



# Mining of Real-world Hypergraphs: Concepts, Patterns, and Generators Part 3. Generative Models



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## Part 3. Generative Models

"How can we generate realistic hypergraphs?"

"What are underlying mechanisms that lead to the observed patterns?"





## Why Generative Models?

- Explaining Patterns: Shed a light on why patterns occur
- Statistical Test: Test the statistical significance of patterns
- Benchmark Data Generation
  - Create large realistic hypergraphs for evaluation of hypergraph algorithms
  - Useful when real hypergraphs are hard/impossible to collect
- Anonymization
  - Generate and publicize synthetic hypergraphs to structurally-similar real ones
  - Useful real hypergraphs cannot be publicized (due to sensitive information etc.)



## Roadmap

- Part 1. Static Structural Patterns
  - Basic Patterns
  - Advanced Patterns

## Part 2. Dynamic Structural Patterns

- Basic Patterns
- Advanced Patterns
- Part 3. Generative Models
  - Static Hypergraph Generator <</li>
  - Dynamic Hypergraph Generator



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# Part 3-1. Static Hypergraph Generative Models

Part 3. demonstrative Models

Ð	Static Models	Full-Hypergraphs	C20, LCS21
		Sub-Hypergraphs	CYLBKS22
	Dynamic Models	Full-Hypergraphs	DYHS20, KKS20, KBCYS23, GLLB23
		Sub-Hypergraphs	BKT18, CK21

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# **C20: Configuration Models**

• G1: Pairwise reshuffling



## **Configuration Models**

 Configuration models generate random hypergraphs while preserving distributions of node degrees and hyperedge sizes.





### **Real-world hypergraph**

Randomized hypergraph

## **Pairwise Reshuffling**

## **Step 1. Hyperedge Pair Sampling**



### <u>Step 1</u>

Sample a pair of hyperedges uniformly at random.

$$(e_i, e_j) \in \begin{pmatrix} E \\ 2 \end{pmatrix}$$

# **Pairwise Reshuffling (cont.)**

## **Step 2. Shuffle Hyperedges**



### <u>Step 2-1</u>

For each node  $v \in e_i \cap e_j$ , add to both  $e'_i$  and  $e'_i$ .

## **Pairwise Reshuffling (cont.)**

## **Step 2. Shuffle Hyperedges**



### Step 2-2

From  $(e_i \cup e_j) - (e_i \cap e_j)$ , sample  $|e_i - e_j|$  nodes and add to  $e'_i$ .

### Step 2-3

Add remaining nodes to  $e'_i$ .



## **LCS21: Static Full-Hypergraph Generator**

- **G1.** HyperCL: <u>Hyper</u>grpaph <u>C</u>hung-<u>L</u>u (Basic model)
- **G2.** HyperLap: <u>Hyper</u>graph Over<u>Lap</u> (Multilevel HyperCL)



# HyperCL: Basic Model

- An approximate configuration model.
- HyperCL fills each hyperedge with sampled nodes.
  - Samples nodes with **probability**  $\propto$  degrees.



Random sampling prob.  $\propto d$ 's degree

## **Evaluation of Configuration Models**

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- Configuration models preserve node degrees and hyperedge sizes.
- They are limited in reproducing realistic overlapping patterns.
- Especially, they fail to produce highly-overlapping hyperedges.



# HyperLap: Multilevel HyperCL

## **Step 1. Random Hierarchical Grouping of Nodes**



# HyperLap: Multilevel HyperCL (cont.)

### **Step 2. Hyperedge Generation**

![](_page_14_Figure_3.jpeg)

### Step 2-1

Select a level with probability

proportional to the given weight of each level  $\{w_1, \dots, w_L\}$ .

# HyperLap: Multilevel HyperCL (cont.)

## **Step 2. Hyperedge Generation**

![](_page_15_Figure_3.jpeg)

#### Step 2-2

Select a group uniformly at random.

# HyperLap: Multilevel HyperCL (cont.)

## **Step 2. Hyperedge Generation**

![](_page_16_Figure_3.jpeg)

### Step 2-3

**Sample nodes** independently with probability proportional to the degree of each node to form a hyperedge.

# **Evaluation of HyperLap**

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- HyperLap produces realistic overlaps of hypereges in many aspects.
- For example, HyperLap yields highly-overlapping hyperedges.

![](_page_17_Figure_3.jpeg)

![](_page_18_Picture_1.jpeg)

# **Evaluation of HyperLap (cont.)**

Question: How can HyperLap yield realistic overlapping patterns of hyperedges?

![](_page_18_Figure_4.jpeg)

### **Answer:**

- HyperLap generates hyperedges from groups of various sizes.
- Hyperedges from small groups highly overlap with each other.
- Hyperedges from large groups
  less overlap with each other.

![](_page_19_Picture_0.jpeg)

## **CYLBKS22: Static Sub-Hypergraph Generator**

• **G1.** MiDaS: <u>Minimum Degree Biased</u> Sampling of Hyperedges

![](_page_19_Picture_3.jpeg)

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# Hypergraph Representative Sampling

### **Question:**

From a hypergraph G, how can we generate a **smaller** hypergraph  $\widehat{G}$  that preserves the structural properties?

## **Answer:**

We sample a **representative sub-hypergraph**  $\widehat{\mathcal{G}}$  from  $\mathcal{G}$ 

![](_page_20_Figure_6.jpeg)

# Hypergraph Representative Sampling (cont.)

**Question:** 

What is a **representative** sub-hypergraph?

### **Answer:**

### We consider **10 structural properties**.

P1. DegreeP5. Singular ValuesP8. DensityP2. Pair DegreeP6. Connected Component SizeP9. OverlapnessP3. SizeP7. Global Clustering CoefficientP10. Effective Diameter

![](_page_21_Picture_7.jpeg)

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P4. Intersection Size

Node-level, hyperedge-level, and hypergraph-level structural properties

![](_page_22_Picture_0.jpeg)

## Simple and Intuitive Approaches

• Node selection (NS) chooses a subset of nodes and returns the sub-hypergraph induced by the nodes.

![](_page_22_Figure_3.jpeg)

• Hyperedge selection (HS) directly chooses a subset of hyperedges.

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# Simple and Intuitive Approaches (cont.)

- RHS (Random Hyperedge Sampling) performs best overall
  - RHS chooses hyperedges uniformly at random

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![](_page_23_Figure_3.jpeg)

## **Random Hyperedge Sampling: Pros**

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• RHS preserves many structural properties surprisingly well.

![](_page_24_Figure_2.jpeg)

M. Choe, J. Yoo, G. Lee, W. Baek, U Kang, K. Shin. "MiDaS: Representative Sampling from Realworld Hypergraphs", **WWW 2022** 

:

![](_page_25_Picture_0.jpeg)

## Random Hyperedge Sampling: Cons

- **RHS** gives a weakly connected sub-hypergraph.
- Especially, RHS suffers from a lack of high-degree nodes.

![](_page_25_Figure_4.jpeg)

## MiDaS-Basic: Main Idea

 To increase the fraction of high-degree nodes, prioritize hyperedges composed of high-degree nodes.

![](_page_26_Figure_3.jpeg)

![](_page_27_Picture_0.jpeg)

## MiDaS-Basic: Main Idea (cont.)

• Sampling a target number of hyperedges with probability proportional to the **minimum degree of nodes** in each hyperedge to the power of  $\alpha$ .

![](_page_27_Figure_3.jpeg)

## **MiDaS-Basic: Empirical Properties**

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- With a proper  $\alpha$  value, degree distributions are well preserved.
- Motivates (full-fledged) MiDaS with a hill-climbing search of  $\alpha$

![](_page_28_Figure_3.jpeg)

M. Choe, J. Yoo, G. Lee, W. Baek, U Kang, K. Shin. "MiDaS: Representative Sampling from Realworld Hypergraphs", **WWW 2022** 

**Details** 

## MiDaS: Evaluation

• **MiDaS** provides overall the most representative samples in terms of both average rankings and Z-scores.

![](_page_29_Figure_3.jpeg)

## MiDaS: Evaluation (cont.)

• MiDaS is the fastest except for the simplest methods.

![](_page_30_Figure_3.jpeg)

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![](_page_31_Picture_0.jpeg)

## Roadmap

- Part 1. Static Structural Patterns
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  - Advanced Patterns

## Part 2. Dynamic Structural Patterns

- Basic Patterns
- Advanced Patterns

## Part 3. Generative Models

- Static Hypergraph Generator
- Dynamic Hypergraph Generator <</li>

![](_page_31_Picture_11.jpeg)

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![](_page_32_Picture_0.jpeg)

# Part 3-2. Dynamic Hypergraph Generative Models

Part 3. df Generative Models

Ð	Static Models	Full-Hypergraphs	C20, LCS21
		Sub-Hypergraphs	CYLBKS22
	Dynamic Models	Full-Hypergraphs	DYHS20, KKS20, KBCYS23, GLLB23
		Sub-Hypergraphs	BKT18, CK21

![](_page_33_Picture_0.jpeg)

## **DYHS20: Dynamic Full-Hypergraph Generator**

• G1. HyperPA: <u>Hyper</u>graph <u>P</u>referential <u>A</u>ttachment

![](_page_33_Picture_3.jpeg)

M. T. Do, S. Yoon, B. Hooi, K. Shin, "Structural Patterns and Generative Models of Real-world Hypergraphs", **KDD 2020** 

## **HyperPA: Preferential Attachment**

- Inspired by the PA model for pairwise graphs [AA02]
  - Preferential attachment or "the rich get richer"
- Main idea: "Subsets get rich together"

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• Groups of nodes appear with **probability**  $\propto$  **"group degrees**."

M. T. Do, S. Yoon, B. Hooi, K. Shin, "Structural Patterns and Generative Models of Real-world Hypergraphs", **KDD 2020** 

![](_page_35_Picture_0.jpeg)

## HyperPA: Preferential Attachment (cont.)

### **Hyperedge Generation**

![](_page_35_Figure_3.jpeg)

### **Group Degrees**

M. T. Do, S. Yoon, B. Hooi, K. Shin, "Structural Patterns and Generative Models of Real-world Hypergraphs", **KDD 2020**


## HyperPA: Preferential Attachment (cont.)

#### **Hyperedge Generation**







#### **Group Degrees**

M. T. Do, S. Yoon, B. Hooi, K. Shin, "Structural Patterns and Generative Models of Real-world Hypergraphs", **KDD 2020** 



## HyperPA: Preferential Attachment (cont.)

#### **Hyperedge Generation**



M. T. Do, S. Yoon, B. Hooi, K. Shin, "Structural Patterns and Generative Models of Real-world Hypergraphs", **KDD 2020** 

## HyperPA: Evaluation (cont.)

- HyperPA generates realistic higher-order structures.
  - HyperPA considers "group degrees."

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• NaivePA (baseline) considers node degrees individually.



Degree distributions of the triangle-level decomposed graphs

M. T. Do, S. Yoon, B. Hooi, K. Shin, "Structural Patterns and Generative Models of Real-world Hypergraphs", **KDD 2020** 

## **KKS20: Dynamic Full-Hypergraph Generator**

• **G1.** HyperFF: <u>Hyper</u>graph <u>Forest</u> <u>Fire</u>



Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 

## **HyperFF: Motivation**

• Inspired by the forest fire model for pairwise graphs [LKF05]



Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 

# HyperFF: (Step 1) Hyperedge Formation

- For a new node, HyperFF simulates a forest fire from an ambassador.
- The forest fire is spread through hyperedges.

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• The new nodes forms a size-2 hyperedge with each burned node.



Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 

# HyperFF: (Step 2) Expansion

• Each size-2 hyperedge is expanded again through a forest fire.



Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 

## **HyperFF: Evaluation**

• HyperFF reproduces static structural patterns in real hypergraphs.



Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 

# HyperFF: Evaluation (cont.)

• HyperFF reproduces static structural patterns in real hypergraphs.



Intersection size distribution

Singular value distribution

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Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 

## HyperFF: Evaluation (cont.)

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• HyperFF reproduces dynamic structural patterns in real hypergraphs.



**Diminishing overlaps** 

Increasing edge density

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Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 

# HyperFF: Evaluation (cont.)

• HyperFF reproduces dynamic structural patterns in real hypergraphs.



**Shrinking diameter** 

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Y. Kook, J. Ko, K. Shin, "Evolution of Real-world Hypergraphs: Patterns and Models without Oracles", **ICDM 2020** 





# How Can HyperFF be Realistic?

- By simplifying HyperFF, several properties can be "proven."
  - Heavy-tailed degree distribution
  - Densification



Simplified HyperFF: nodes are burned with prob.

depending on the distance in a hierarchy tree

J. Ko, Y. Kook, K. Shin, "Growth patterns and models of real-world hypergraphs", **Knowledge and Information Systems (2022)** 



### **KBCYS23: Dynamic Full-Hypergraph Generator**

- G1. Naïve THera: Preliminary Version
- **G2.** THera: <u>Transitive</u> <u>Hypergraph</u> Gen<u>era</u>tor



## **Recap: Transitivity of Hypergraphs**

• Real-world hypergraphs exhibit transitivity.

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• The level of transitivity introduced by HyperPA and HyperPA often deviates much from that in real-world hypergraphs.





## **Naïve-THera: Preliminary Version**

- Naïve-THera assigns each node to a community and generates intra-community hyperedges.
- The level of transitivity can be controlled by the size of communities.



# Naïve-THera: Preliminary Version (cont.)

- However, Naïve-THera generates unrealistic hypergraphs:
  - Near-uniform node degree distribution

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Divided and disconnected hypergraphs



1.0 b 0.5 0.5 0.0 Beal-world THera Naïve-THera 50 Node Degree



#### **THera: Transitivity-Preserving Generator**

• **THera** generates two types of hyperedges:

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- Intra-community edges consist of nodes within the same community.
- Hierarchical edges consist of nodes from different communities.
- Hierarchical edges address disconnectivity by bridging communities.

Intra-community edge

## **THera: Transitivity-Preserving Generator (cont.)**

- Hierarchical edges lead to a skewed node degree distribution.
  - Tree-like hierarchy of nodes is assumed.

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• Each node appears in edges with priority based on the level it belongs to.



### **THera: Transitivity-Preserving Generator (cont.)**

• The number of levels in hierarchy grows over time.

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• This growth models the growth of real-world hypergraphs.



#### **THera: Evaluation**

• THera reproduces a realistic level of transitivity while addressing

the obvious limitations of Naïve-THera.

	Generator	email		NDC		contact		coauthorship			q&a		
		enron	eu	classes	substances	high	primary	dblp	geology	history	ubuntu	server	math
-	Real World	0.195	0.125	0.052	0.019	0.345	0.336	0.007	0.005	0.002	0.005	0.005	0.025
	THERA	0.192	0.124	0.052	0.019	0.344	0.334	0.007	0.005	0.002	0.004	0.004	0.025
Г	HyperCL [33]	0.078	0.053	0.008	0.005	0.119	0.223	0.000*	$0.000^{*}$	0.000*	0.014	0.017	0.040
	HyperPA [16]	0.090	0.110	0.070	-	0.121	0.153	-	-	-	0.003	-	-
$\left\{ \right\}$	HyperFF [30]	0.176	0.125	0.006	0.003	0.006	0.007	0.047	0.048	0.048	0.051	0.050	0.054
	HyperLap [33]	0.123	0.085	0.008	0.008	0.220	0.301	0.001	$0.000^{*}$	$0.000^{*}$	0.016	0.015	0.004
	HyperLap+ [33]	0.231	0.144	0.026	0.016	0.322	0.338	0.042	0.019	0.005	0.029	0.023	0.007

#### Hypergraph Transitivity

#### competitors



### **GLLB23: Dynamic Full Hypergraph Generator**

- G1. Discrete Auto Regressive Hypergraph (DARH) model
- G2. Cross-memory DARH (cDARH) model



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### **Reproduction of Temporal Dynamics**



**Question:** Given a set of hyperedges, how can we produce a realistic **sequence of hypergraph snapshots** over time?



Answer: Exploit intra-order and cross-order correlations in real-world hypergraphs!

L. Gallo, L. Lacasa, V. Latora, and F. Battiston, "Higher-order Correlations Reveal Complex Memory in Temporal Hypergraphs", **arXiv (2023)** 

## **Recap: Empirical Observations**

• Intra-order correlations: Temporal correlations emerge between hyperedges of the same sizes.



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Real-world	Random
Size 2 hyperedges	Size 2 hyperedges
🛑 Size 3 hyperedges	Size 3 hyperedges
Size 4 hyperedges	Size 4 hyperedges
Size 5 hyperedges	Size 5 hyperedges

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## **Recap: Empirical Observations (cont.)**

• Cross-order correlations: Temporal correlations emerge between hyperedges of different sizes.



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## **Discrete Auto Regressive Hypergraph**

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- In **Discrete Auto Regressive Hypergraph** (**DARH**), each hyperedge evolves based on an independent stochastic process.
- At each time *t*, it determines whether each hyperedge occurs or not.



L. Gallo, L. Lacasa, V. Latora, and F. Battiston, "Higher-order Correlations Reveal Complex Memory in Temporal Hypergraphs", **arXiv (2023)** 

## **Discrete Auto Regressive Hypergraph (cont.)**

- Step 1. Determine the criterion of the hyperedge's occurrence
- Step 2. Sample from the past occurrences of the hyperedge

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Step 2

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## **Cross-memory DARH (cDARH) model**

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• cDARH samples an occurrence also from the occurrences of supersets & subsets to model cross-order correlations.



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## Cross-memory DARH (cDARH) model (cont.)

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• cDARH reproduces intra-order temporal correlations of hyperedges.



## Cross-memory DARH (cDARH) model (cont.)

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• cDARH reproduces cross-order temporal correlations of hyperedges.



## **BKT18: Dynamic Sub-Hypergraph Generator**

• G1. Correlated Repeated Unions (CRU) model



### **Next Hyperedge Prediction**

**Question:** 

Given a (sub-)sequence of temporal hyperedges, how can we predict the **next hyperedge**?

#### **Answer**:

The CRU model predicts the next hyperedge based on three empirical observations: (1) repeat behavior, (2) subset correlation, and (3) recency bias.





#### **Recap: Three Empirical Observations**

#### **Repeat Behavior**

Temporal hyperedges tend to **repeat** previous ones.

#### **Subset Correlation**

Subsets of nodes tend to be **correlated**.

#### **Recency Bias**

Temporal hyperedges tend to be similar to recent ones.



### **CRU: Correlated Repeated Unions (cont.)**

#### **Step 0. Initialization**



Recer	Recency weight vector w							
0.08	0.15	0.29	0.48					
t-4	t-3	t-2	t-1					
Correlation probability $p = 0.80$								

Two parameters of CRU

## **CRU: Correlated Repeated Unions (cont.)**

#### **Step 1. Sample an existing hyperedge**

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### **CRU: Correlated Repeated Unions (cont.)**

**Step 2. Sample nodes** 

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Intuition: p controls the subset correlation. A larger  $p \rightarrow$  More correlation in selecting items from the same hyperedge



#### **CRU: Trained Parameters**

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- Correlation probability p and recency weight vector w are trained
- Recency bias and subset correlation are observed




# **CK21: Dynamic Sub-Hypergraph Generator**

- G1. Temporal order prediction model
- G2. Temporal reconstruction model



C. Comrie, J. Kleinberg, "Hypergraph Ego-networks and Their Temporal Evolution", ICDM 2021

# **Task 1: Temporal Order Prediction**

#### **Question:**

Has the given dynamic ego-network evolved reasonably?

#### **Answer:**

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- A supervised **binary classification** task is defined.
- Are the hyperedges in a given dynamic ego-network correctly or randomly ordered?





#### **Recap: Four Empirical Observations**

#### **Intersection Size of Ego-networks**

Temporally adjacent hyperedges in ego-networks are similar.

#### **Spread of Alter-networks**

Spread of alter-networks are temporally local.

#### Anthropic Principle of Ego-networks

The arrival of ego-nodes occurs after pre-dated hyperedges.

#### **Novelty of Ego-networks**

Novelty decreases in ego-networks.

# **Temporal Order Prediction (cont.)**

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- We extract six features based on the patterns to train a classifier.
- Compared to random guessing (baseline), the trained classifier significantly outperforms on all datasets and ego-network types.

	Star ego-network		Radial ego-network		Contracted ego-network	
	Random	Proposed	Random	Proposed	Random	Proposed
coauth-DBLP	0.50	0.93 ± 0.01	0.50	0.91 ± 0.01	0.50	0.85 ± 0.01
email-Avocado	0.50	<b>0.84</b> ± <b>0.09</b>	-	Omittad dua	to their oir	-
threads-ask-ubuntu	0.50	$\textbf{0.72} \pm \textbf{0.05}$	-			-

#### **Classification accuracy**

C. Comrie, J. Kleinberg, "Hypergraph Ego-networks and Their Temporal Evolution", ICDM 2021

### **Task 2: Temporal Reconstruction**

Question: How can we properly reconstruct the temporal order of hyperedges in the given ego-network?

#### **Answer:**

A local search algorithm is used to iteratively update the temporal order



#### **Step 1. Swap pairs**





All possible swaps



Step 2. Predict the order based on Fitness ( $\mathcal{M}$ : Model for Task 1)





#### **Step 3. Multiple trials**



#### Best orders from each trial

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• The proposed algorithm shows a **non-trivial improvement** over random guessing (baseline).

	Star ego-network		Radial ego-network		Contracted ego-network	
	Random	Proposed	Random	Proposed	Random	Proposed
coauth-DBLP	0.50	0.65 ± 0.08	0.50	0.56 ± 0.05	0.50	<b>0.65</b> ± <b>0.08</b>
email-Avocado	0.50	0.63 ± 0.11	-		to the in sim	-
threads-ask-ubuntu	0.50	<b>0.70</b> ± <b>0.07</b>	-	Omitted due	to their siz	.es -

Reconstruction accuracy, i.e., the ratio of corrected predicted pairs of hyperedges

### Part 3. Hypergraph Generative Models



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### Conclusions

- Hypergraph modeling of group interactions
  - Provides a new perspective ("set of sets")
  - Reveals new structural patterns that are previously overlooked
- Hypergraph mining tools and measures
  - Many tools (e.g., hypergraph motifs) and measures are available
- Hypergraph generative models
  - Shed a light on why the patterns occur
  - Applications: statistical testing, anonymization, benchmark data generation

### **Future Research Directions**

- Mining of directed hypergraphs (e.g., chemical reactions)
  - How do real-world directed hypergraphs look and evolve time?
- Hypergraph representation learning
  - How can we embed hyperedges while preserving their structural properties?
- Anomaly detection

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• How can we identify abnormal group interactions?

### **Tutorial Materials**

- https://sites.google.com/view/hypergraph-tutorial
  - Slides 🔑 📴
  - Videos 🕟
  - Code and Datasets

#### References

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#### Mining of Real-world Hypergraphs: Concepts, Patterns, and Generators



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