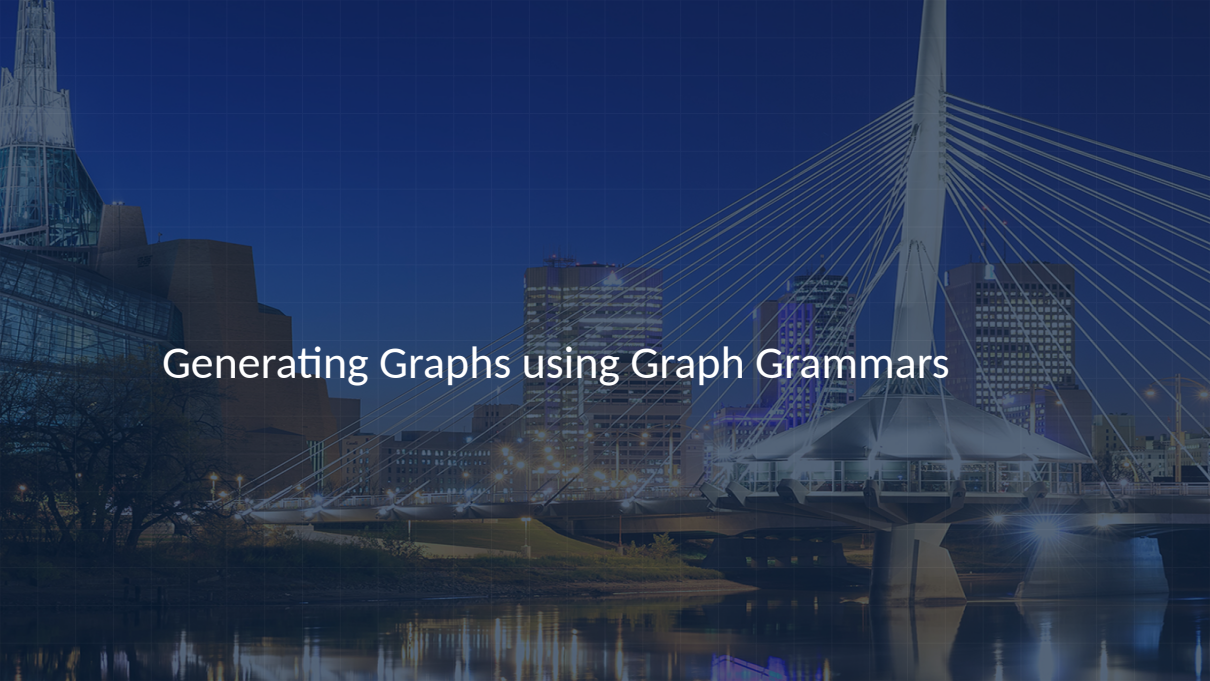
Edge Mixing Matrix



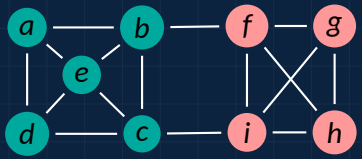
6 Most-frequent Rule RHSs

Graph Grammar Pipeline Revisited

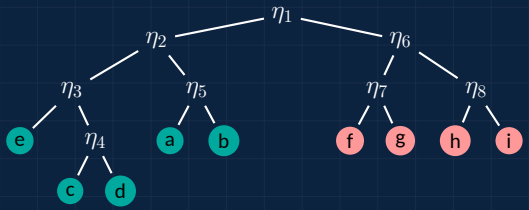



Generating Graphs using Graph Grammars

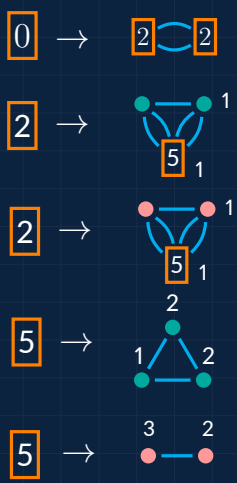
Attributed NCE Grammars



Graph H



Dendrogram $\mathcal{D}$



Extracted ANCE rules

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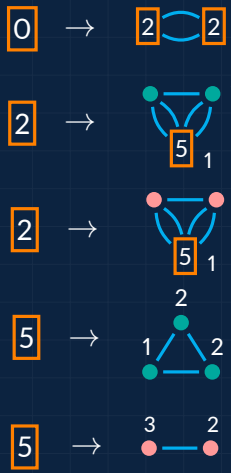

Extracted ANCE Rules

$\mathcal{S}$

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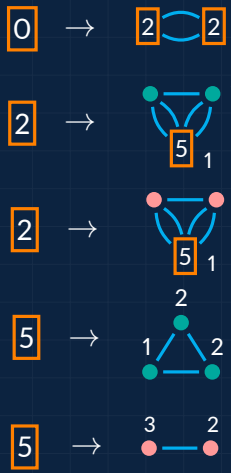

Extracted ANCE Rules

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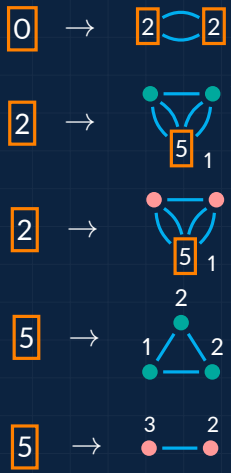

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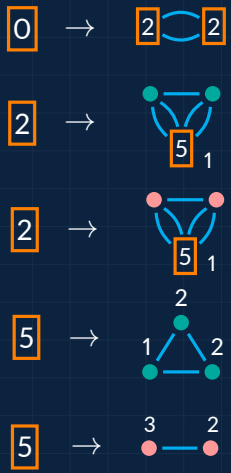

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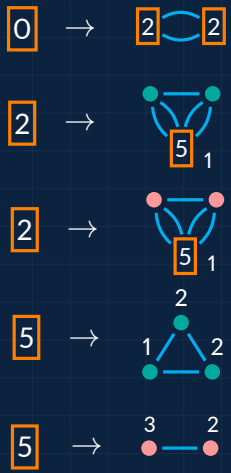

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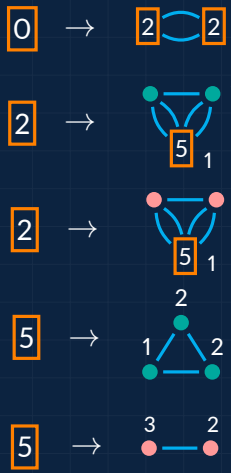

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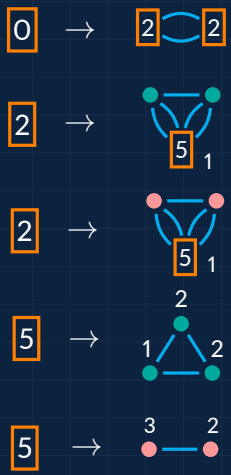

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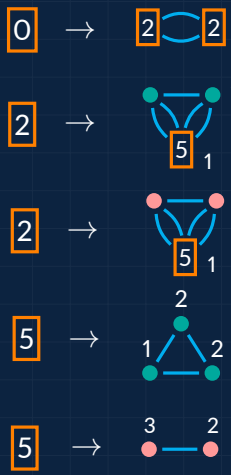

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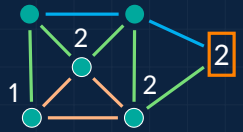

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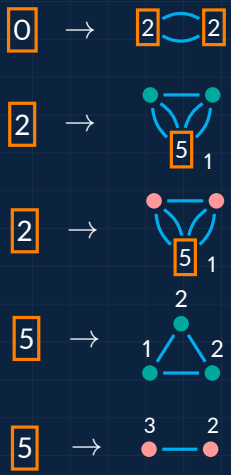

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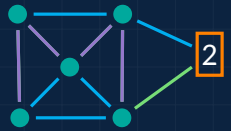

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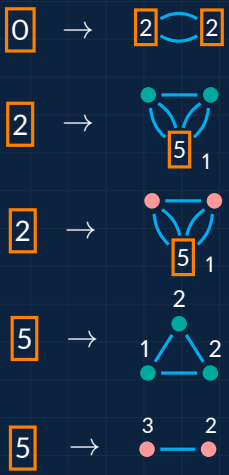

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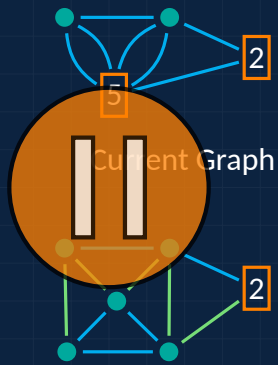

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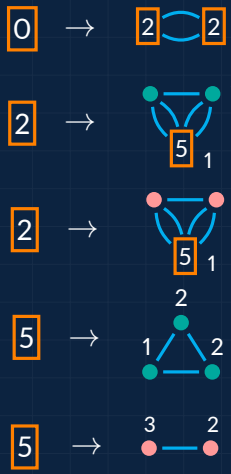

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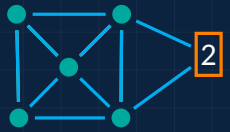

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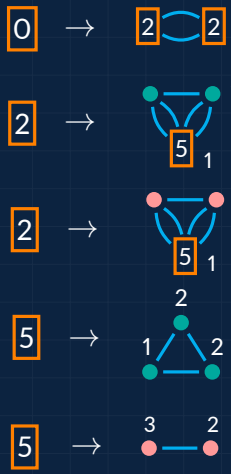

Extracted ANCE Rules

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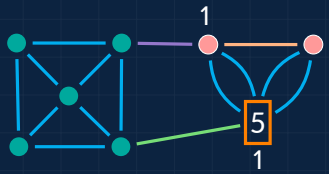

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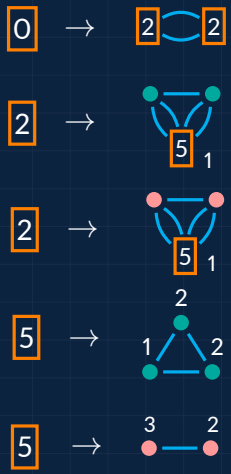

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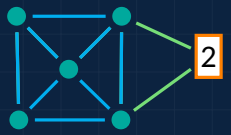

Current Graph H'

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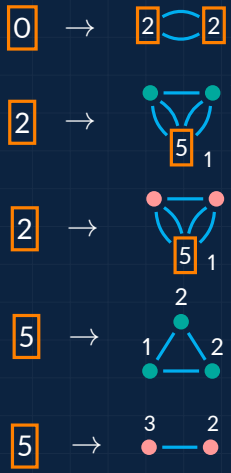
Generating Graphs from an ANCE V



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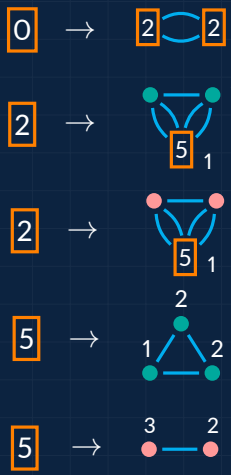

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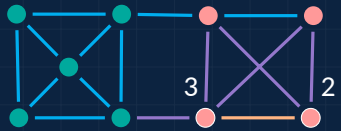

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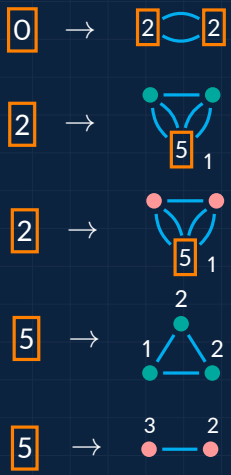

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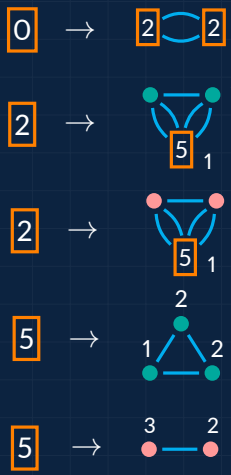

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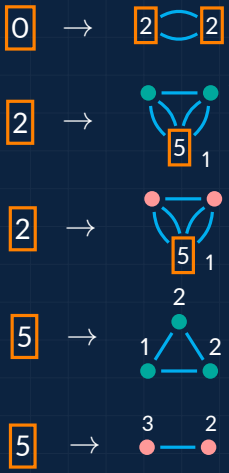

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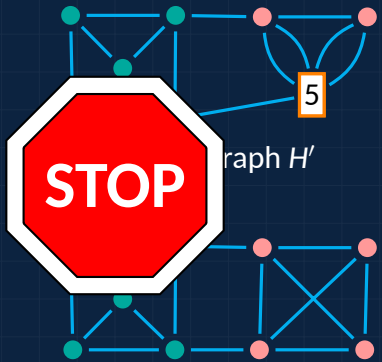
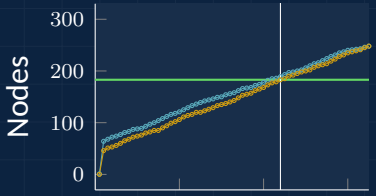
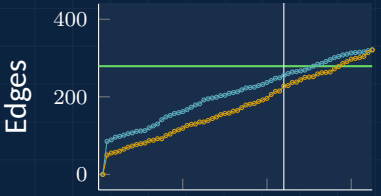


Next Graph $\hat{H}$

Language of Graphs Described by a Grammar

Examining the Graph Growth Process





Whole Graph Terminal Graph Input Graph Metric Input Graph Size

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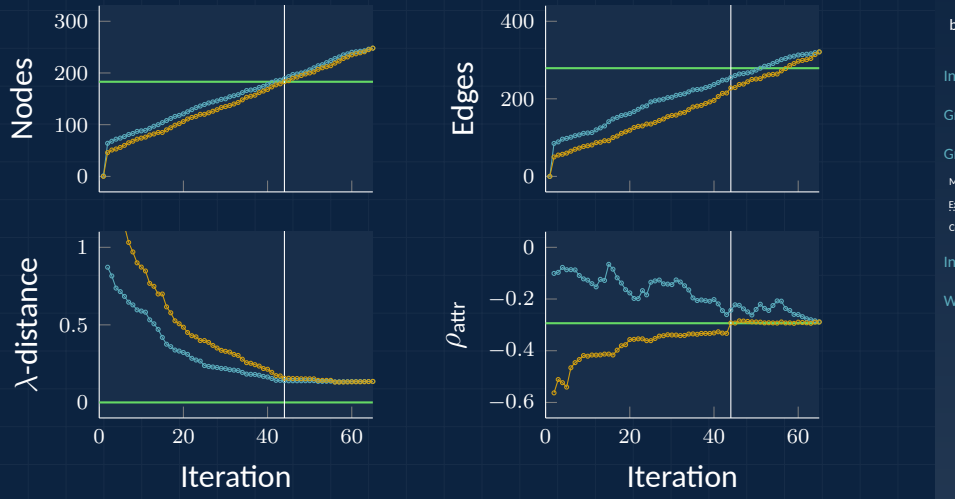
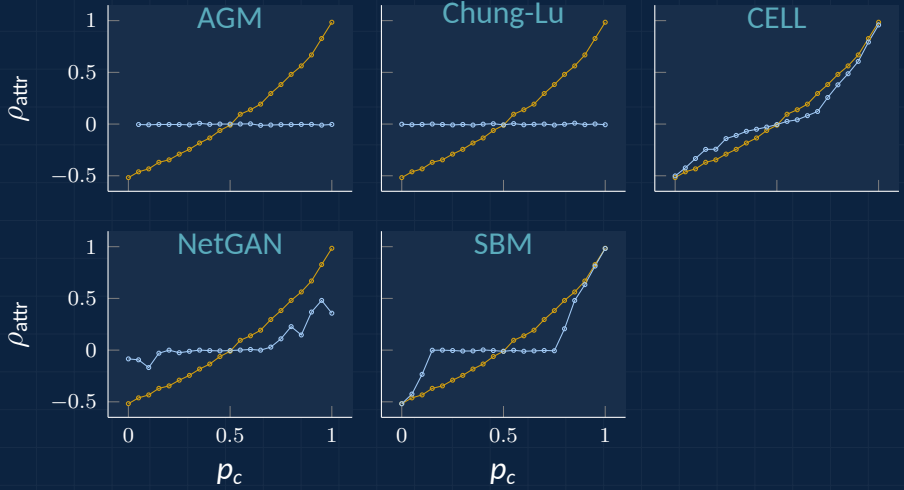


CABAM Graphs



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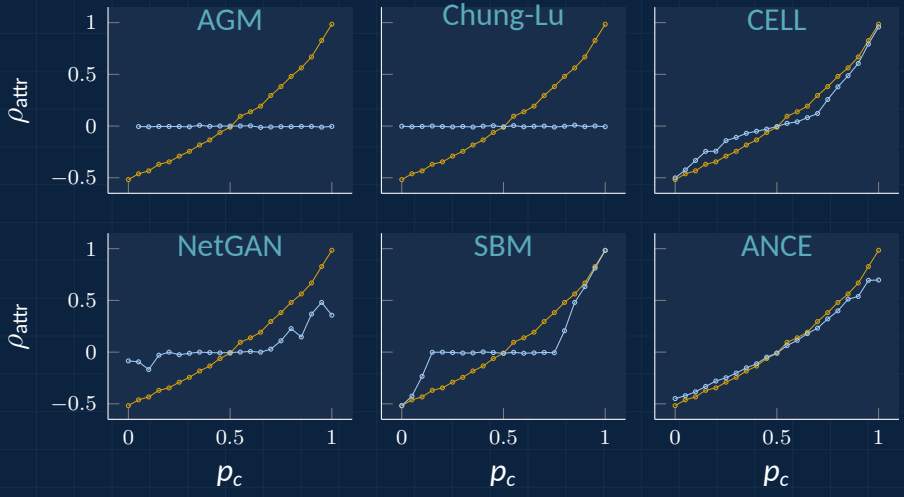

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Main Takeaways

- *Simple* and *interpretable* formalism from formal languages

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Shortcomings

- Dependence on the *dendrogram*

Takeaways

Main Takeaways

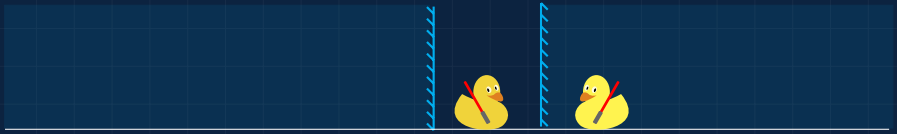
- *Simple* and *interpretable* formalism from formal languages
- *Scalable* to medium-large graphs
- *Faithful* graph generation: topology and attribute

Shortcomings

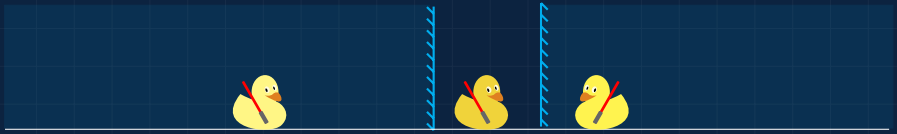
- Dependence on the *dendrogram*
- Rule extraction process is *non-deterministic*

The Infinity Mirror Test for Graph Models

Infinity Mirror Test for Duck Vader



Infinity Mirror Test for Duck Vader



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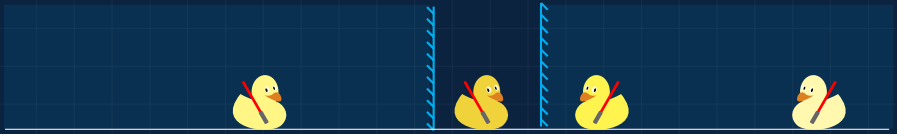

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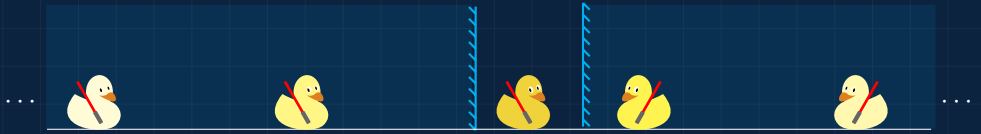

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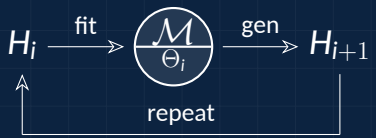
Infinity Mirror Test for Graph Models

Key Idea

Forcing a model to fit and re-fit the generated graphs amplifies biases



Scalable and Interpretable Graph Modeling with Graph Grammars

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Infinity Mirror Test for Graph Models

Key Idea

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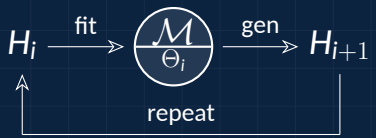
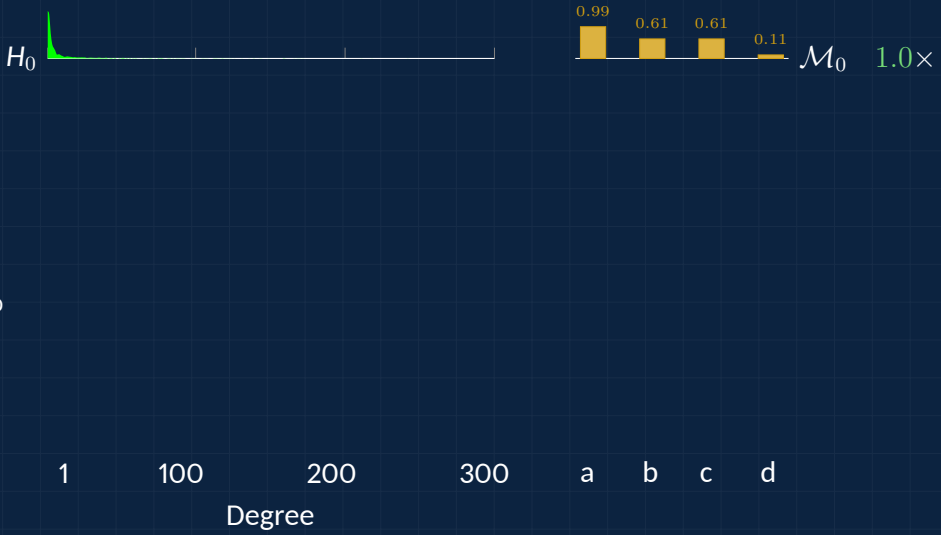
Evaluation Plan

Compare H_i and H_0 to observe *incremental* degradation



Kronecker Degree Distribution Ridge Plot

$\mathcal{M} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$



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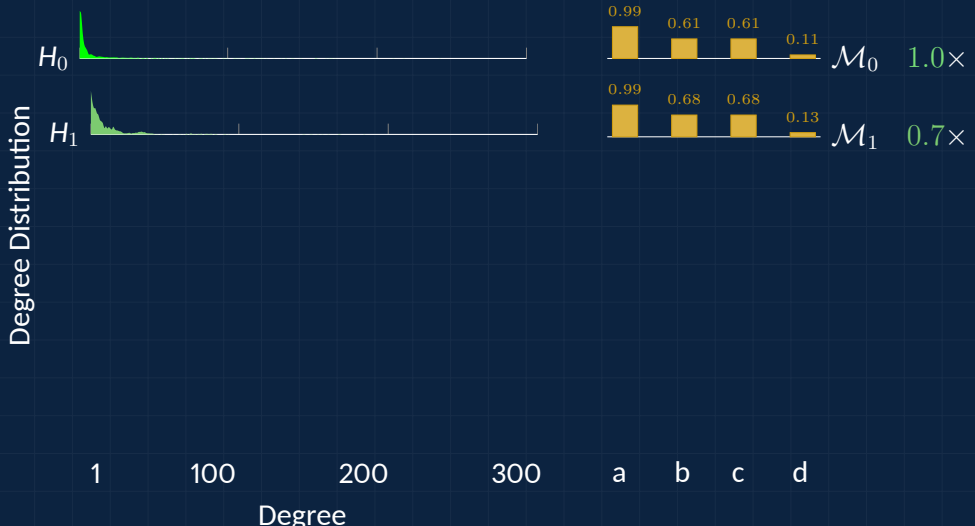

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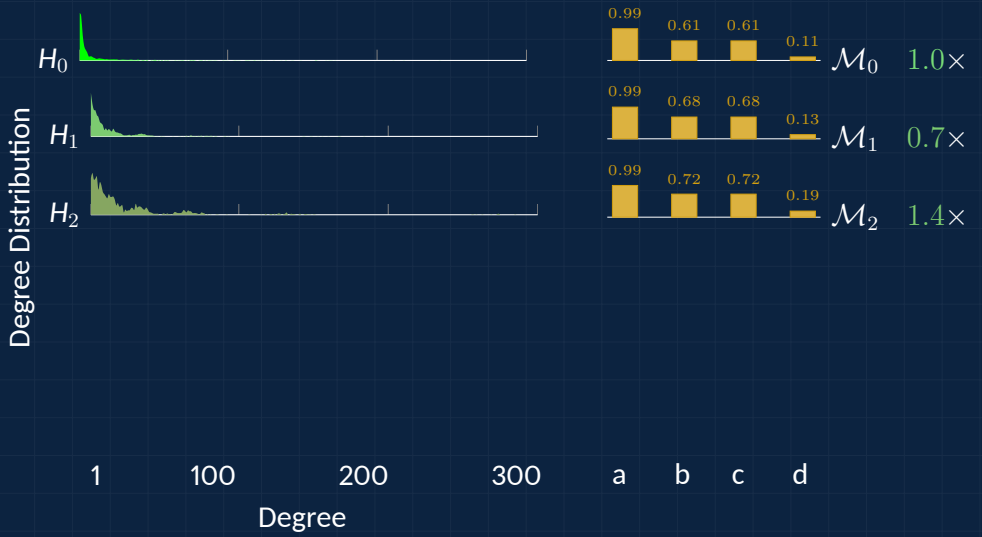

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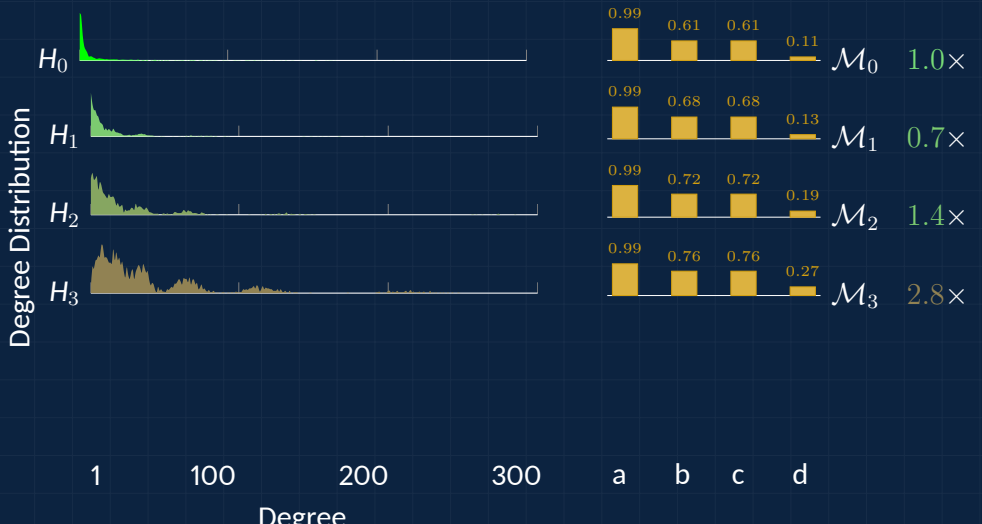

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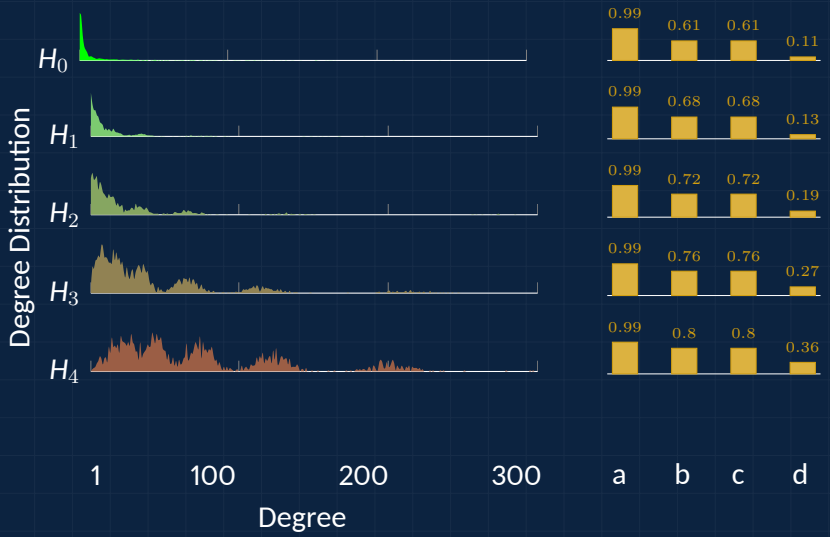

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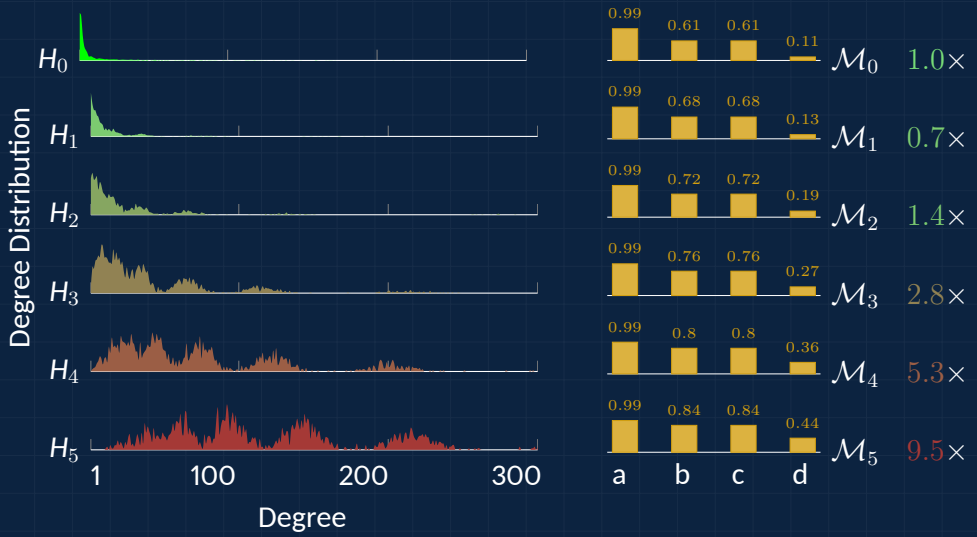

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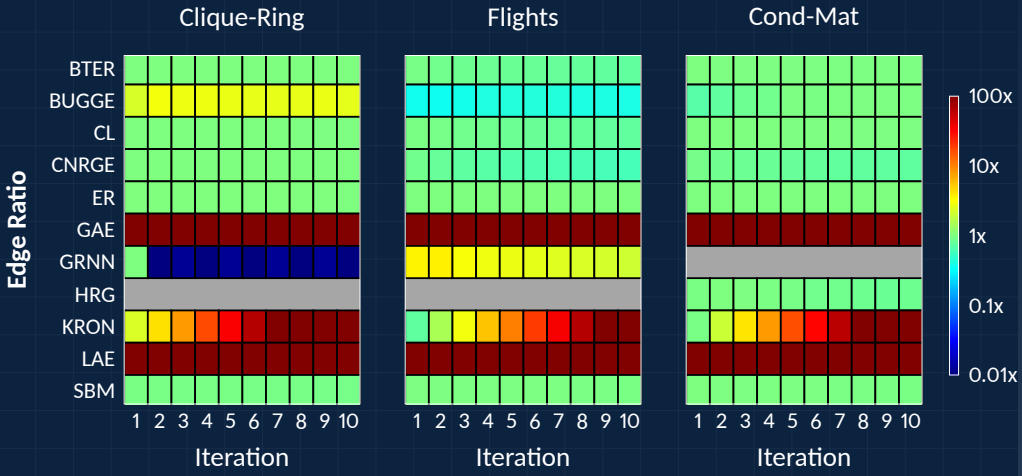
First-order Graph Statistics



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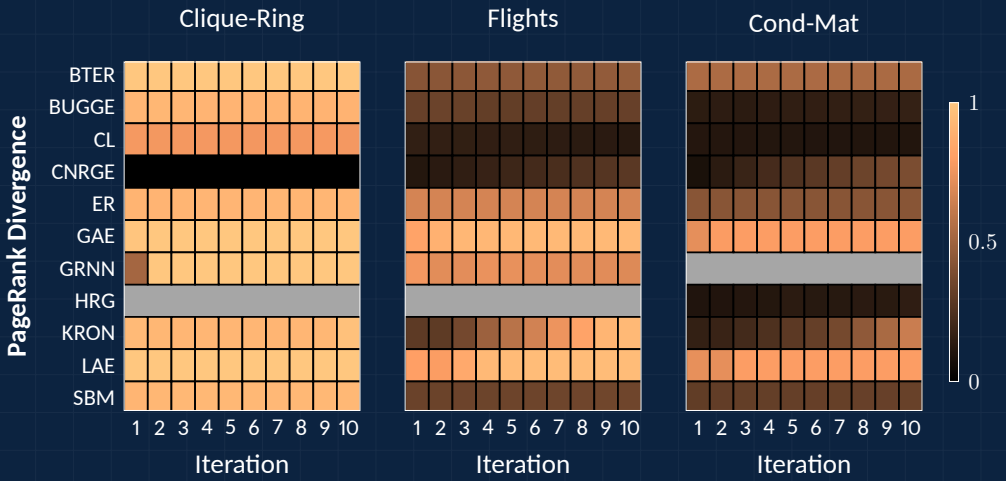

Tracking Evolution: Clustering & Geodesics

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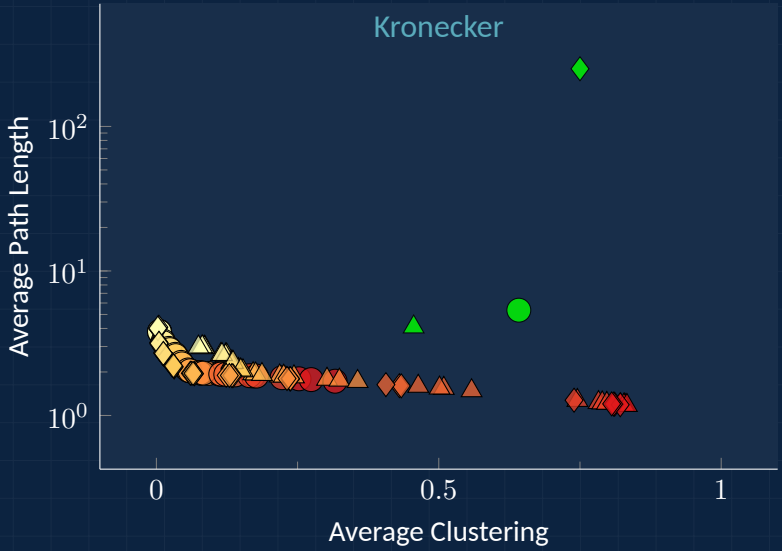

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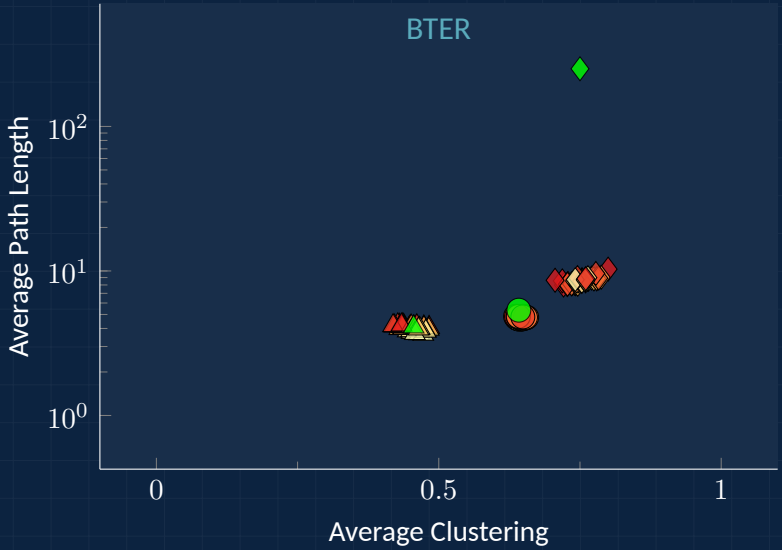

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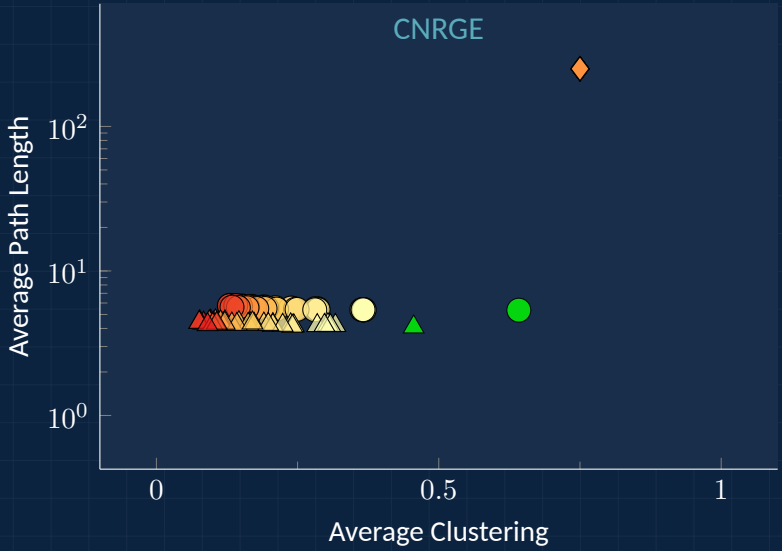

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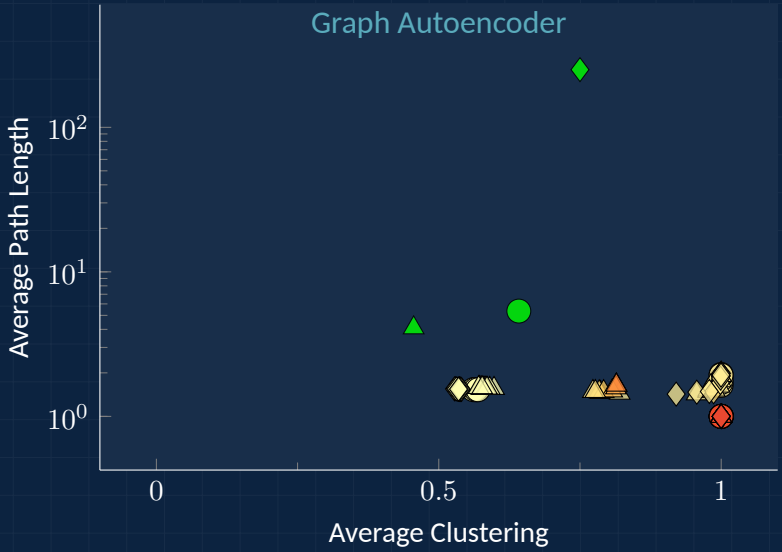

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Takeaways

Main Takeaways

- *Confirms* previously known biases in Kronecker graphs

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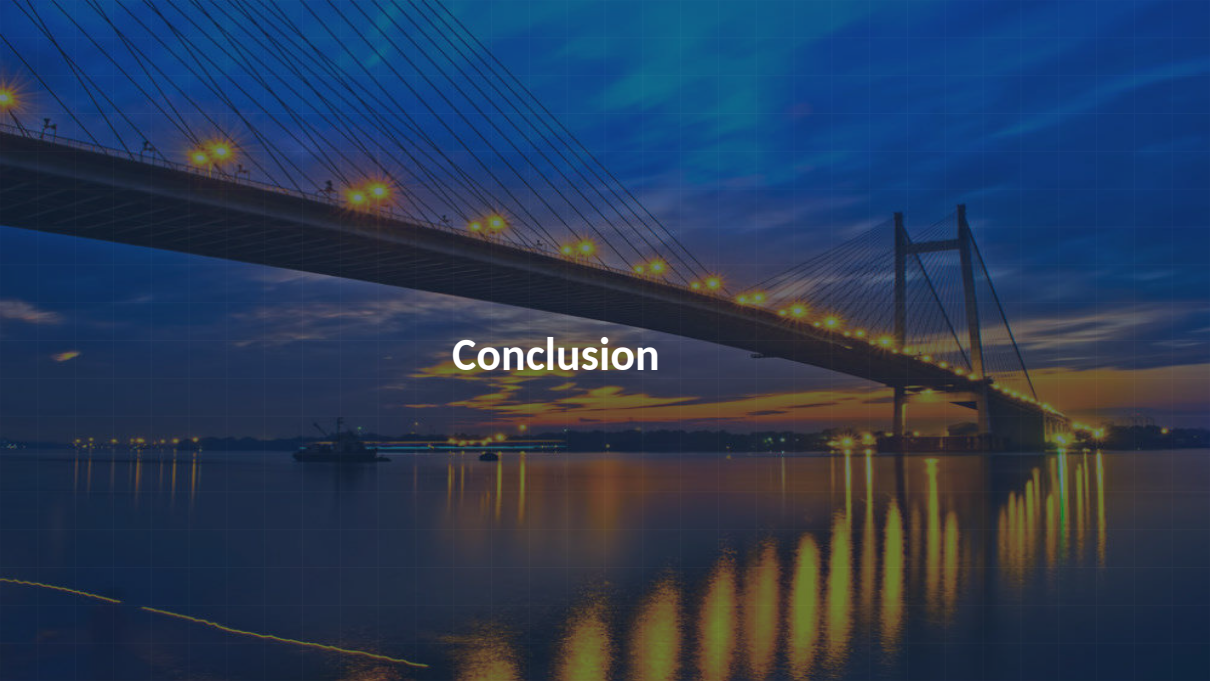
- *Confirms* previously known biases in Kronecker graphs
- Uncovers *unique* distortion patterns in popular graph models
- A tool to design *better*, more parsimonious models



Conclusion

Summary

Vertex Replacement Grammars

- A new class of *scalable*, *interpretable* graph models
- Preserves both *topology* and *attribute* similarities

Summary

Vertex Replacement Grammars

- A new class of *scalable*, *interpretable* graph models
- Preserves both *topology* and *attribute* similarities

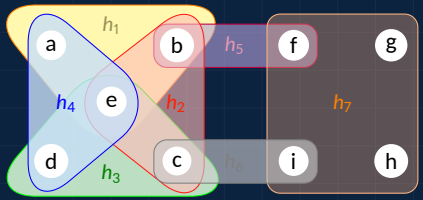
Infinity Mirror Test

- A *novel* stress-test for graph models
- Reveals new *biases* prompting further investigation

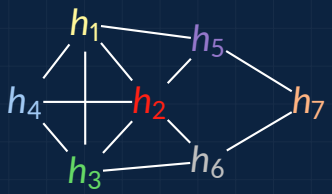
What's Next

Hypergraph Grammars

- New extraction method for HRGs *bypassing* tree decompositions
- Should improve both *stability* and scalability



Hypergraph *H*



Line Graph of *H*

Life at Indiana University

What's Next

Postdoctoral Fellow @ IU

- Work with *Santo Fortunato* on the MINERVA project
- Understanding the *process* of scientific discovery
- Studying the *dynamics* of citation and collaboration networks

Thank You!

Minimum Description Length Principle

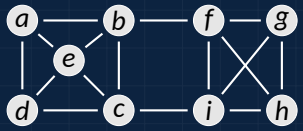
The Core Idea

- The best model is the one that leads to the best compression

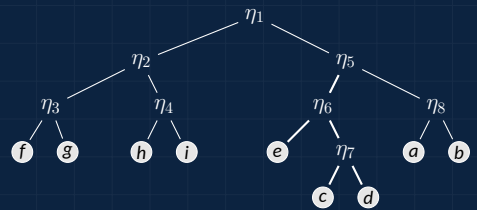
$$\mathcal{M}^* = \text{argmin} \{ \mathcal{L}(\mathcal{M}) + \mathcal{L}(\mathcal{D} \mid \mathcal{M}) \}$$

- $\mathcal{L}(\mathcal{M})$ is the length of the model
- $\mathcal{L}(\mathcal{D} \mid \mathcal{M})$ is the length of data compressed by the model

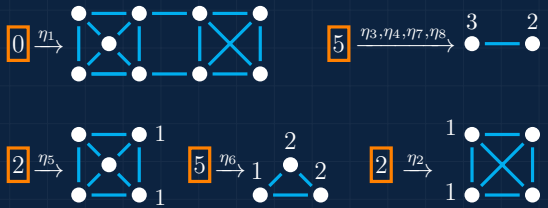
CNRG extraction and MDL



(a) Example graph H with 9 nodes and 16 edges



(b) An example dendrogram $\mathcal{D}$



(c) All possible rules that can be obtained from $\mathcal{D}$

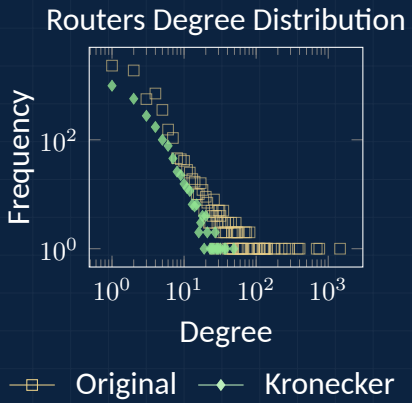
Comparing Graphs

Distribution Based

- Degree distribution
- PageRank centrality
- . . .

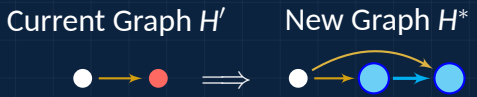
Topology Based

- Graph Edit Distance (GED)
- Graphlet Correlation Distance (GCD)
- DeltaCon - Personalized PR
- . . .



Kemp-Tenenbaum (KT) Graph Grammars

(A) A KT grammar rule



(B) Example of rule application

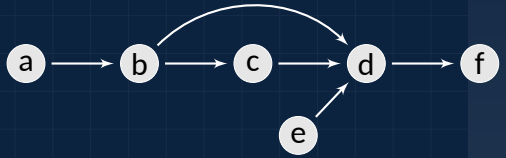
replaced new boundary

Bottom-up Graph Grammar Extraction (BUGGE)

$(\mu = 2)$

(1) Enumerate Subgraphs

- Specify *max* rule size μ
- Find *connected* sets of up to size μ



Enumerating all connected size μ subgraphs in *H*

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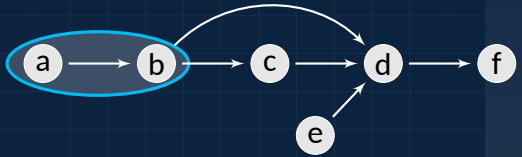

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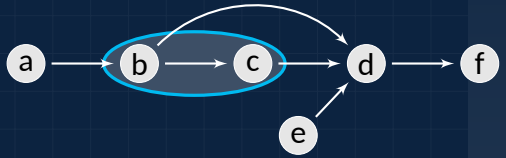

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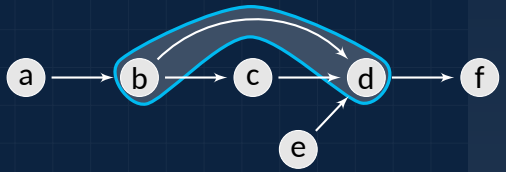

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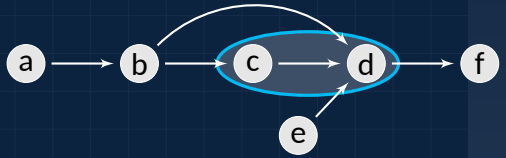

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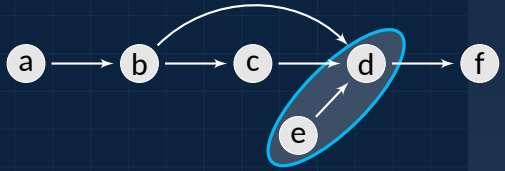

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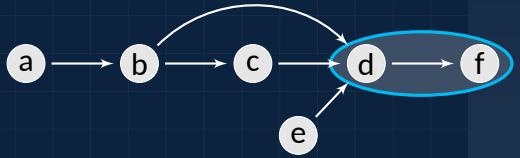

Enumerating all connected size μ subgraphs in *H*

Bottom-up Graph Grammar Extraction (BUGGE)

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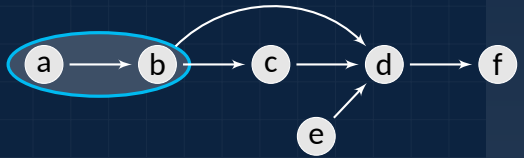
(1) Enumerate Subgraphs

(2) Best Rule Selection

Use MDL principle to find the rule which *compresses* the graph the most

(A) Best rule *R*



(B) *R* appears 4 times in Graph *H*

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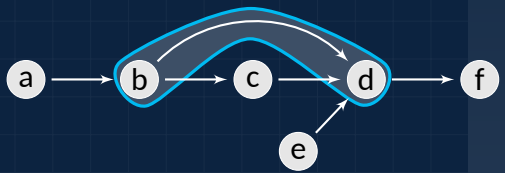

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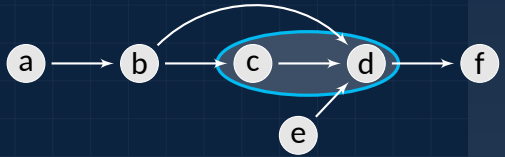

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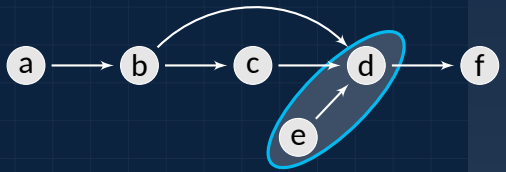

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- Match rule *RHS* in the graph
- *Collapse* matched nodes
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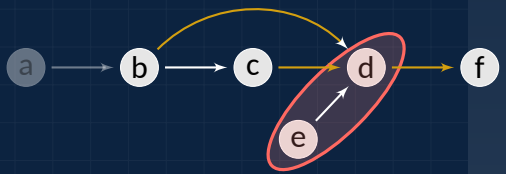
(A) Best rule *R*



(B) Current graph *H*

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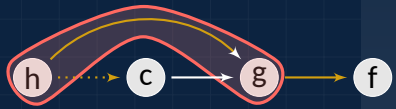

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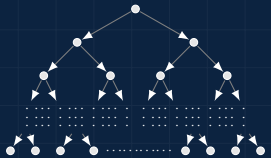
Results from Synthetic Graphs

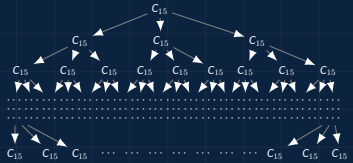
I: Balanced Binary Tree

II: Tree of Directed C_{15} Rings

III: Regular Ring Lattice

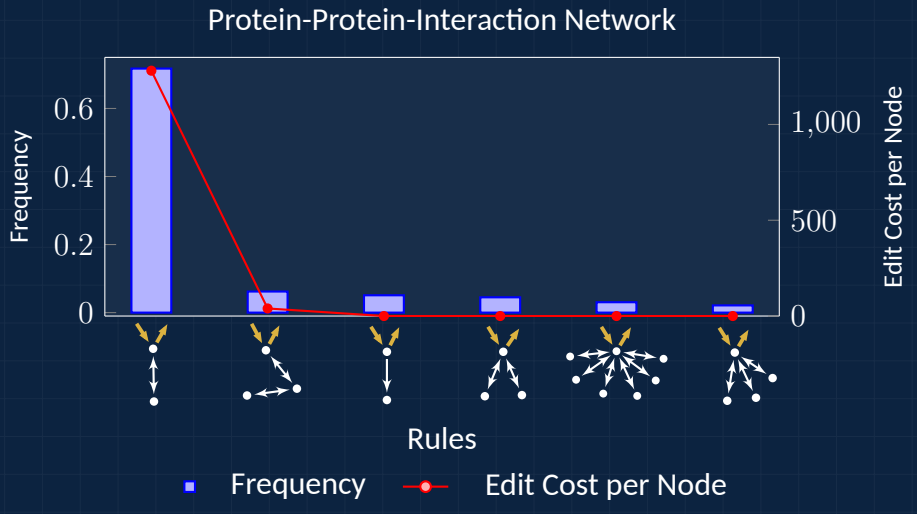
Synthetic Graphs





BUGGE Rules

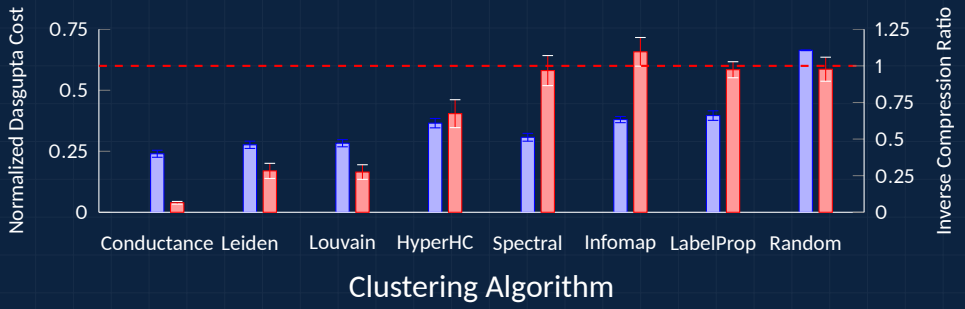
Most Frequent Rules Extracted from a PPI Network



CNRG Results

	EuCore		PolBlogs		OpenFlights	
	GCD	λ-dist	GCD	λ-dist	GCD	λ-dist
ChungLu	0.409	**0.803**	0.466	**1.234**	1.1116	**0.614**
HRG	0.229	8.091	1.196	4.407	1.2442	2.761
DC-SBM	**0.180**	2.057	0.262	4.186	0.8414	3.534
BTER	–	–	0.352	7.505	0.832	4.936
Kronecker	0.3164	11.802	1.302	14.31	1.83	10.459
CNRGE	0.233	4.969	**0.212**	4.276	**0.2832**	3.581

CNRG Results

	GrQc		PGP		Gnutella	
	GCD	λ-dist	GCD	λ-dist	GCD	λ-dist
ChungLu	2.657	**0.389**	2	**0.64**	1.02	0.42
HRG	1.99	4.41	–	–	2	5
DC-SBM	2.065	2.202	1.39	2.29	–	–
BTER	2.231	0.439	1.61	0.832	1.10	0.474
Kronecker	3.87	5.468	2.882	3.54	3.31	5.96
CNRGE	**1.067**	0.723	**0.448**	1.329	**0.41**	**0.20**

Dendrogram Selection