


Scalable and Interpretable Graph Modeling with Graph Grammars

Satyaki Sikdar

Ph.D. Defense

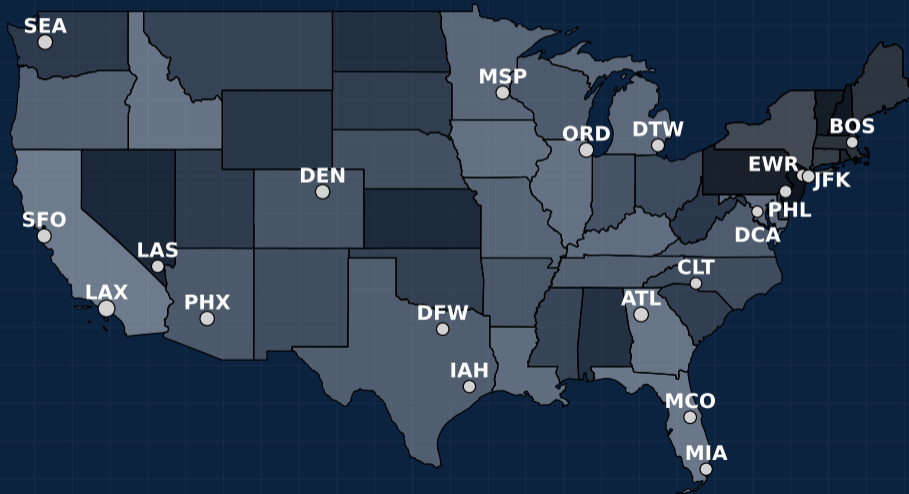
Committee: Dr. Tim Weninger, Chair

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

An aerial, high-angle view of Prague, Czech Republic, showing the Vltava River and several bridges. The most prominent bridge in the foreground is the Charles Bridge, with its multiple stone arches. Behind it, the New Bridge and the Starobratrská Bridge are visible. The city's architecture, including domes and spires, is visible in the background. The image has a dark, muted color palette, and the text 'Introduction' is overlaid in the center.

Introduction

US Flights Network in 2011



Scalable and
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Modeling with
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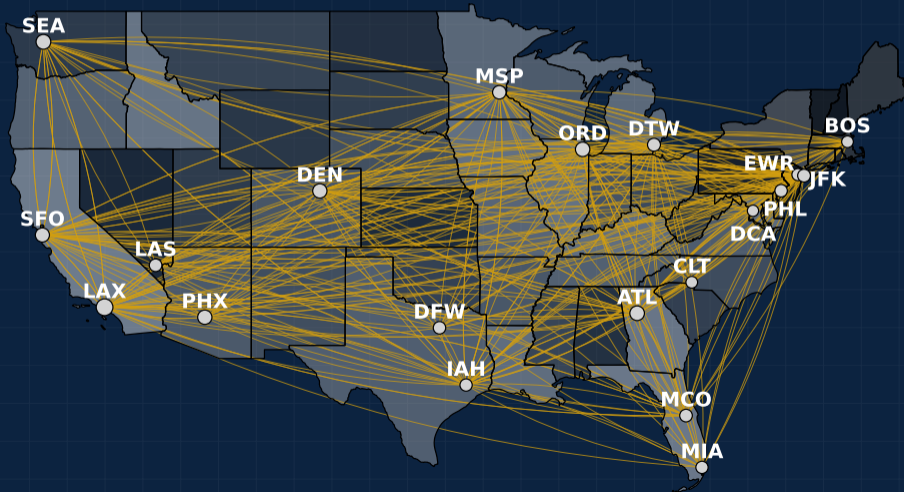
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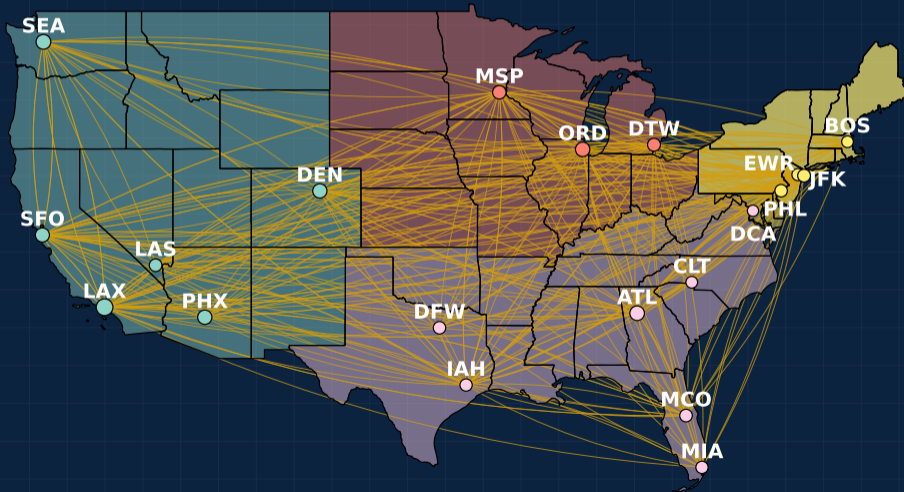
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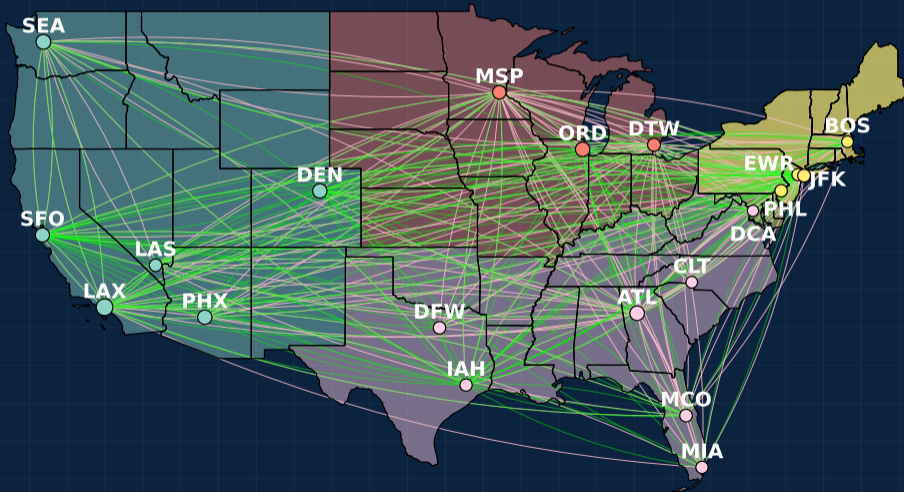
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How to Study Graphs?

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Subgraph Mining

- ◆ Extract *statistically significant* patterns



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Subgraph Mining

- ◆ Extract *statistically significant* patterns

Graph Representation Learning

- ◆ Learn low-dimensional *embedding* of nodes



Graph Generative Models

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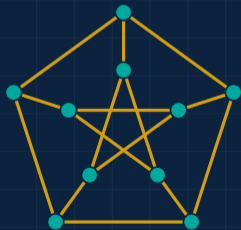
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Original Graph H



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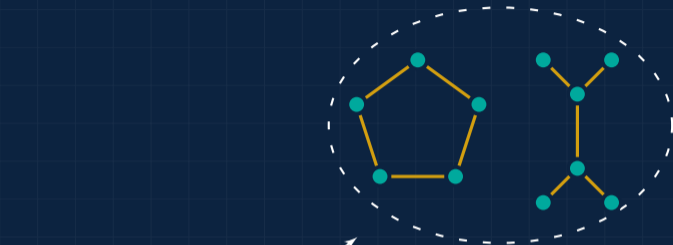
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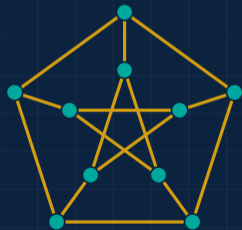
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Extracted Features Θ



Original Graph H

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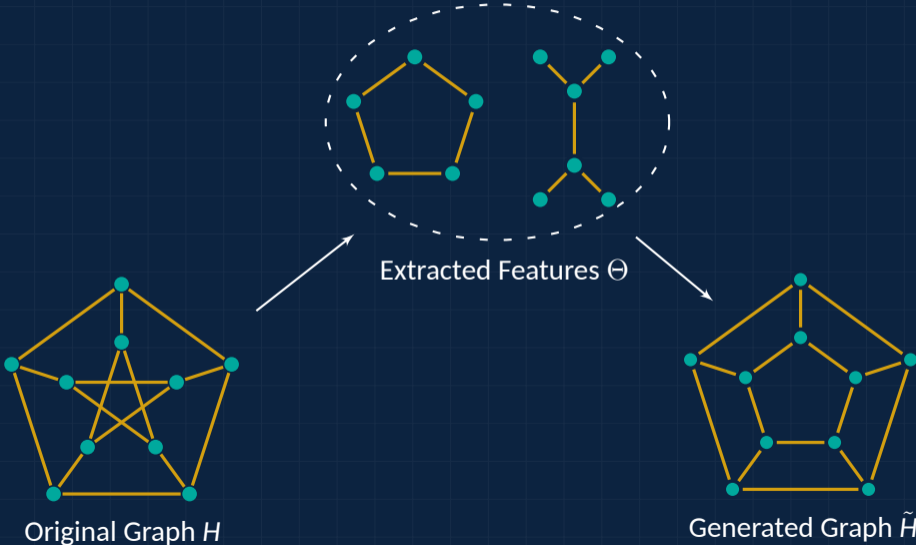
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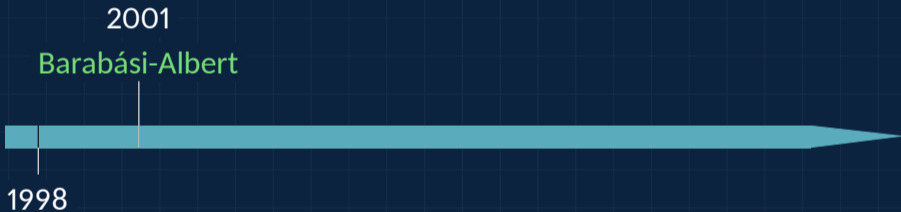
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2001

Barabási-Albert

1998

Watts-Strogatz



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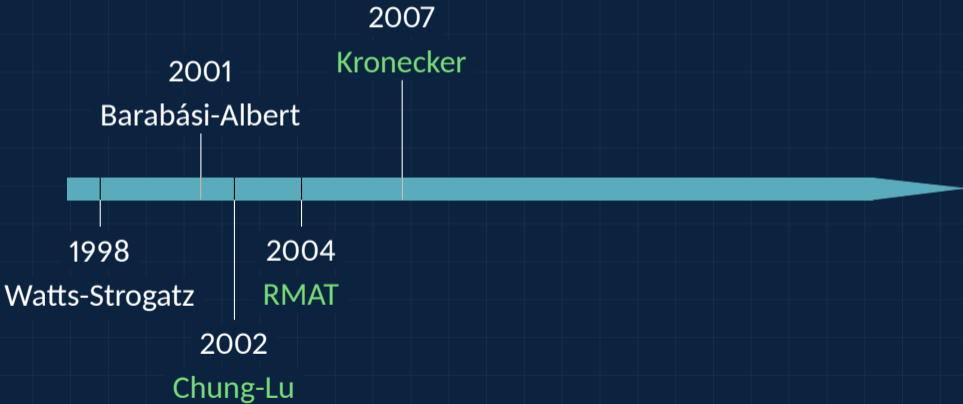
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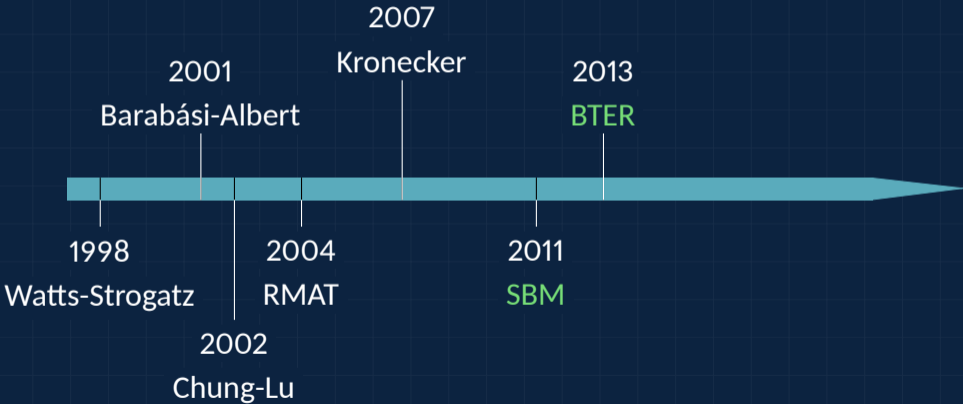
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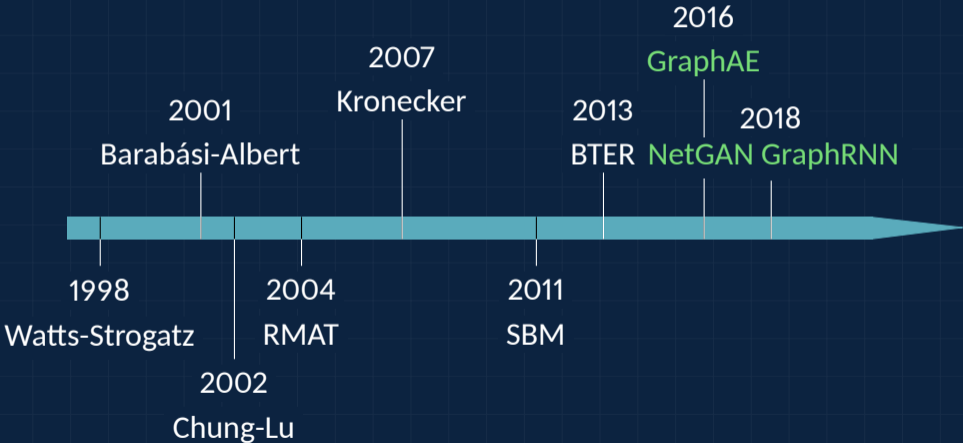
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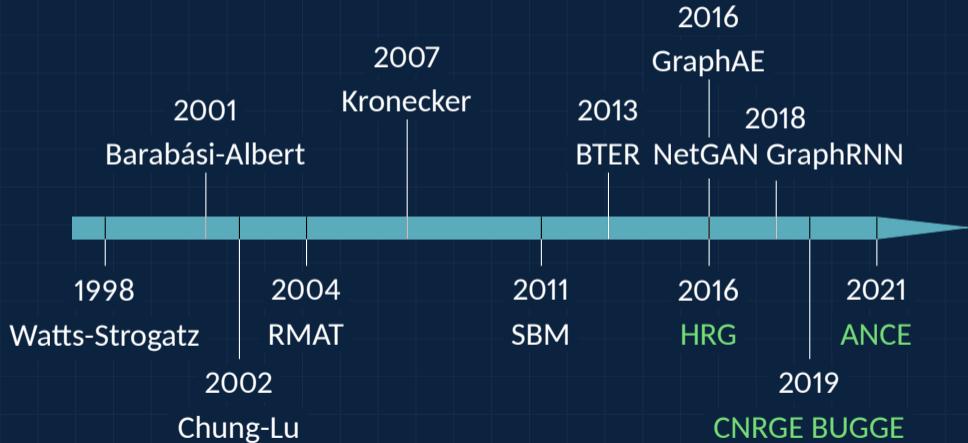
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A Fork in the Road

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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.*

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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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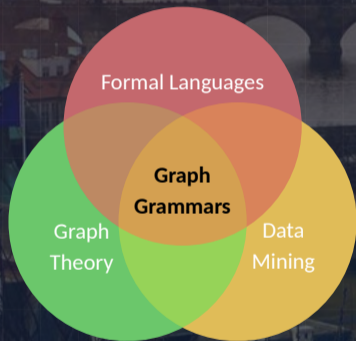
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ICDM 19 *Modeling Graphs with Vertex Replacement Grammars*

WSDM 22* *Attributed Vertex Replacement Graph Grammars*

The Big Picture

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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

- ◆ $S \rightarrow NP VP$
- ◆ $NP \rightarrow \text{the } N$
- ◆ $VP \rightarrow V NP$
- ◆ $N \rightarrow \text{cat} \mid \text{song}$
- ◆ $V \rightarrow \text{sings} \mid \text{eats}$

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$S \Rightarrow NP VP$



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$S \Rightarrow NP VP \Rightarrow \text{the } N VP$

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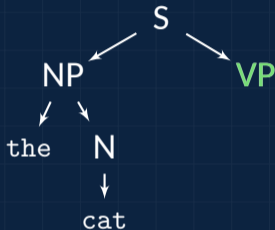
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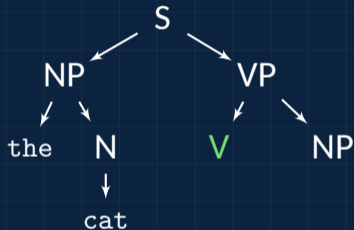
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$S \Rightarrow NP VP \Rightarrow the N VP \Rightarrow the cat VP \Rightarrow the cat V NP$

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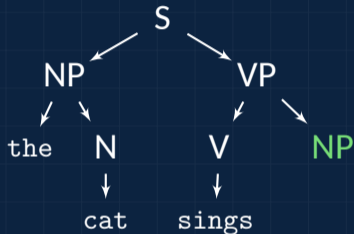
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String Grammars

CFG Production Rules

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$S \Rightarrow NP VP \Rightarrow \text{the } N VP \Rightarrow \text{the cat } VP \Rightarrow \text{the cat } V NP$
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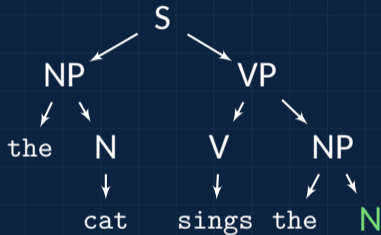
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- ◆ $VP \rightarrow V NP$
- ◆ $N \rightarrow cat | song$
- ◆ $V \rightarrow sings | eats$



$S \Rightarrow NP VP \Rightarrow the N VP \Rightarrow the cat VP \Rightarrow the cat V NP$
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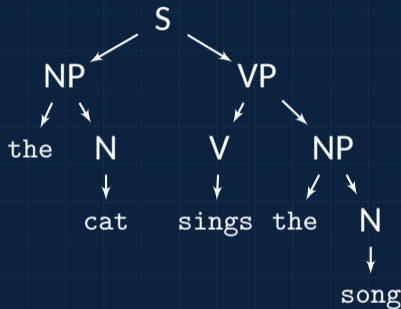
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- ◆ $VP \rightarrow V NP$
- ◆ $N \rightarrow cat \mid song$
- ◆ $V \rightarrow sings \mid eats$



$S \Rightarrow NP VP \Rightarrow the N VP \Rightarrow the cat VP \Rightarrow the cat V NP$
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Context Free Graph Grammars

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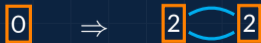
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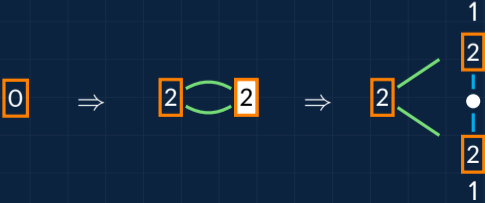
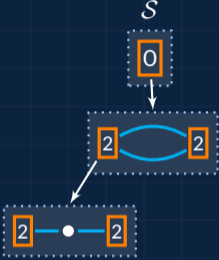
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NCE Production Rules

- ◆ $0 \rightarrow$ 
- ◆ $2 \xrightarrow{1}$ 
- ◆ $2 \rightarrow$ 



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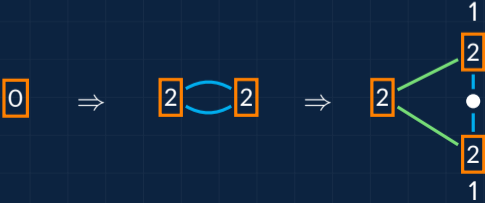
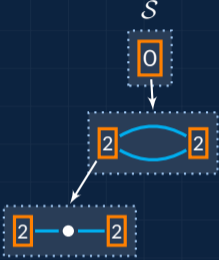
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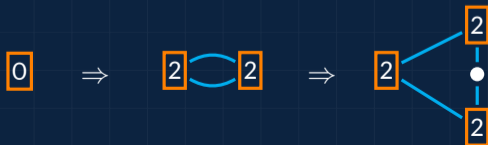
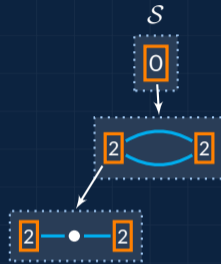
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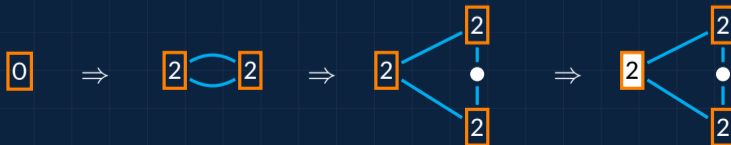
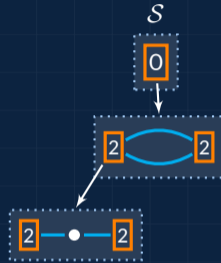
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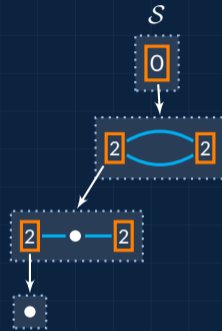
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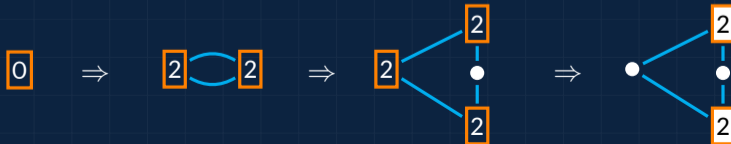
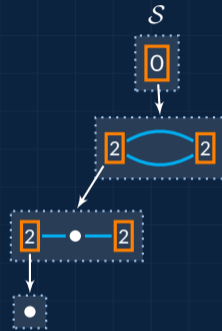
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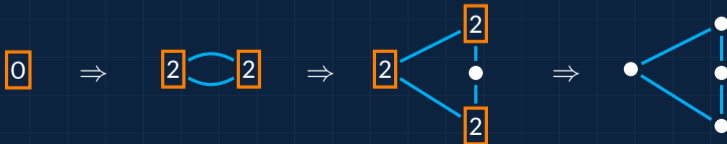
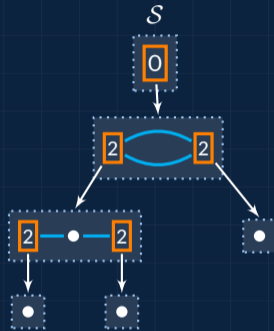
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Input Graph H

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Random, Attribute-aware



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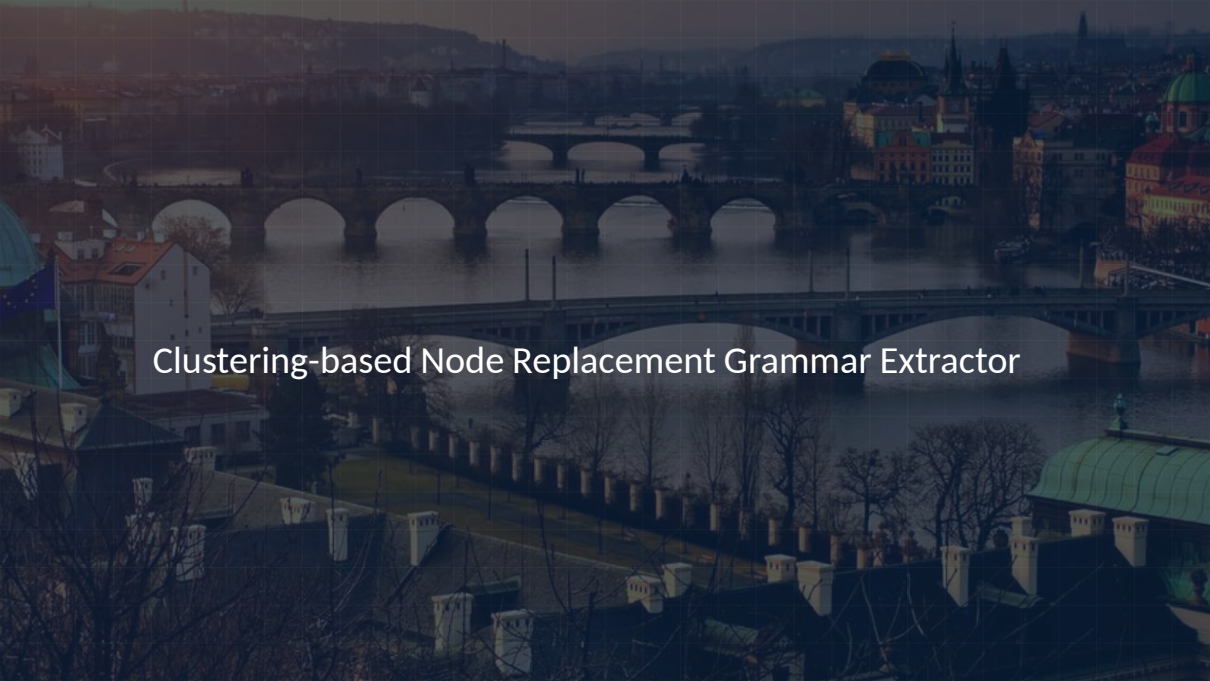


Output Graphs $\langle \tilde{H} \rangle$

Grammar Extractor

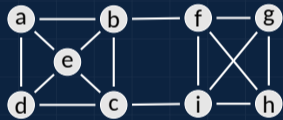
Graph Generator



An aerial photograph of Prague, Czech Republic, showing the Vltava river and several bridges. The most prominent bridge is the Charles Bridge, with its many arches. Other bridges are visible in the background. The city buildings and hills are visible in the distance. The image is dimly lit, with a dark overlay.

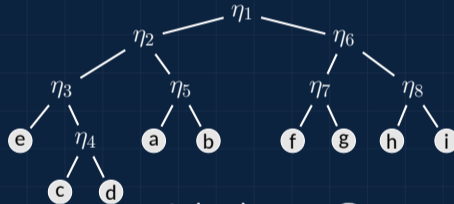
Clustering-based Node Replacement Grammar Extractor

Hierarchical Graph Clustering



Graph H

Leiden
Louvain
Spectral
MinCut



A dendrogram \mathcal{D}

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Infinity Mirror Test

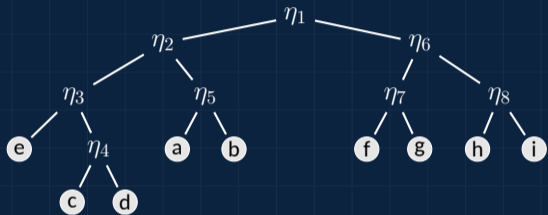
Wrapping Up

Extracting NCE Rules I

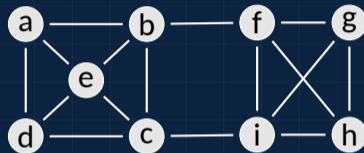
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Current Graph H

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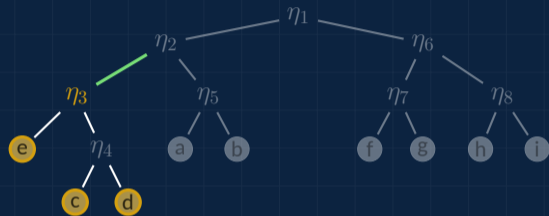


Extracting NCE Rules I

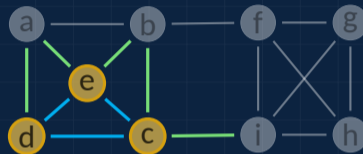
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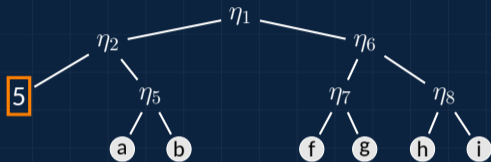
Infinity Mirror Test

Wrapping Up

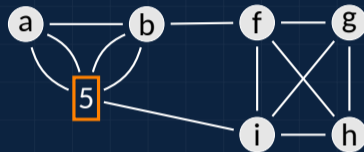


Extracting NCE Rules I

$(\mu = 3)$



Updated Dendrogram \mathcal{D}'



Updated Graph H'

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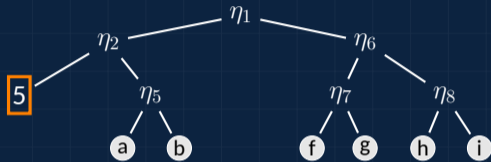


Extracting NCE Rules II

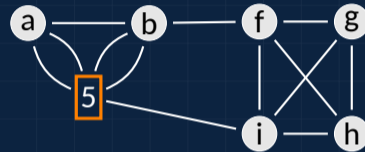
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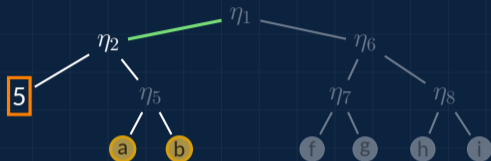


Extracting NCE Rules II

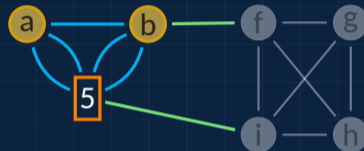
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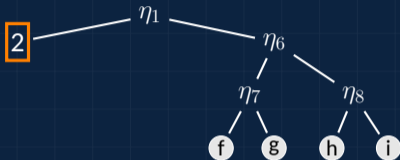


Extracting NCE Rules II

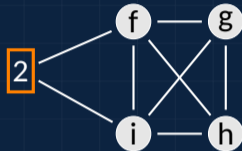
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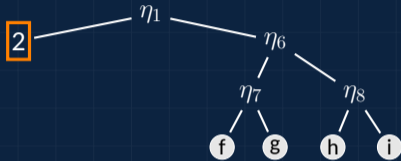


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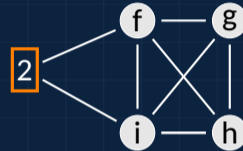
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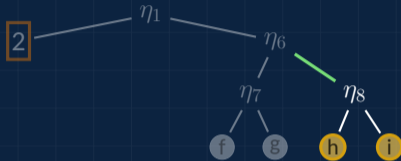


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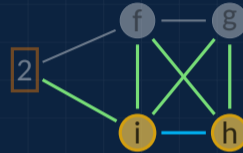
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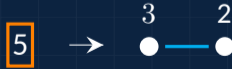
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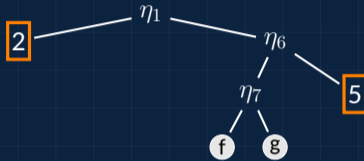


Extracting NCE Rules III

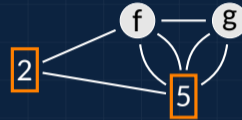
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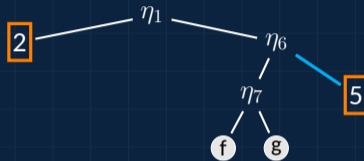


Extracting NCE Rules IV

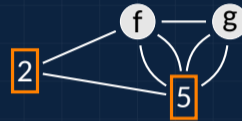
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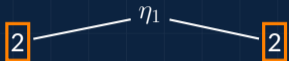


Extracting NCE Rules IV

$(\mu = 3)$

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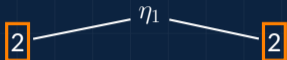
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Extracting NCE Rules V

$(\mu = 3)$



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Current Graph H



Extracted NCE Rule

Extracting NCE Rules V

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0

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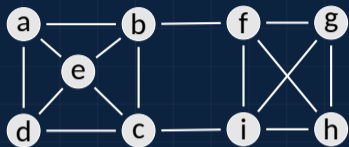
Graph Generation

Infinity Mirror Test

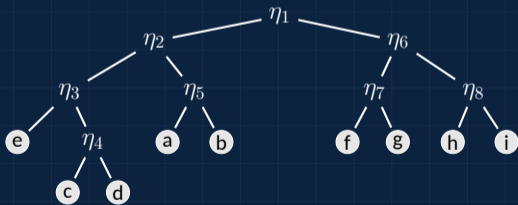
Wrapping Up



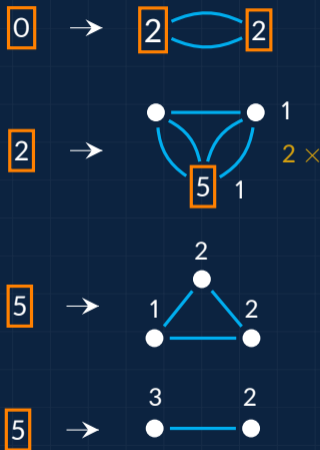
Extracted NCE Grammar



Graph H

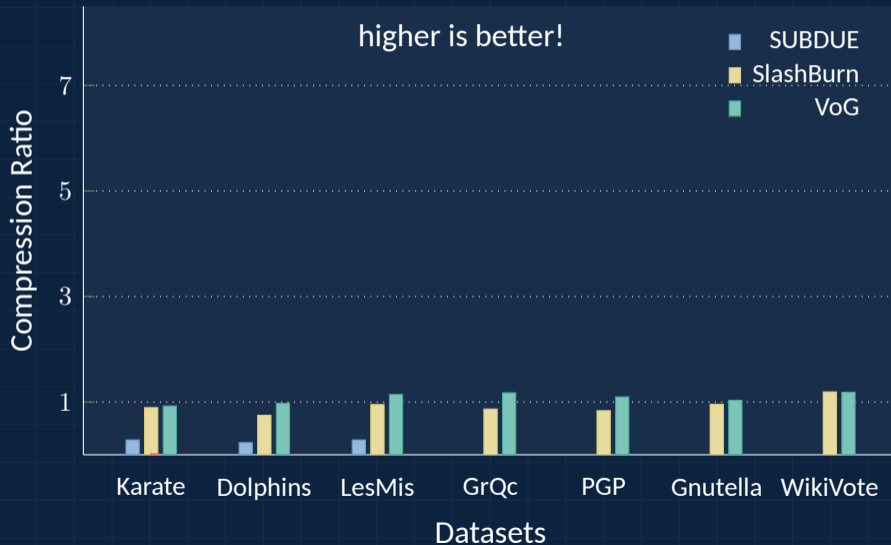


Dendrogram \mathcal{D}

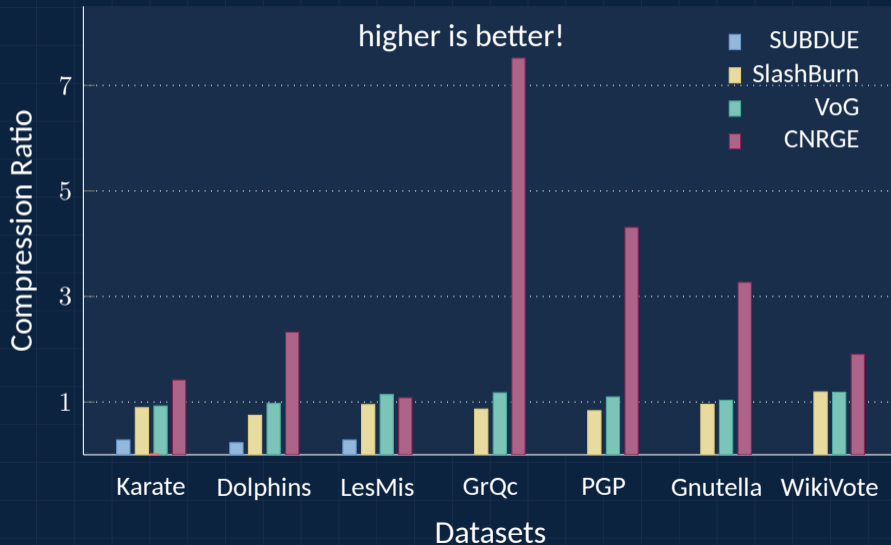


Extracted NCE rules

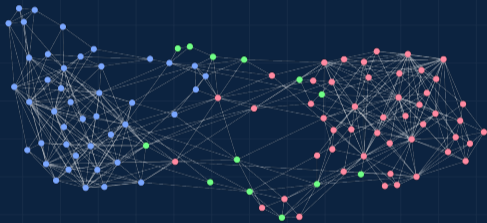
Model Size Comparison



Model Size Comparison



Attributed Graphs



Homophily in PolBooks graph

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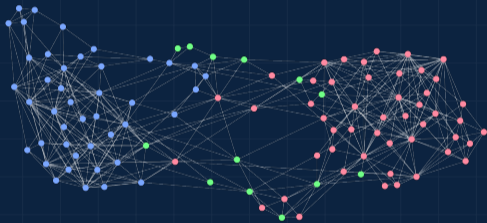
Rule Extraction

Attributed Graphs

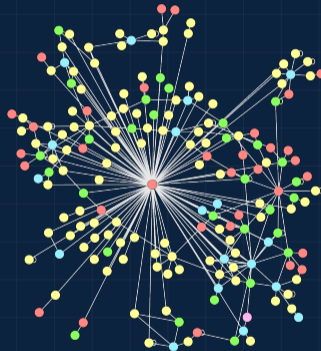
Graph Generation

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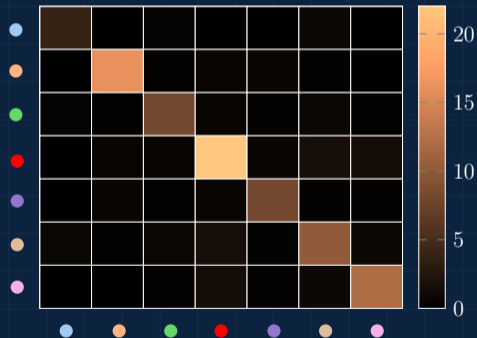
Homophily in PolBooks graph



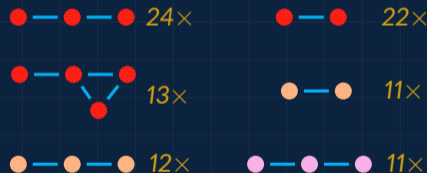
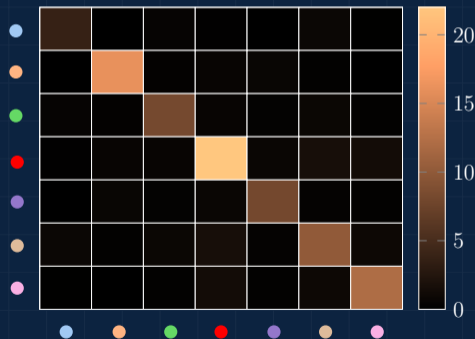
Heterophily in Texas CS website



Real-world Grammars: Cora



Real-world Grammars: Cora



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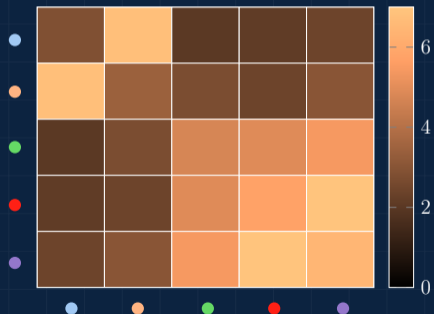
Real-world Grammars: Chameleon

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20% 20.2% 19.9% 22.9% 17%

Node Distribution



Edge Mixing Matrix

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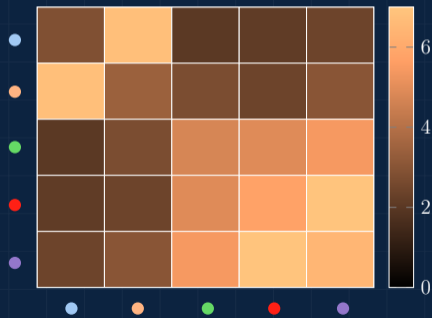
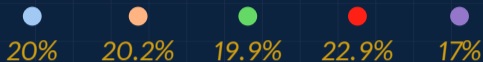
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Real-world Grammars: Chameleon



Graph Grammar Pipeline Revisited

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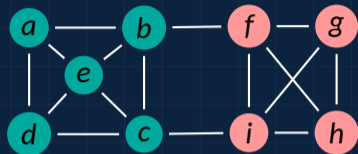
Graph Generator



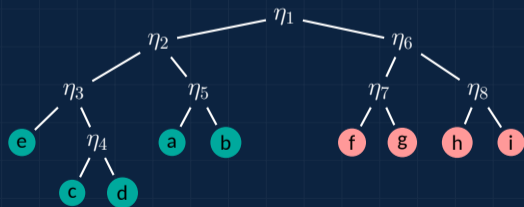


Generating Graphs using Graph Grammars

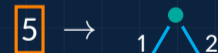
Attributed NCE Grammars



Graph H

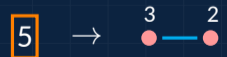


Dendrogram \mathcal{D}



Extracted ANCE rules

Generating Graphs from an ANCE I



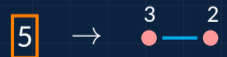
Extracted ANCE Rules

S
0

Current Graph H'

Next Graph \hat{H}

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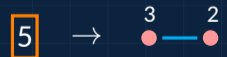
Extracted ANCE Rules

S
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Current Graph H'

Next Graph \hat{H}

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Extracted ANCE Rules

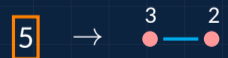


Current Graph H'



Next Graph \hat{H}

Generating Graphs from an ANCE II



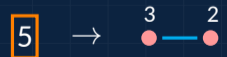
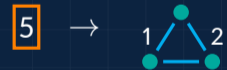
Extracted ANCE Rules



Current Graph H'

Next Graph \hat{H}

Generating Graphs from an ANCE II



Extracted ANCE Rules

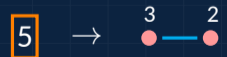
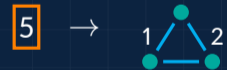


Current Graph H'



Next Graph \hat{H}

Generating Graphs from an ANCE II



Extracted ANCE Rules

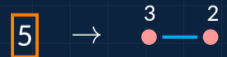


Current Graph H'



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Extracted ANCE Rules



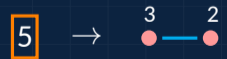
Current Graph H'

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Generating Graphs from an ANCE III



Extracted ANCE Rules

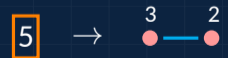


Current Graph H'



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Extracted ANCE Rules

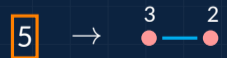


Current Graph H'

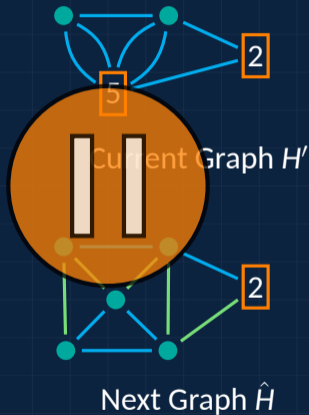


Next Graph \hat{H}

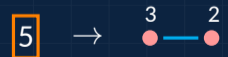
Generating Graphs from an ANCE III



Extracted ANCE Rules



Generating Graphs from an ANCE IV



Extracted ANCE Rules



Current Graph H'

Next Graph \hat{H}

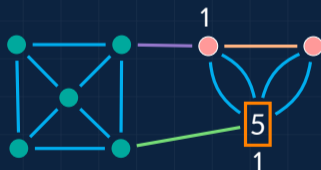
Generating Graphs from an ANCE IV



Extracted ANCE Rules

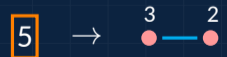


Current Graph H'



Next Graph \hat{H}

Generating Graphs from an ANCE IV



Extracted ANCE Rules

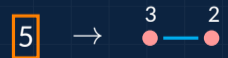


Current Graph H'



Next Graph \hat{H}

Generating Graphs from an ANCE V



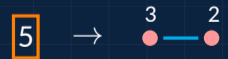
Extracted ANCE Rules



Current Graph H'

Next Graph \hat{H}

Generating Graphs from an ANCE V



Extracted ANCE Rules

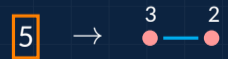


Current Graph H'



Next Graph \hat{H}

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Extracted ANCE Rules



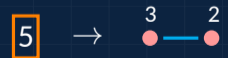
Current Graph H'



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Generating Graphs from an ANCE V



Extracted ANCE Rules

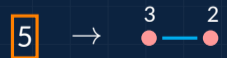


Current Graph H'

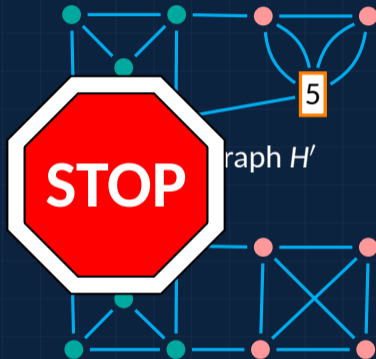


Next Graph \hat{H}

Generating Graphs from an ANCE V



Extracted ANCE Rules



Language of Graphs Described by a Grammar

Scalable and
Interpretable Graph
Modeling with
Graph Grammars

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Experimental Results

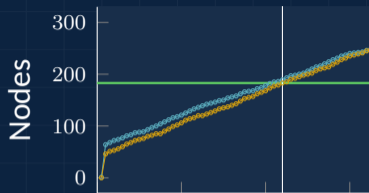
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Examining the Graph Growth Process



—○— Whole Graph —●— Terminal Graph — Input Graph Metric — Input Graph Size

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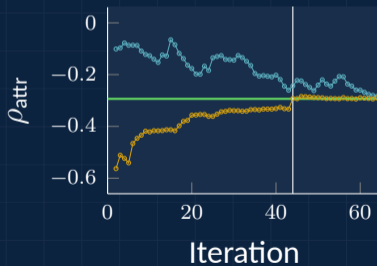
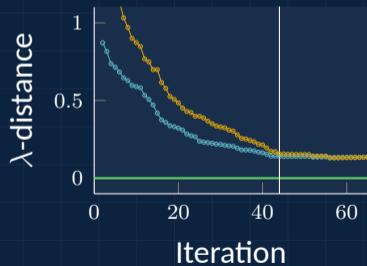
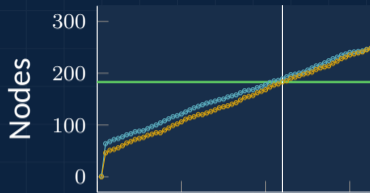
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CABAM Graphs

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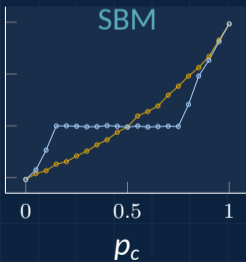
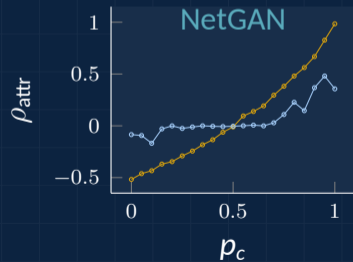
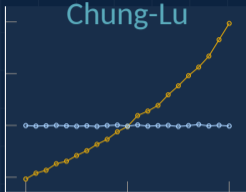
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● Original ● Model



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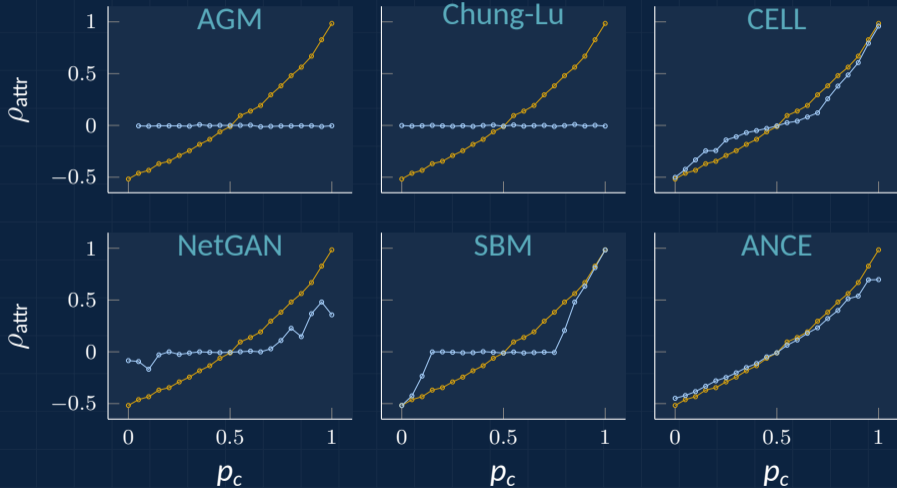
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—●— Original —●— Model



Takeaways

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Main Takeaways

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

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Main Takeaways

- ◆ *Simple* and *interpretable* formalism from formal languages
- ◆ *Scalable* to medium-large graphs

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Main Takeaways

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

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Main Takeaways

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

- ◆ Dependence on the *dendrogram*

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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*

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An aerial photograph of a coastal city at dusk, featuring a beach, ocean, and dense urban development. A semi-transparent grid is overlaid on the entire image. The title text is centered in the middle of the frame.

The Infinity Mirror Test for Graph Models

Infinity Mirror Test for Duck Vader

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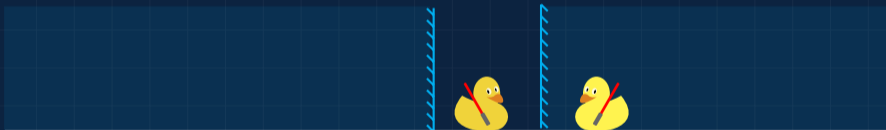
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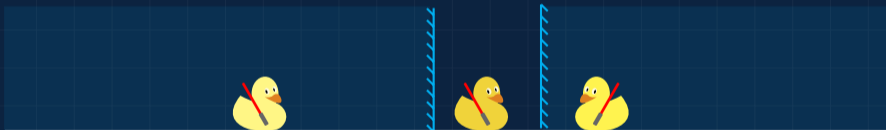
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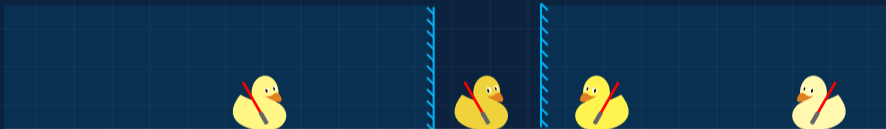
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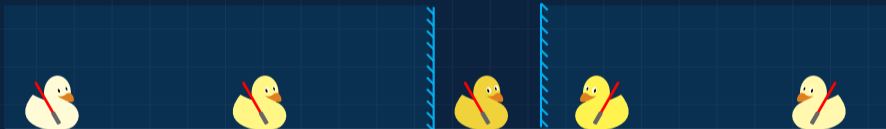
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Infinity Mirror Test for Graph Models

Key Idea

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



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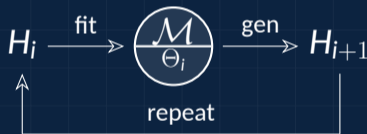
Infinity Mirror Test for Graph Models

Key Idea

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

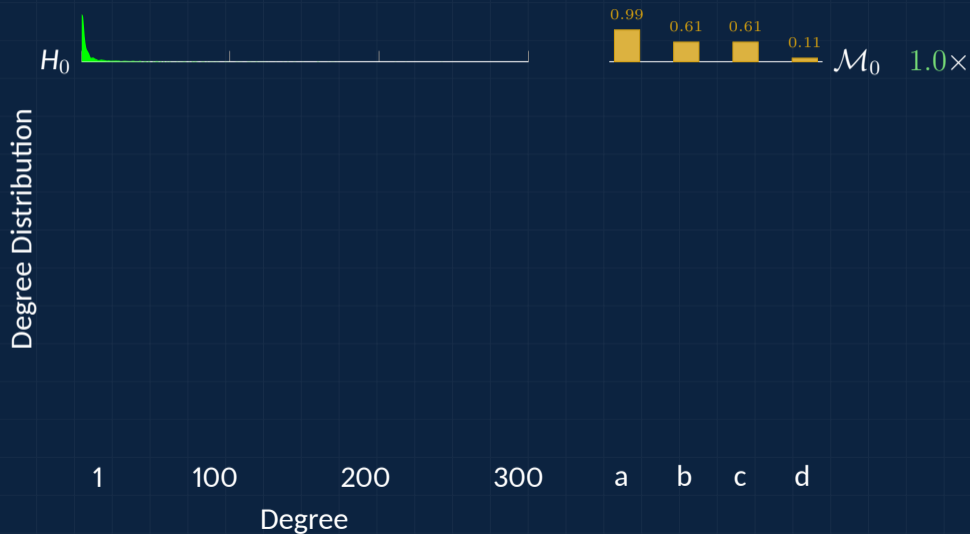
Evaluation Plan

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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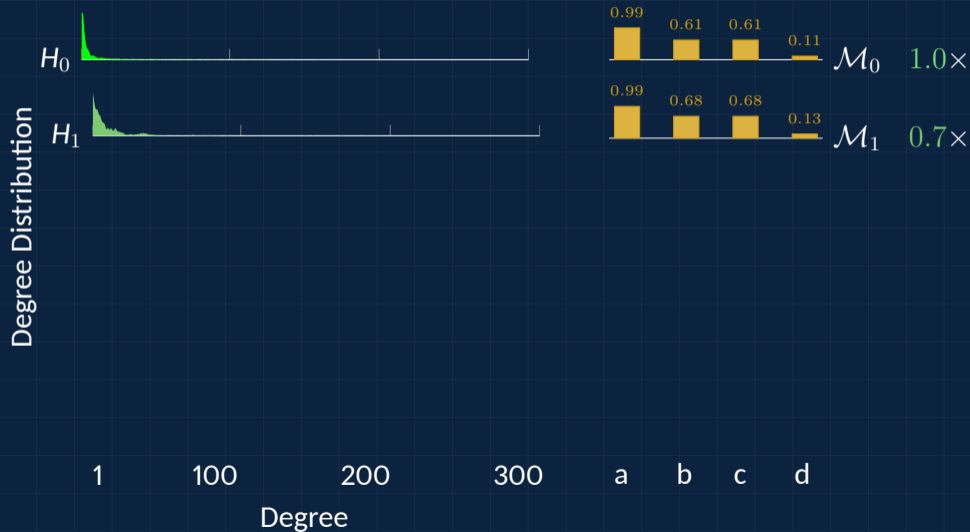
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Kronecker Degree Distribution Ridge Plot

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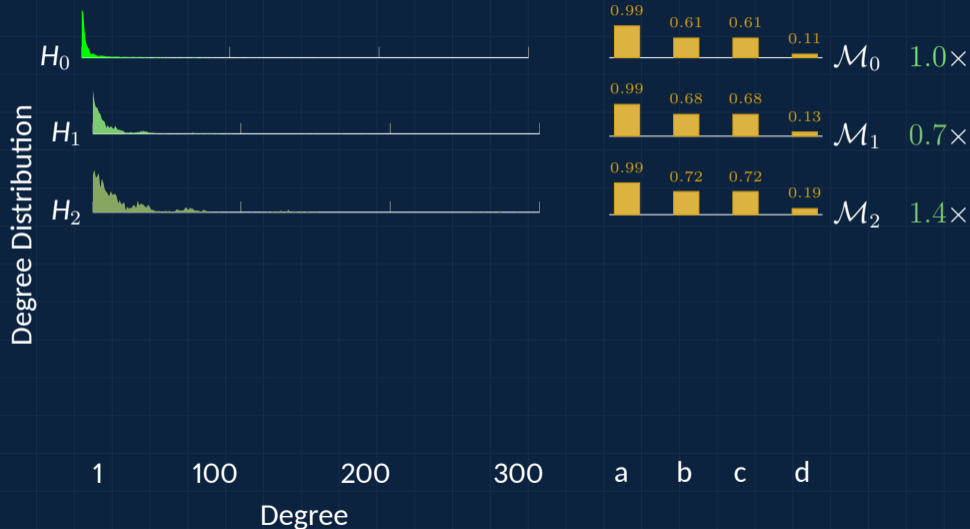
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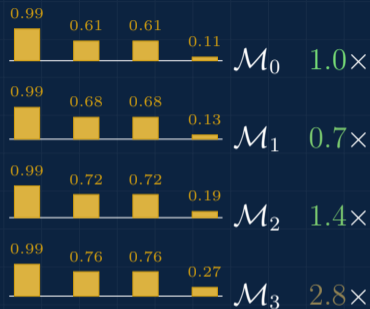
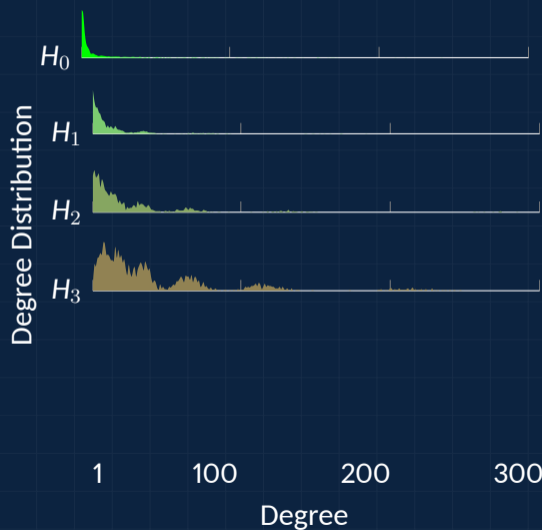
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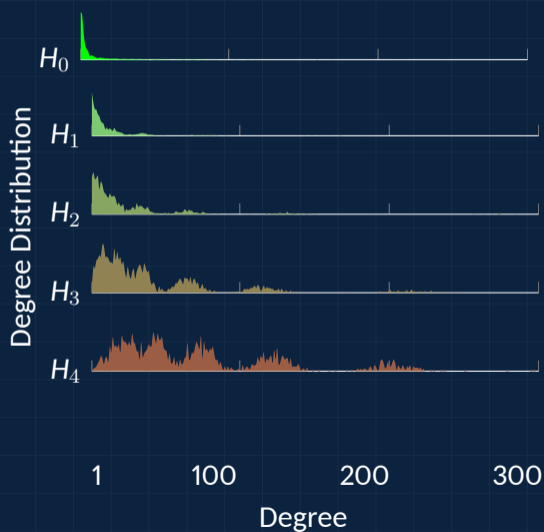
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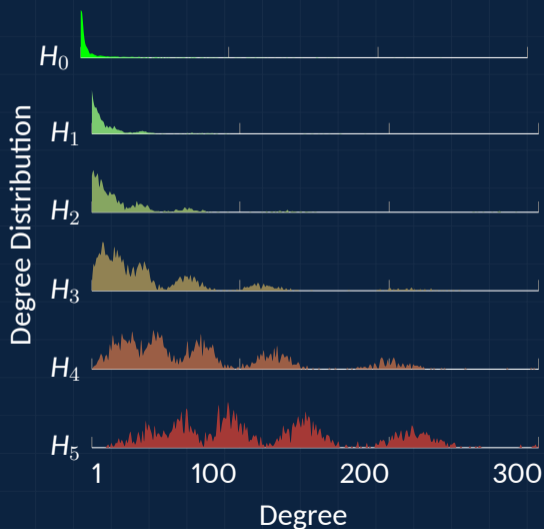
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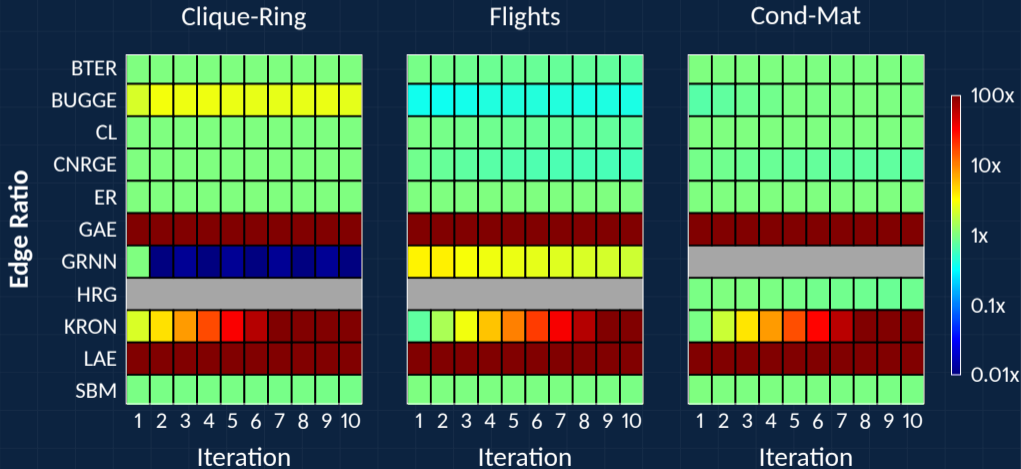
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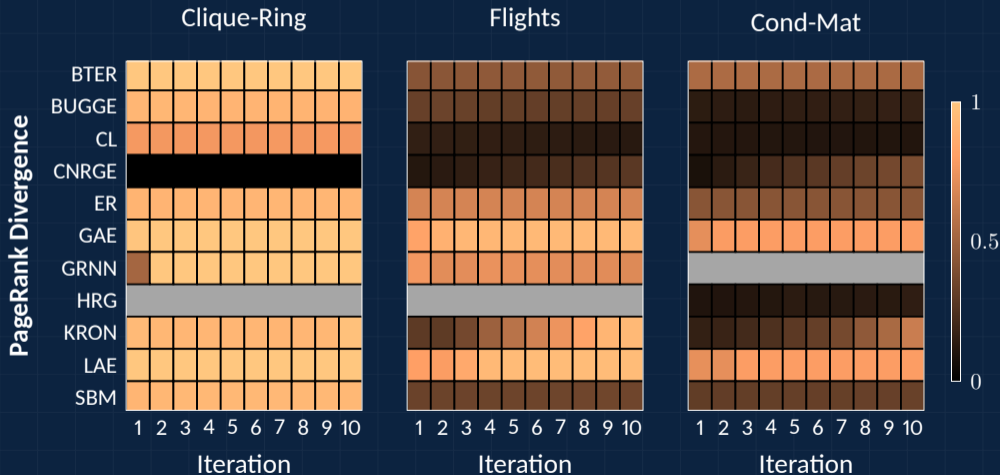
First-order Graph Statistics



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First-order Graph Statistics



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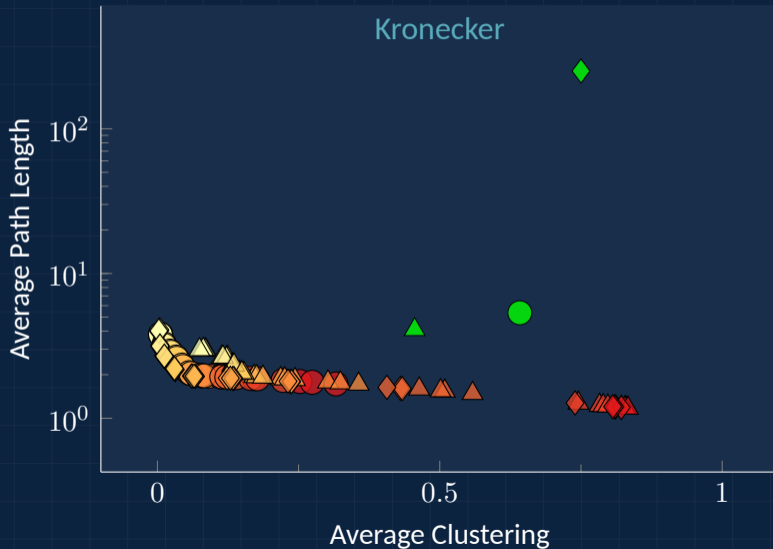
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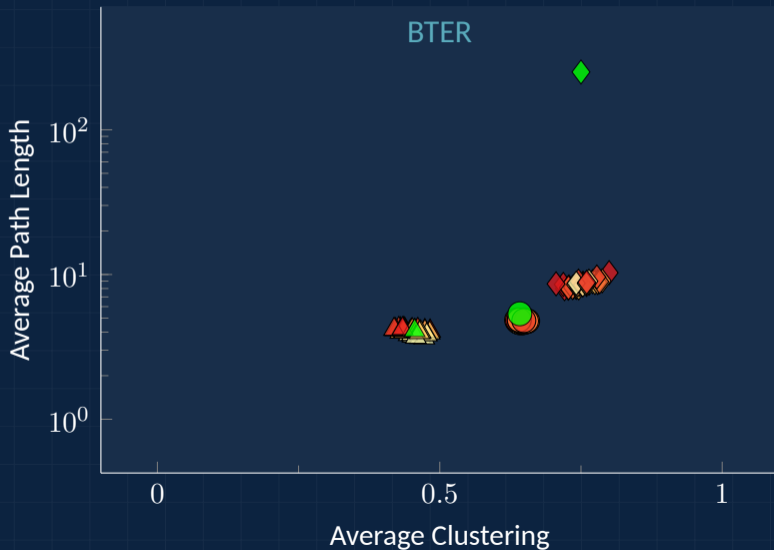
Tracking Evolution: Clustering & Geodesics



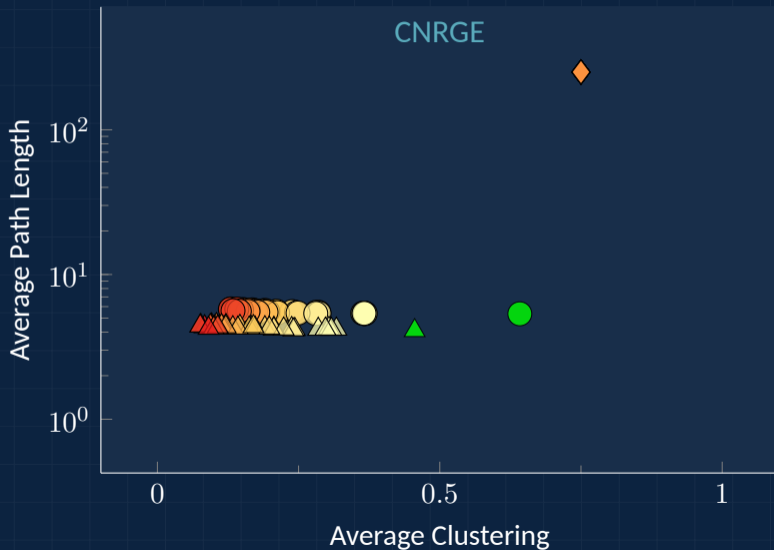
Tracking Evolution: Clustering & Geodesics



Tracking Evolution: Clustering & Geodesics



Tracking Evolution: Clustering & Geodesics



Tracking Evolution: Clustering & Geodesics

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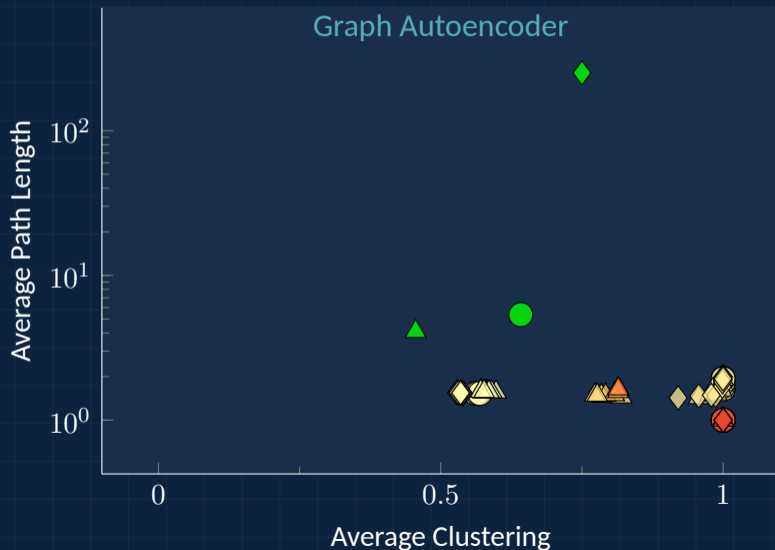
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Main Takeaways

- ◆ *Confirms* previously known biases in Kronecker graphs



Takeaways



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- ◆ *Confirms* previously known biases in Kronecker graphs
- ◆ Uncovers *unique* distortion patterns in popular graph models

Takeaways



Main Takeaways

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

A cable-stayed bridge is shown at dusk, with its lights reflecting on the water below. The sky is a deep blue, and the bridge's structure is silhouetted against the twilight. The word "Conclusion" is centered in white text over the bridge.

Conclusion

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What's Next

Vertex Replacement Grammars

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



Summary

Vertex Replacement Grammars

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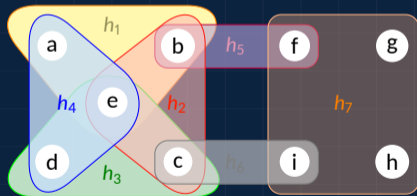
Infinity Mirror Test

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

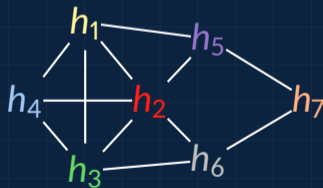
What's Next

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

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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



An aerial photograph of a university campus, likely Georgetown University, featuring a prominent building with a large golden dome and a tall, pointed Gothic-style church spire. The campus is surrounded by dense green trees and a body of water is visible in the upper right. The text "Thank You!" is overlaid in the center in a white, sans-serif font.

Thank You!

Minimum Description Length Principle

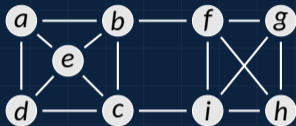
The Core Idea

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

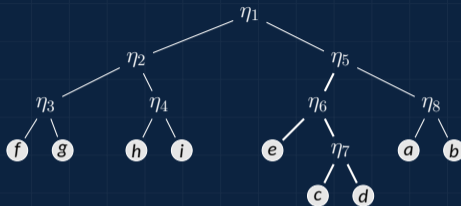
$$\mathcal{M}^* = \operatorname{argmin} \{ \mathcal{L}(\mathcal{M}) + \mathcal{L}(\mathcal{D} | \mathcal{M}) \}$$

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

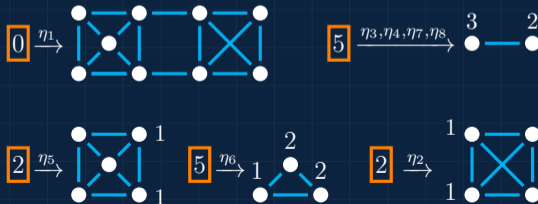
CNRG extraction and MDL



(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

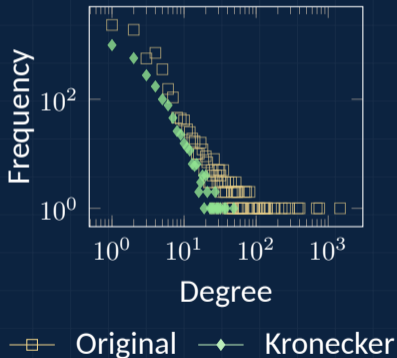
Distribution Based

- ◆ Degree distribution
- ◆ PageRank centrality
- ◆ ...

Topology Based

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

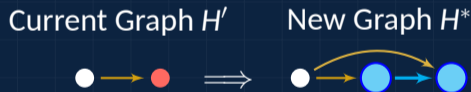
Routers Degree Distribution



Kemp-Tenenbaum (KT) Graph Grammars



(A) A KT grammar rule



(B) Example of rule application

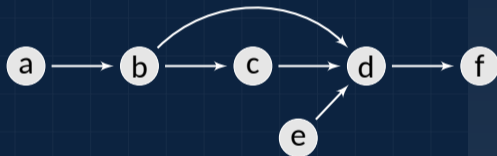
● replaced ● → new → boundary

Bottom-up Graph Grammar Extraction (BUGGE)

$(\mu = 2)$

(1) Enumerate Subgraphs

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



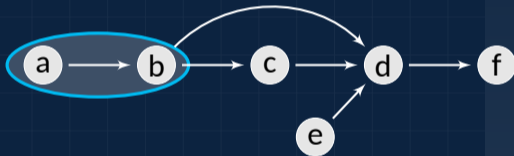
Enumerating all connected size μ
subgraphs in H

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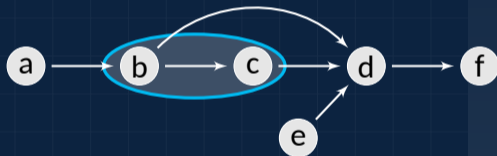
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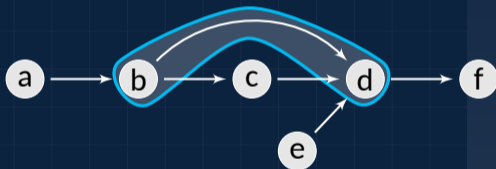
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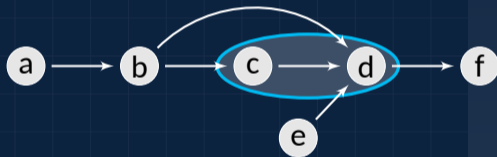
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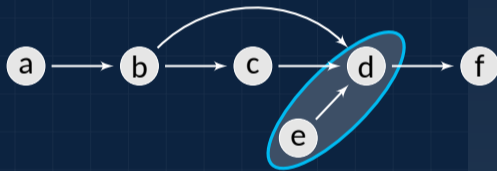
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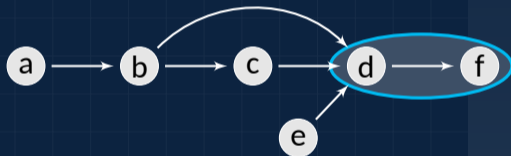
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Enumerating all connected size μ
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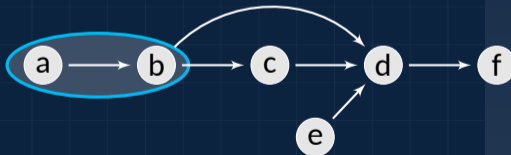
(1) Enumerate Subgraphs

(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

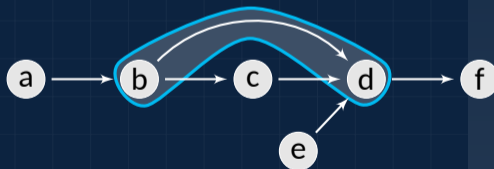
Bottom-up Graph Grammar Extraction (BUGGE)

$(\mu = 2)$

(1) Enumerate Subgraphs

(2) Best Rule Selection

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



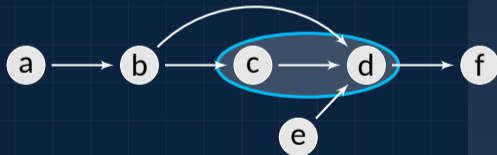
Bottom-up Graph Grammar Extraction (BUGGE)

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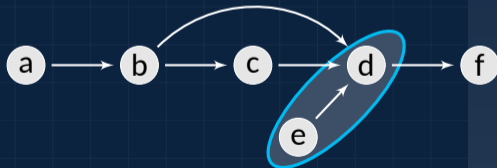
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Bottom-up Graph Grammar Extraction (BUGGE)

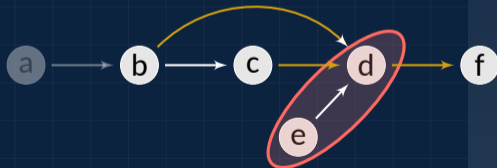
$(\mu = 2)$

(1) Enumerate Subgraphs

(2) Best Rule Selection

(3) Extract Best Rule

- ◆ Match rule *RHS* in the graph
- ◆ *Collapse* matched nodes
- ◆ *Repeat* until the graph is empty



Bottom-up Graph Grammar Extraction (BUGGE)

$(\mu = 2)$

(1) Enumerate Subgraphs

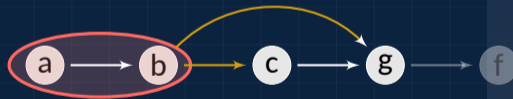
(2) Best Rule Selection

(3) Extract Best Rule

- ◆ Match rule *RHS* in the graph
- ◆ *Collapse* matched nodes
- ◆ *Repeat* until the graph is empty



(A) Best rule R



(B) Current graph H

Bottom-up Graph Grammar Extraction (BUGGE)

$(\mu = 2)$

(1) Enumerate Subgraphs

(2) Best Rule Selection

(3) Extract Best Rule

- ◆ Match rule *RHS* in the graph
- ◆ *Collapse* matched nodes
- ◆ *Repeat* until the graph is empty



(A) Best rule *R*



(B) Current graph *H*

Bottom-up Graph Grammar Extraction (BUGGE)

$(\mu = 2)$

(1) Enumerate Subgraphs

(2) Best Rule Selection

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Bottom-up Graph Grammar Extraction (BUGGE)

($\mu = 2$)

(1) Enumerate Subgraphs

(2) Best Rule Selection

(3) Extract Best Rule

- ◆ Match rule *RHS* in the graph
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(A) Best rule *R*



(B) Current graph *H*

Bottom-up Graph Grammar Extraction (BUGGE)

$(\mu = 2)$

(1) Enumerate Subgraphs

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- ◆ Match rule *RHS* in the graph
- ◆ *Collapse* matched nodes
- ◆ *Repeat* until the graph is empty



(A) Best rule *R*

k



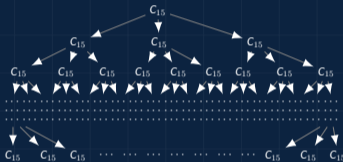
Results from Synthetic Graphs

Synthetic
Graphs

I: Balanced Binary Tree



II: Tree of Directed C_{15} Rings



III: Regular Ring Lattice

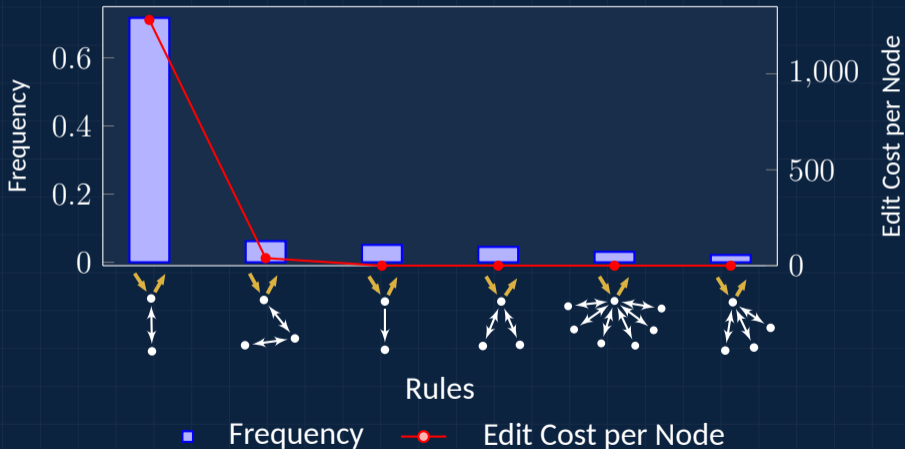


BUGGE
Rules



Most Frequent Rules Extracted from a PPI Network

Protein-Protein-Interaction Network



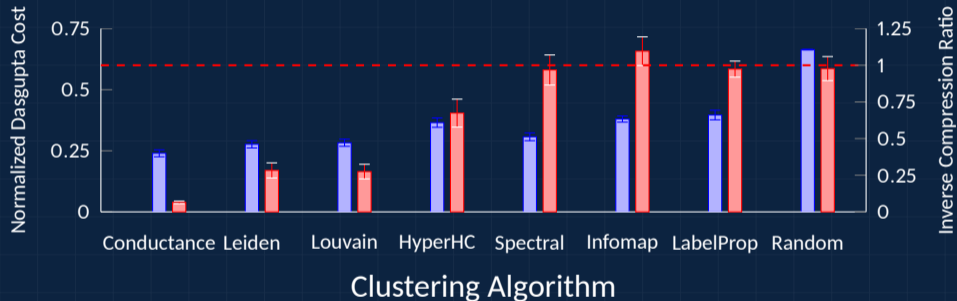
CNRG Results

	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



■ Normalized Dasgupta Cost ■ Inverse Compression Ratio