CCS + 2023 +

COMPLEX SYSTEMS SOCIETY

# Deriving Dynamical Model Equations from Temporal Network Data Using a Graph Rewriting Framework


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# WARNING

- **This is a very, very preliminary progress report** of a newly funded project:

科研費 KAKENHI

JSPS KAKENHI Grant # 23H03414: Automatic derivation of dynamical models from temporal network data using a graph rewriting system

  - Algorithms and software still under initial development
  - Feedback most welcomed!!

# Motivation

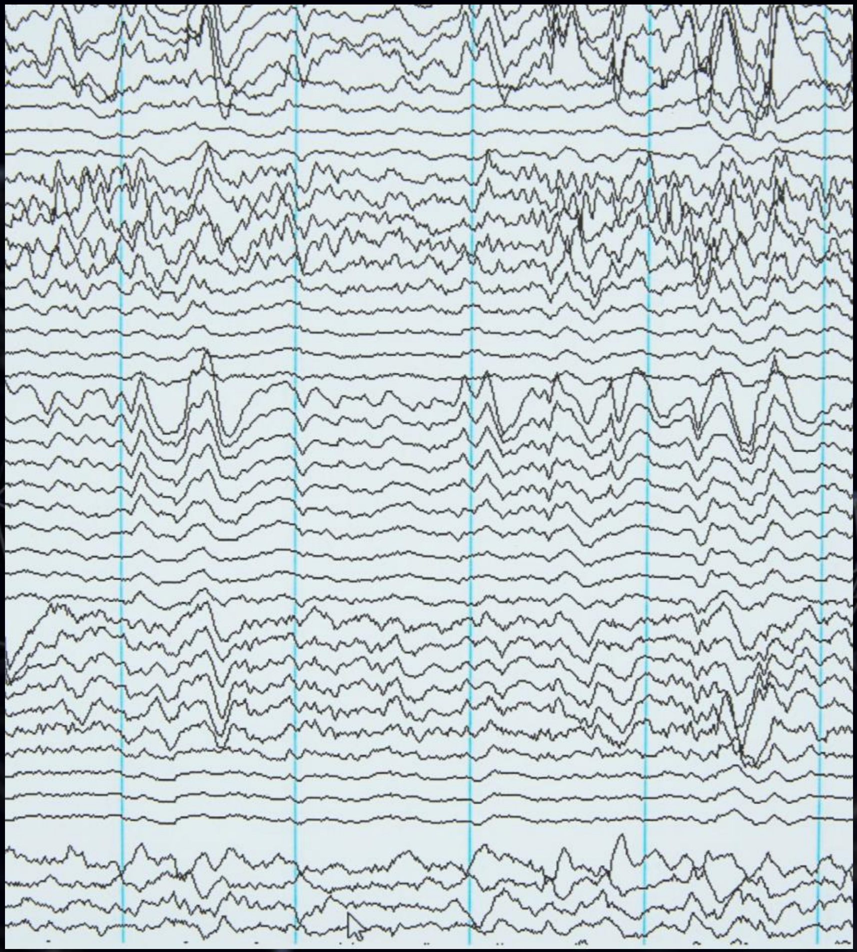
**Pattern Discovery**

**vs.**

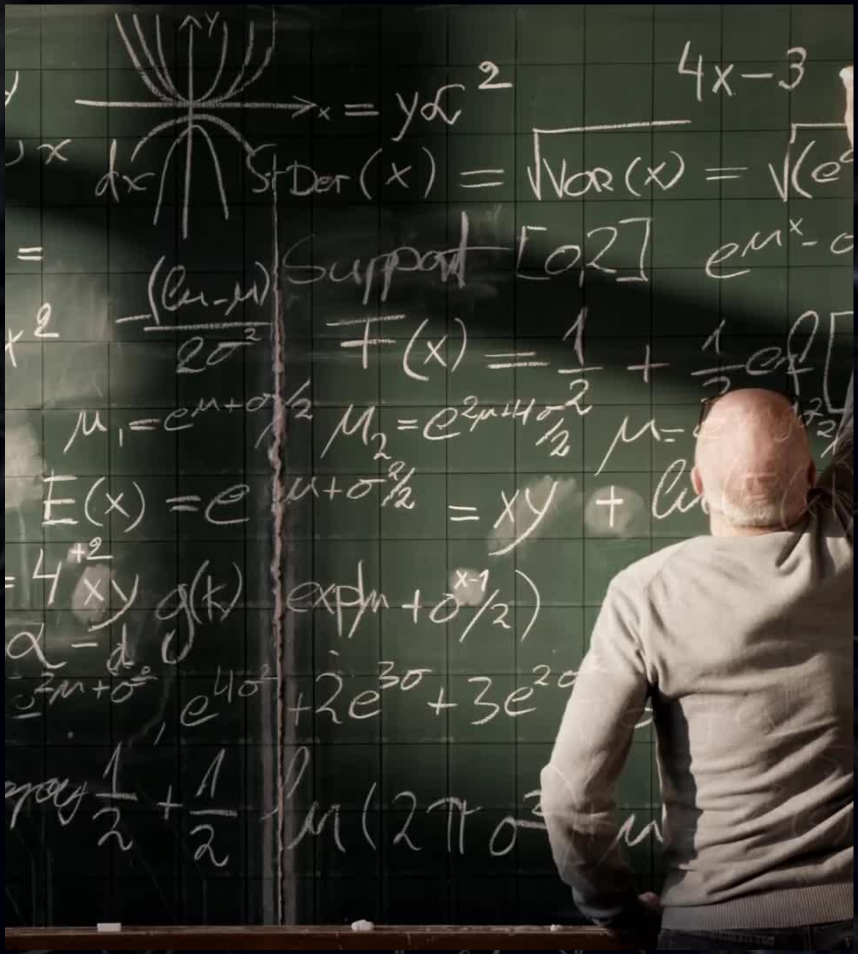
**Mechanistic Modeling**

# Pattern Discovery (Descriptive Modeling)

- Identifying and summarizing patterns in the data
  - Descriptive statistics
  - Machine learning, data science, AI
  - Classification, prediction, clustering

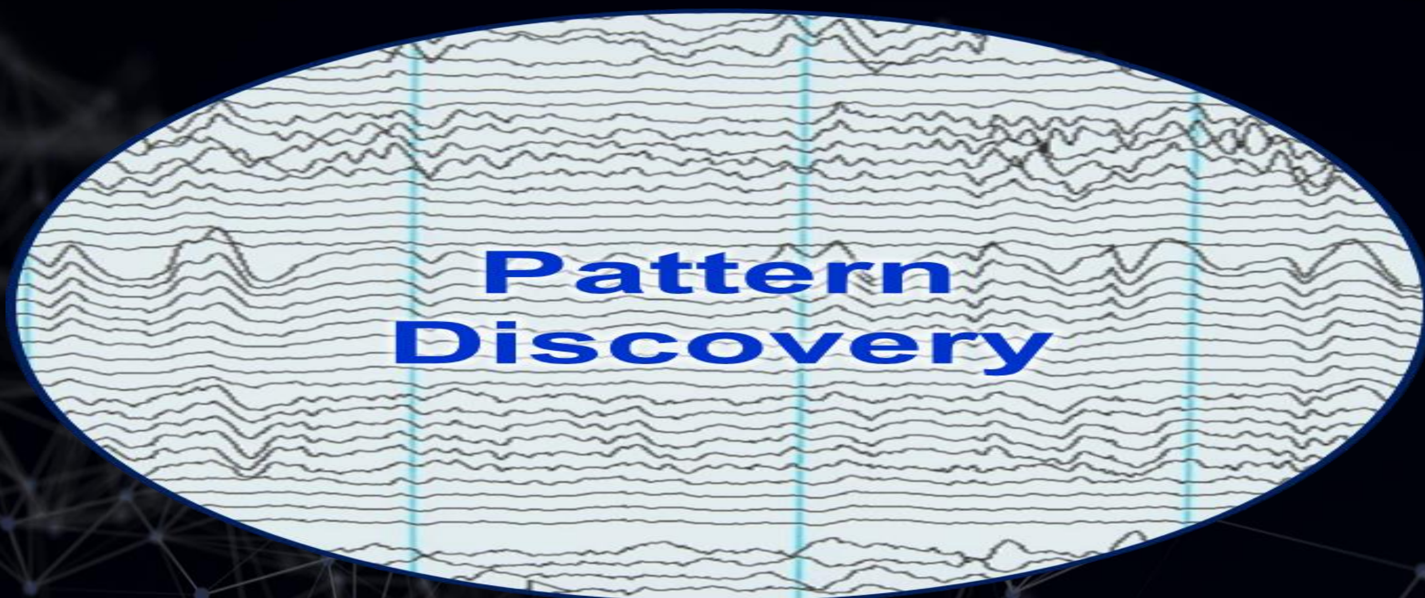


# Mechanistic Modeling (Rule-Based Modeling)



- Explaining the hidden mechanisms and rules that may have produced the observed patterns
  - Theories, principles, dynamical equations, simulations
  - Can provide deeper understanding and insight
  - "System identification"

# Current State of DS/ML/AI





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# We Want Balance and Integration


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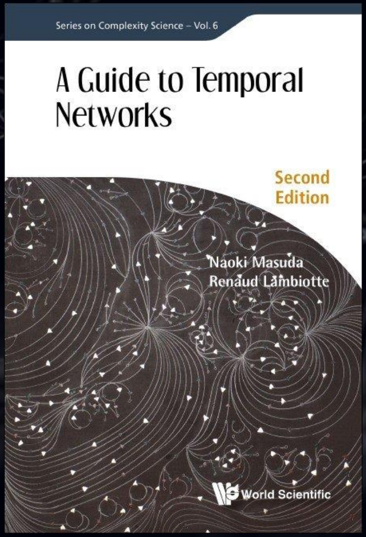
# Specific Application Domain: Temporal Networks

- Complex networks whose topologies change over time
  - Network analysis extended to time-varying network data
  - Relevant to epidemic modeling and social media analysis
  - Mostly descriptive on topological changes only (i.e., no dynamics)





Holme, P., & Saramäki, J. (2012). *Physics Reports*, *519*(3), 97-125.
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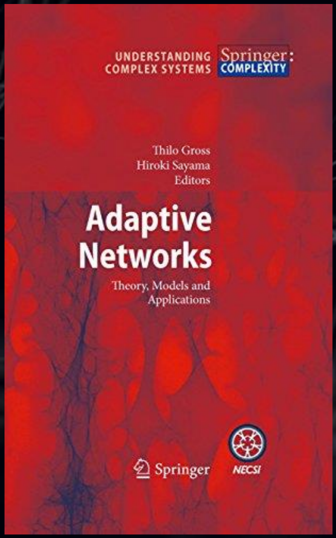
# Dynamical Systems Counterpart: Adaptive Networks

- Complex networks whose states and topologies co-evolve, often over similar time scales
  - Node states adaptively change according to link states
  - Link states (weights, connections) adaptively change according to node states




Gross, T., & Sayama, H. (2009). *Adaptive Networks.* Springer.
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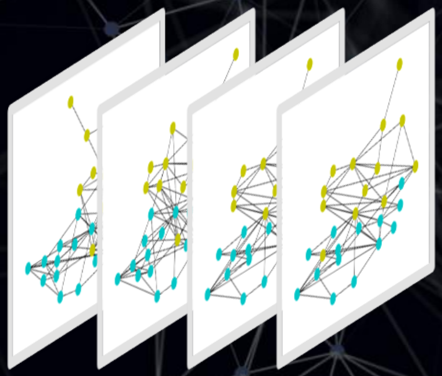
# Research Objective

- To develop a novel modeling method that can derive dynamical model equations of temporal network behaviors directly from real-world temporal network data
  - Toward understanding of "how" and "why"



$$\frac{d}{dt}x = F(x)$$



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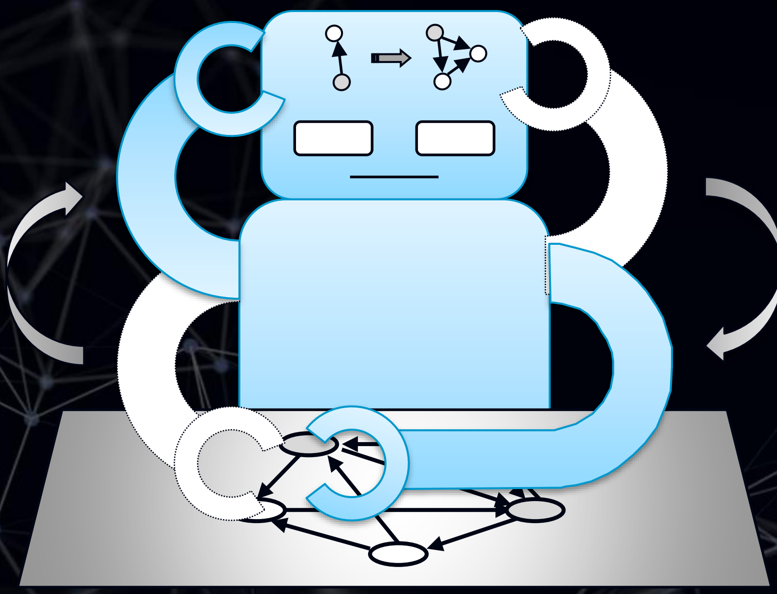
# Basic Approach: Graph Rewriting

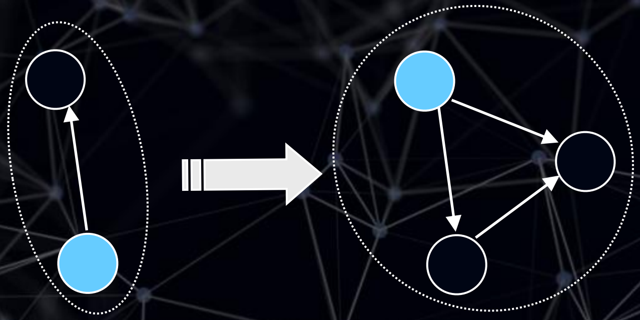
- Temporal network dynamics represented by extraction and replacement of (labeled) subgraphs
  - Partly based on "Generative Network Automata"



Sayama, H. (2007). *Proc. 2007 IEEE SSCI/ALIFE* (pp. 214-221). IEEE.
Sayama, H., Pestov, I., Schmidt, J., Bush, B. J., Wong, C., Yamanoi, J., & Gross, T. (2013). *Comput. Math. with Appl.*, 65(10), 1645-1664.

# Modeling the Dynamics of Subgraph Densities

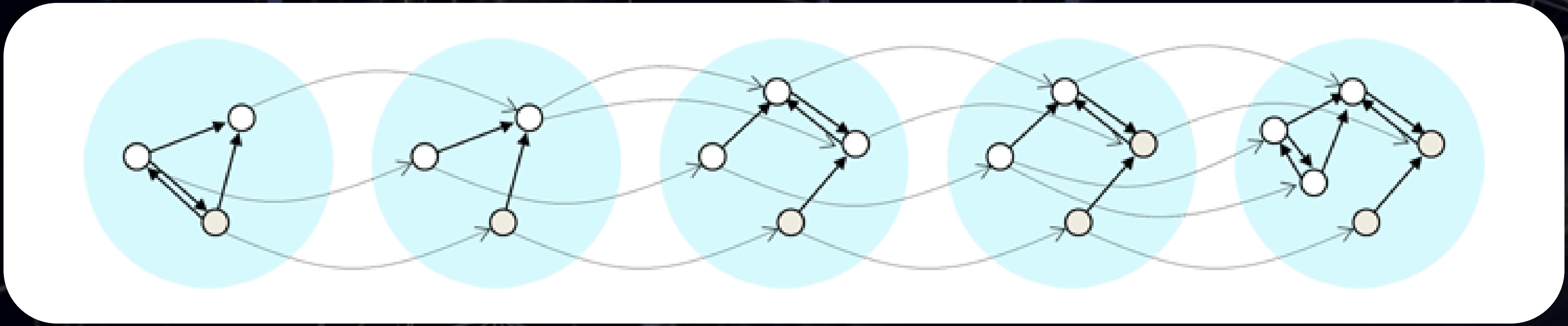
- Each rewriting "rule" removes subgraphs on the LHS and adds subgraphs on the RHS



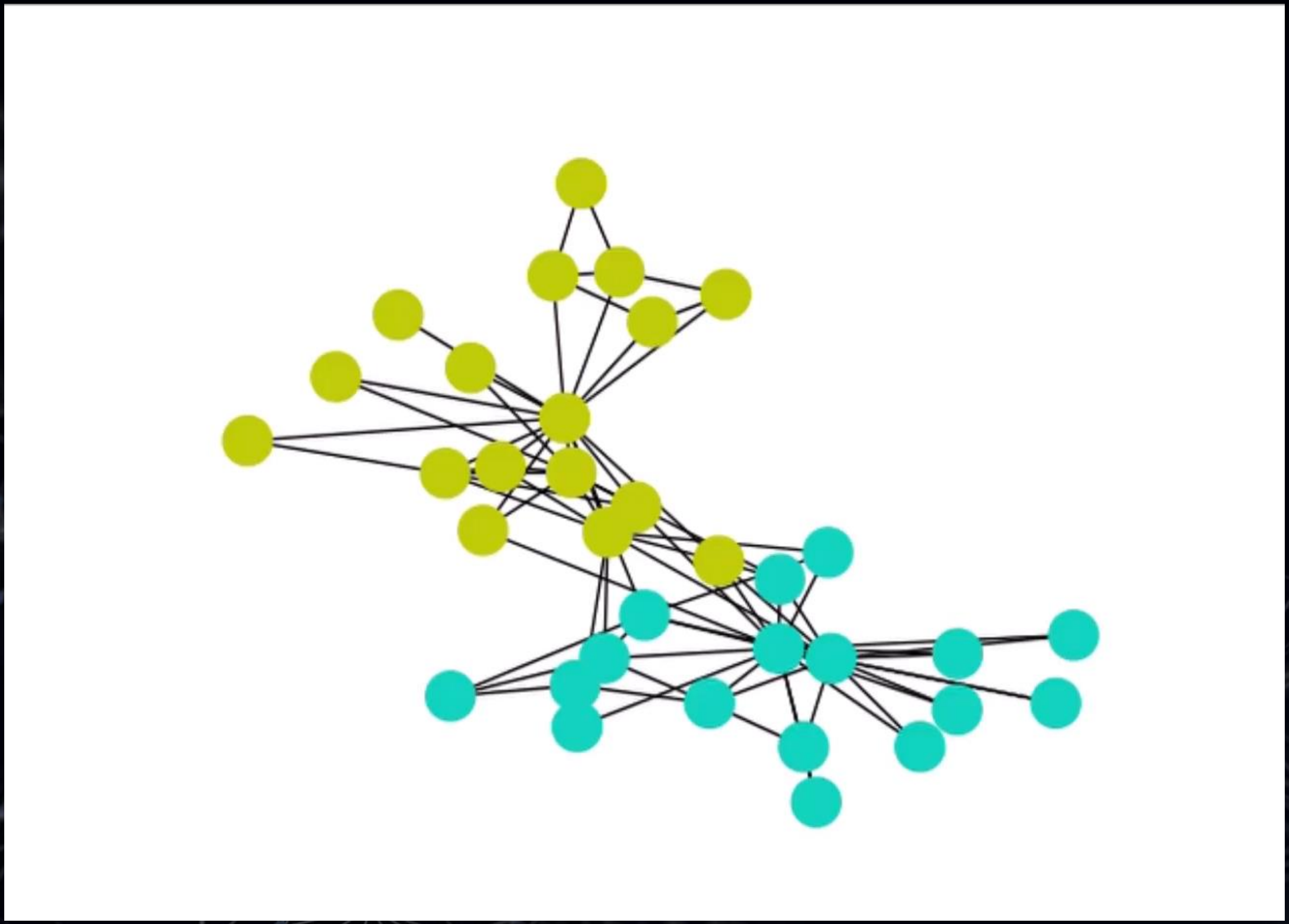
  - Subgraph rewriting events can be converted to a dynamical model of density changes of the involved subgraphs (and beyond)

# Assumptions

- Temporal network data are given in the form of a discrete-time sequence of (labeled) network configurations
- Correspondences of node identities are given between every consecutive pair of network configurations



# Testing with Synthetic Data: ZKC Evolution Model





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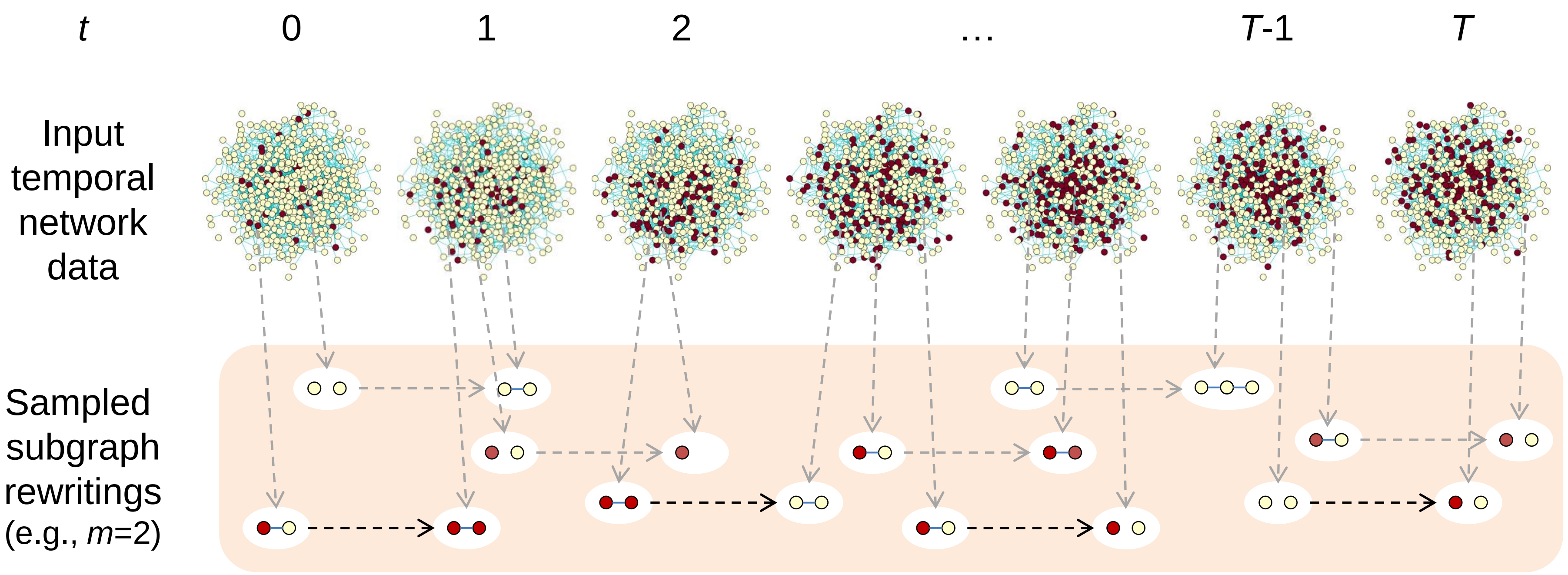
# Prototype Implementation in Python/NetworkX

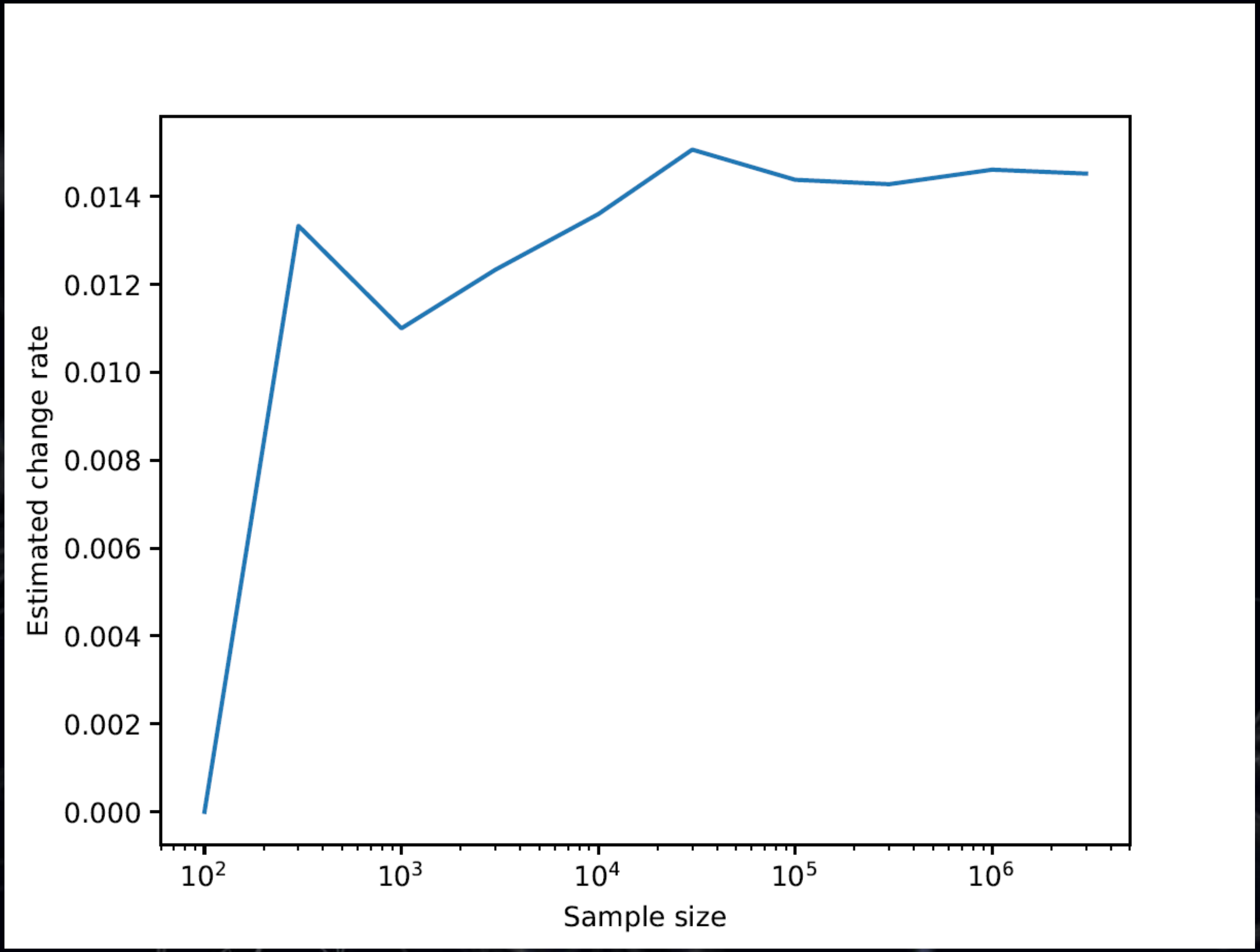
jupyter

NetworkX
Network Analysis in Python

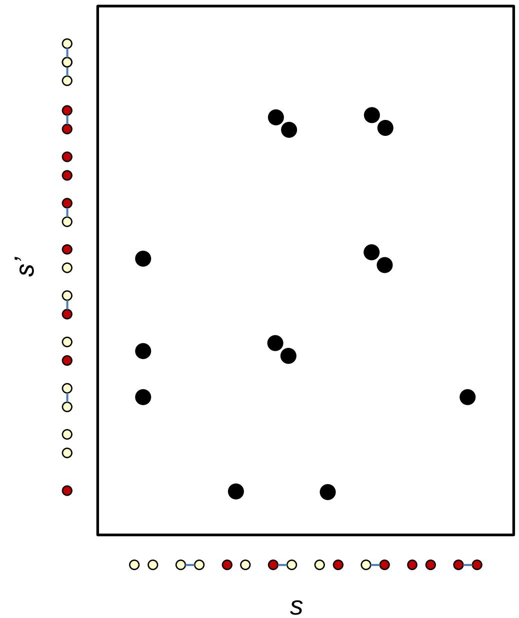
# Step 1: Sampling Subgraph Rewritings

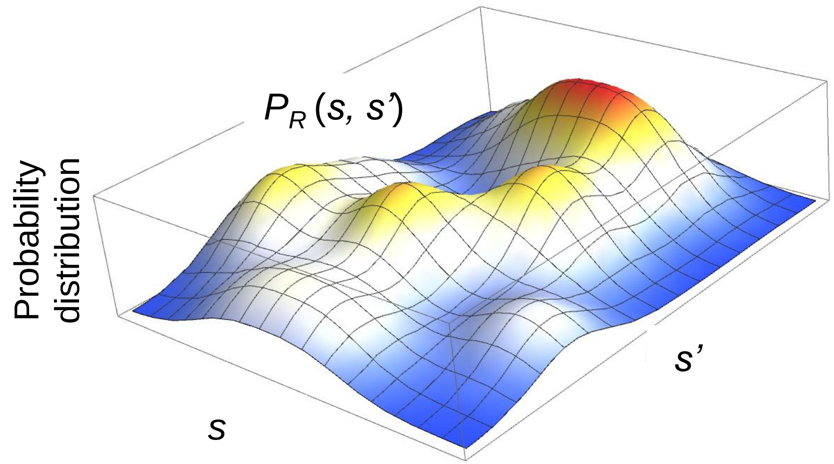


# Checking Convergence of Sampling



# Step 2: Representing Subgraph Rewriting Probability Density




* In this pilot study, the probability distributions were represented non-parametrically with the collected frequency data themselves

# Step 3: Constructing Dynamical Equations

$dx_i/dt = \sum_s \sum_r x_s P_R(r|s) * (\ r.\text{count(i)} - s.\text{count(i)}\ )$

$i$, $s$, $r$: subgraph types

$$\frac{d}{dt}x_0 = -0.0011976047904191 6x_0 + 0.000380372765310004x_1$$

$$\frac{d}{dt}x_1 = -0.00323316850513503x_1 + 6.5321052975374 \cdot 10^{-5}x_2$$

$$\frac{d}{dt}x_2 = 0.00133130467858501x_1 - 0.000348378949201994x_2 + 1.91308107446285 \cdot 10^{-6}x_3 + 0.00108108108108108x_7$$

$$\frac{d}{dt}x_3 = 0.000283057896226621x_2 - 0.000195134269595211x_3$$

$$\frac{d}{dt}x_4 = 0.00119760479041916x_0 - 0.00583373845405931x_4 + 0.000486854917234664x_5$$

$$\frac{d}{dt}x_5 = 0.00152149106124002x_1 + 0.000486144871171609x_4 - 0.00194741966893866x_5$$

$$\frac{d}{dt}x_6 = 0.00194457948468644x_4 - 0.00137835975189524x_6 + 0.00036036036036036x_7 + 0.00033838084764 4023x_8$$

$$\frac{d}{dt}x_7 = 0.00146056475170399x_5 - 0.00324324324324324x_7$$

$$\frac{d}{dt}x_8 = 0.00137835975189524x_6 - 0.000845952119110058x_8$$

$$\frac{d}{dt}x_9 = 0.000193221188520748x_3 + 0.0018018018018018x_7 + 0.000507571271466035x_8 - 0.000216826384485744x_9$$

$$\frac{d}{dt}x_{10} = -0.0139664804469274x_{10} + 0.00340301409820126x_4$$

$$\frac{d}{dt}x_{11} = 0.00418994413407821x_{10} - 0.0054249547920434x_{11} + 0.00120192307692308x_{14}$$

$$\frac{d}{dt}x_{12} = 1.28267617557271 \cdot 10^{-5}x_{15}$$

$$\frac{d}{dt}x_{13} = 0.00837988826815642x_{10}$$

$$\frac{d}{dt}x_{14} = 0.0054249547920434x_{11} - 0.00721153846153846x_{14}$$

$$\frac{d}{dt}x_{15} = 0.00600961538461538x_{14} - 0.000205228188091634x_{15} + 0.000216826384485744x_9$$

$$\frac{d}{dt}x_{16} = 0.00139664804469274x_{10}$$

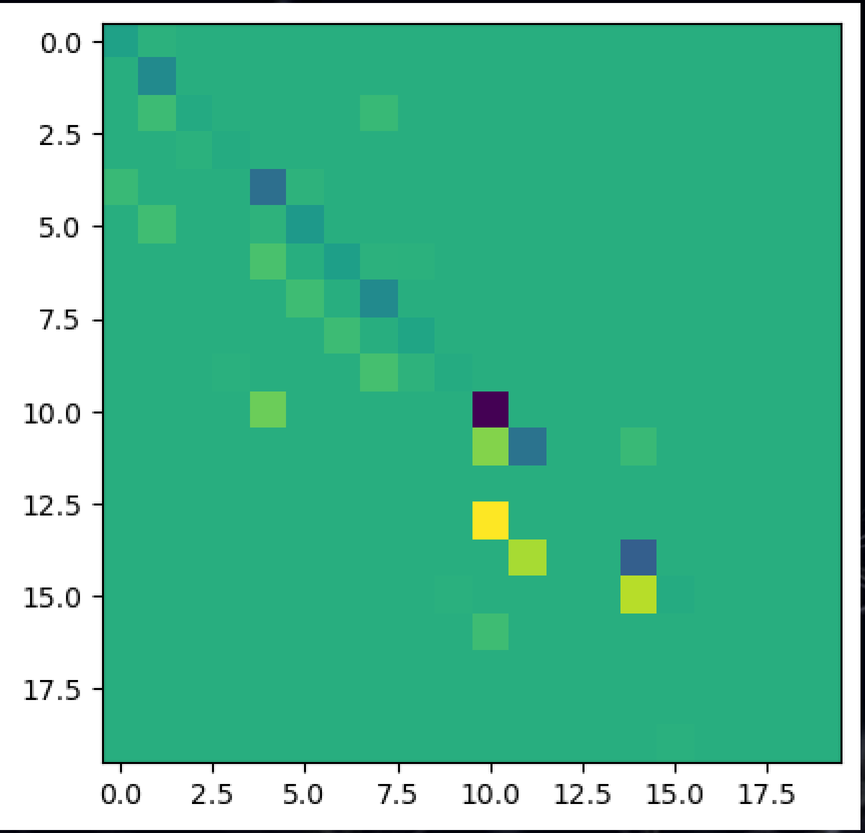
$$\frac{d}{dt}x_{17} = 0$$

$$\frac{d}{dt}x_{18} = 0$$

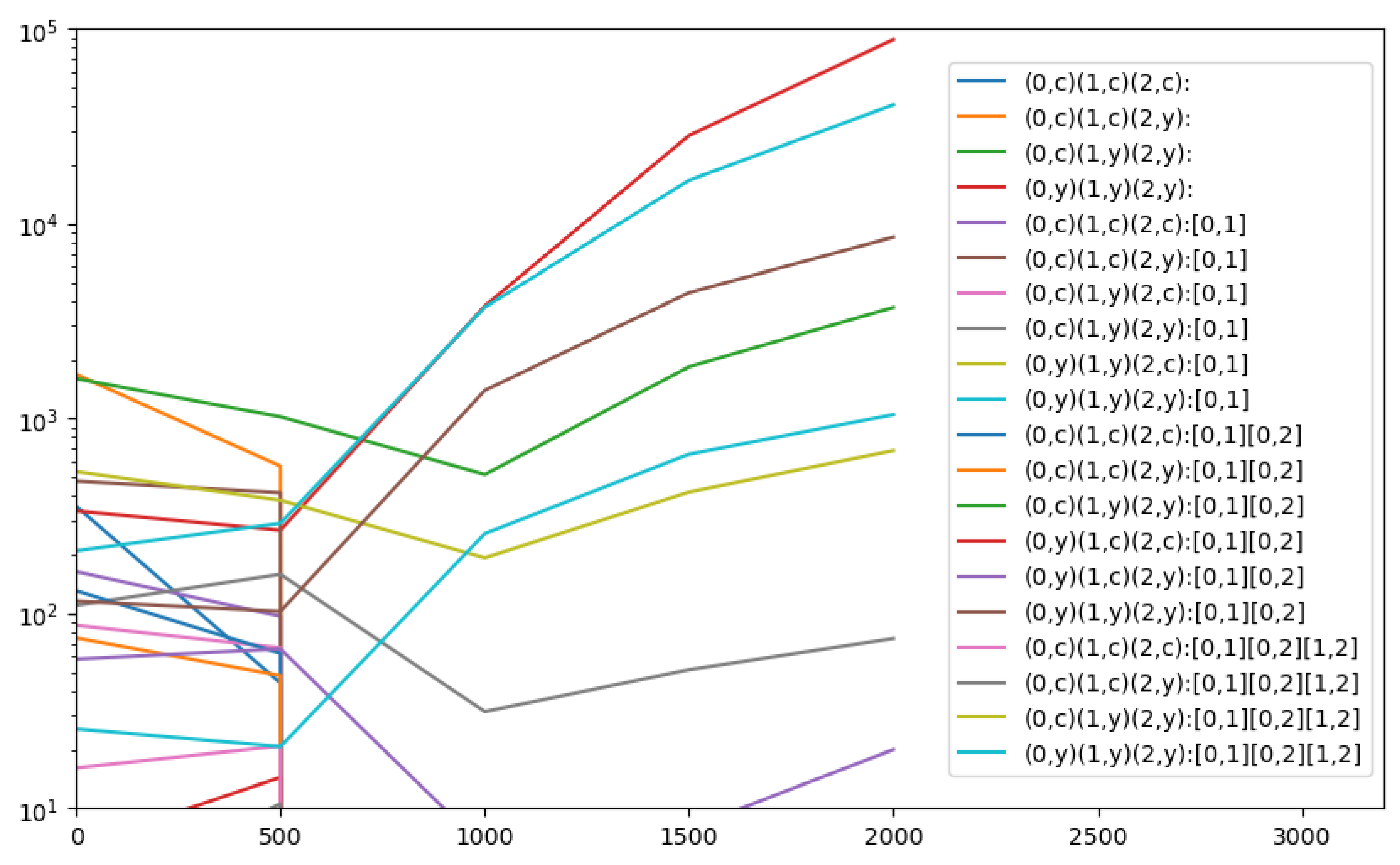
$$\frac{d}{dt}x_{19} = 0.000192401426335907x_{15}$$

# Then You Get a Linear System Model!!

$$\frac{d\vec{x}}{dt} = A\vec{x}$$



# Actual Subgraph Density Dynamics



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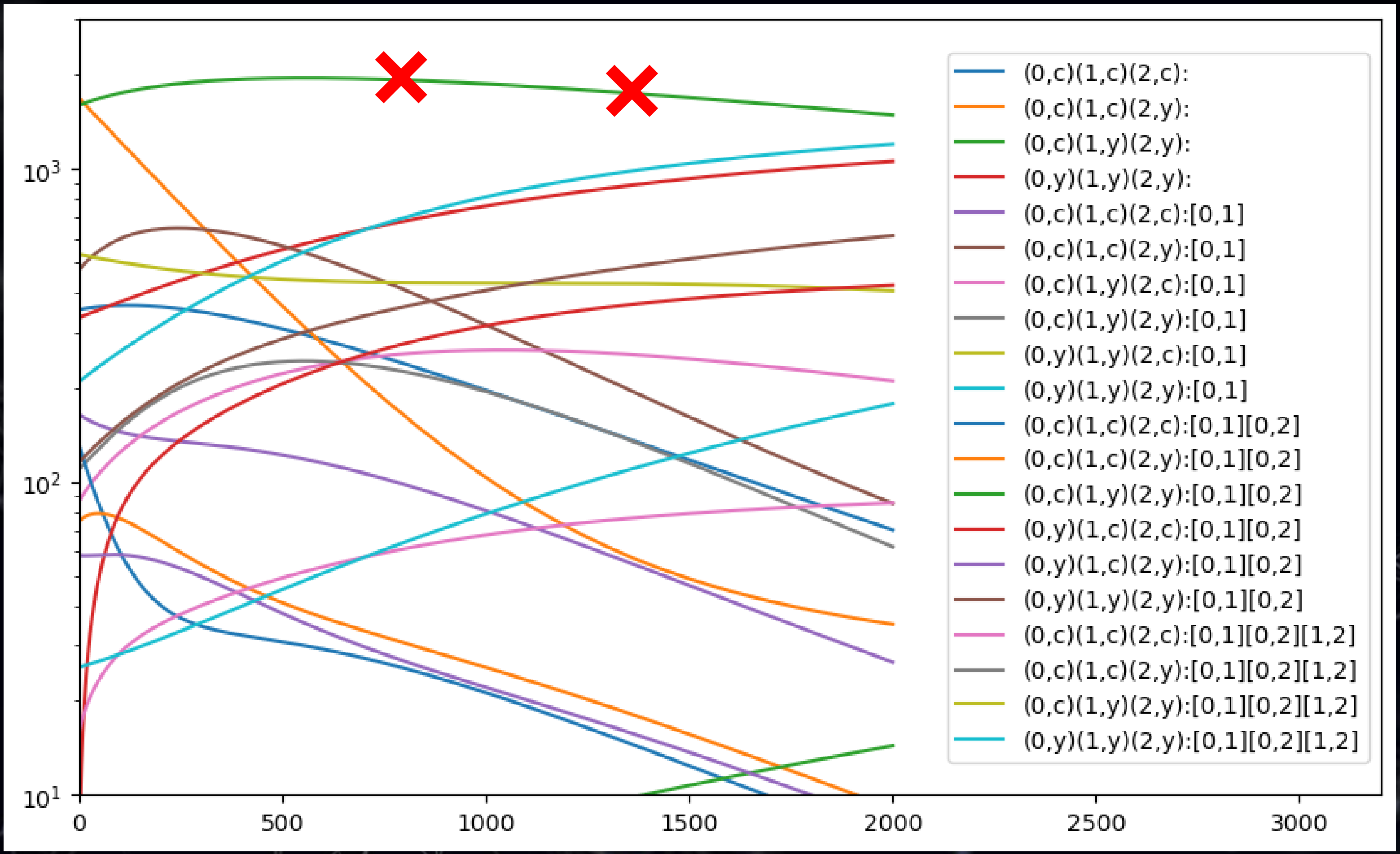
# Predicted Subgraph Density Dynamics



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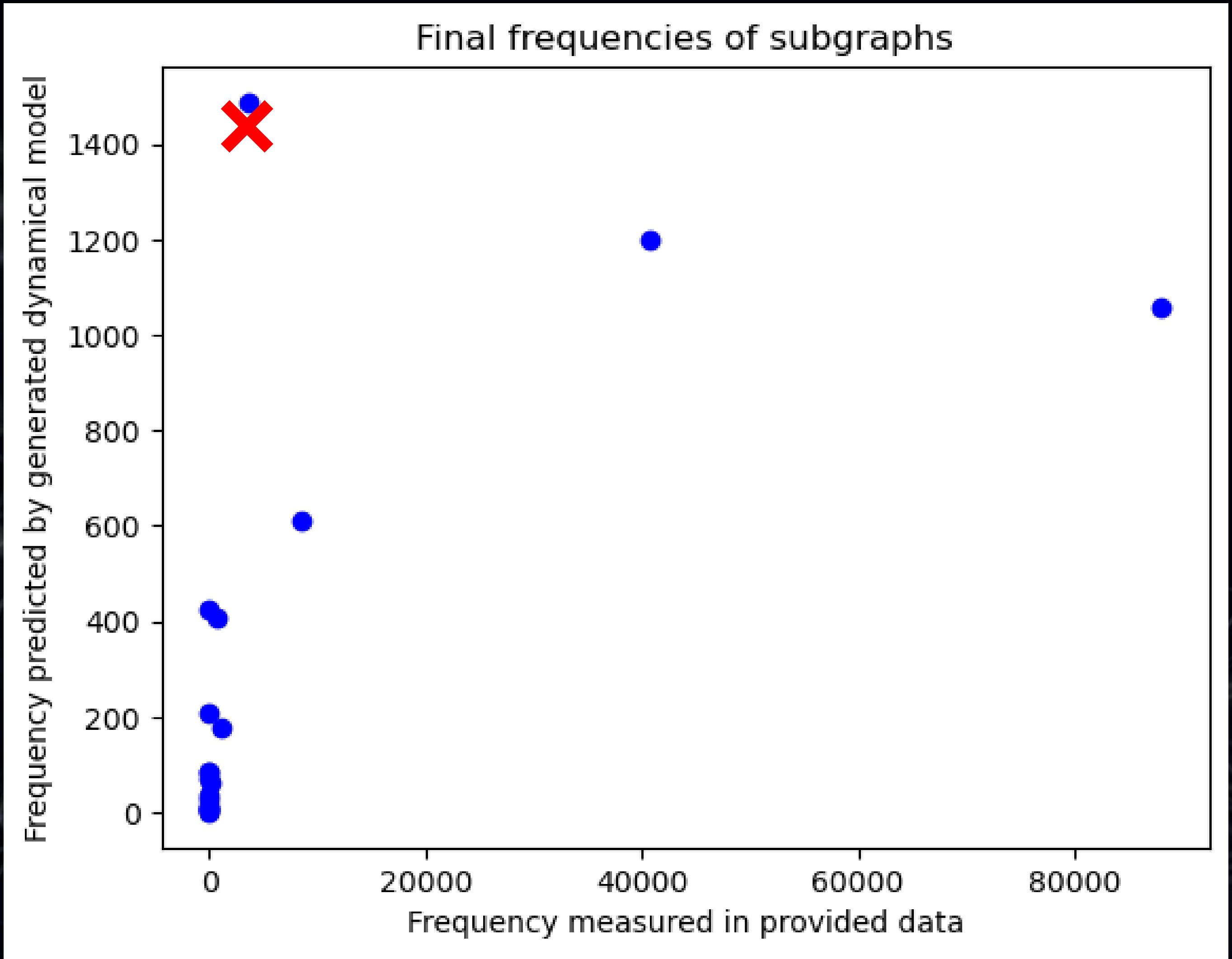
# Comparison



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# Summary

- Proposed a method to automatically derive mechanistic model equations of subgraph density dynamics from temporal network data
- Proof of concept with small synthetic data
- Algorithm and software still at initial development stage with inaccurate results

# Next Steps: So Many Things to Do!

- Addressing indirect (nonlinear) interactions among distant subgraphs and subgraphs with different sizes
  - With moment closure?
- Making sampling faster by adaptive sampling methods
- Improving graph isomorphism accuracy
  - Currently using only approximation
- Constructing smoother, parametric functions for rewriting probability distributions
- Testing with larger-scale real-world datasets

# Thank You

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  - JSPS KAKENHI Grant # 23H03414

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- Special thanks to contributors in earlier stages of this research:
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