Detecting Path Anomalies in Sequential Data on Networks

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This Talk

Motivation: Understanding mechanisms behind sequential data on networks

Today:

Motivate the study of **path anomalies**

Introduce **de Bruijn graph** representation of sequential data

Develop tractable **null model** to measure deviation of path data from expectation

Validate null model in synthetic data + compare with naïve baseline method

Application of methodology to a real system

Intuitive Example: Passenger Flight Data

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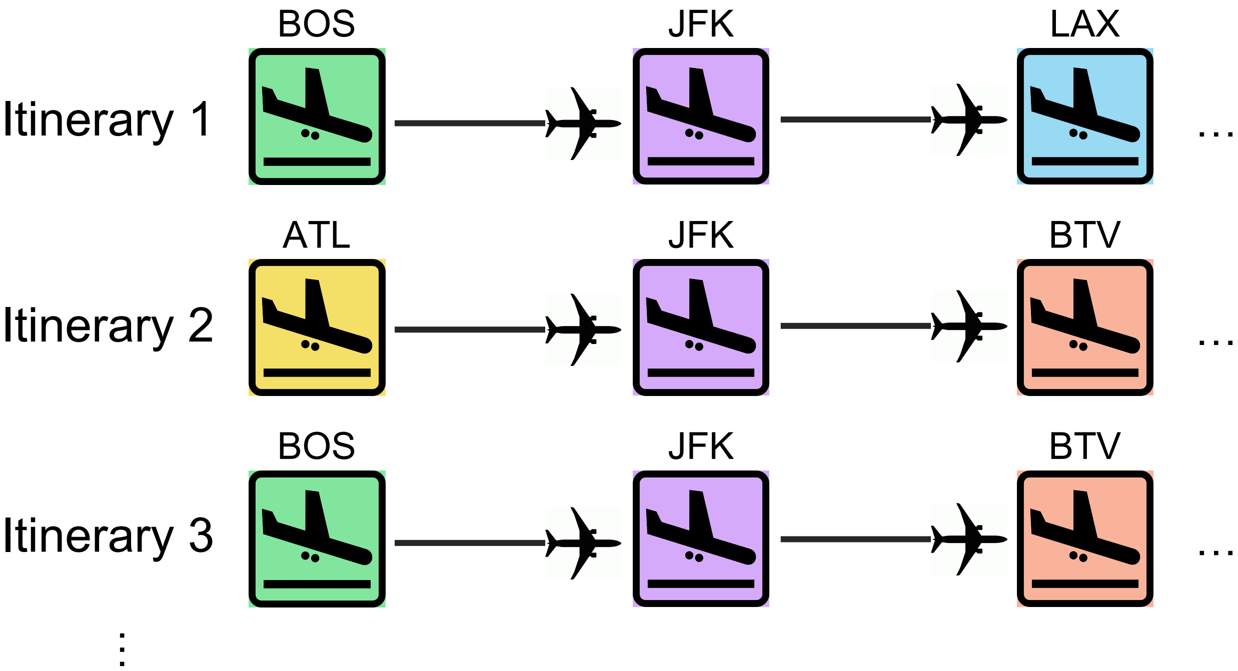
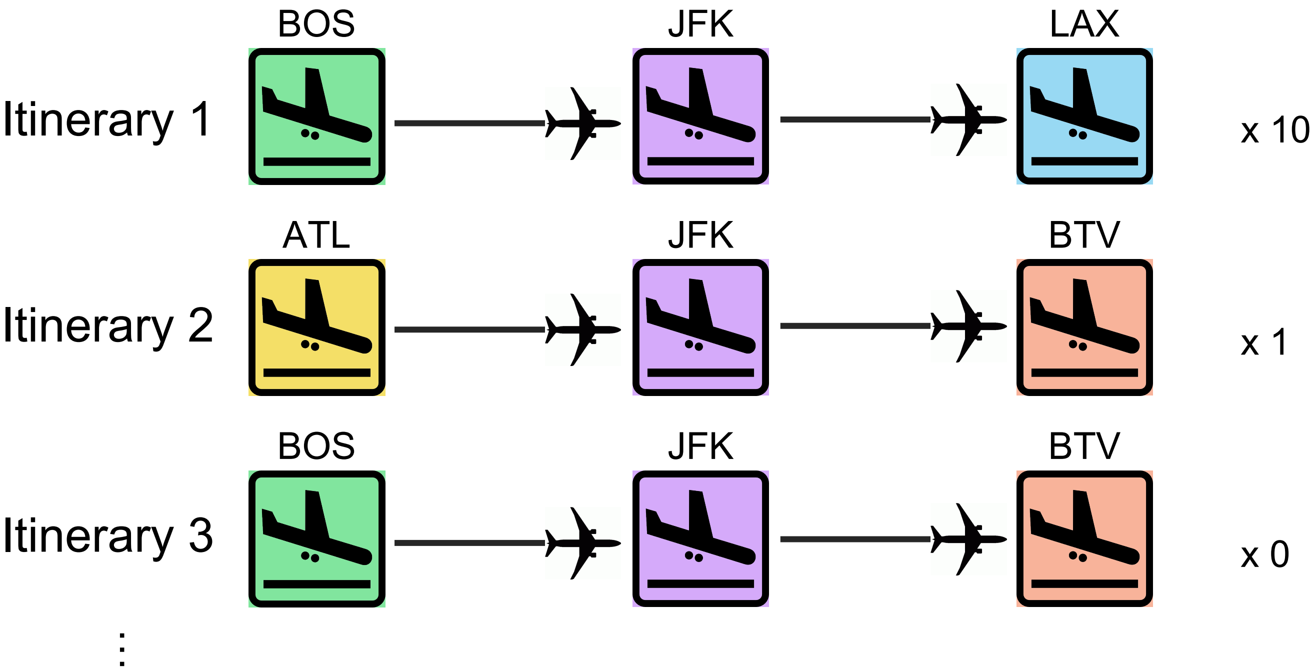


Intuitive Example: Passenger Flight Data



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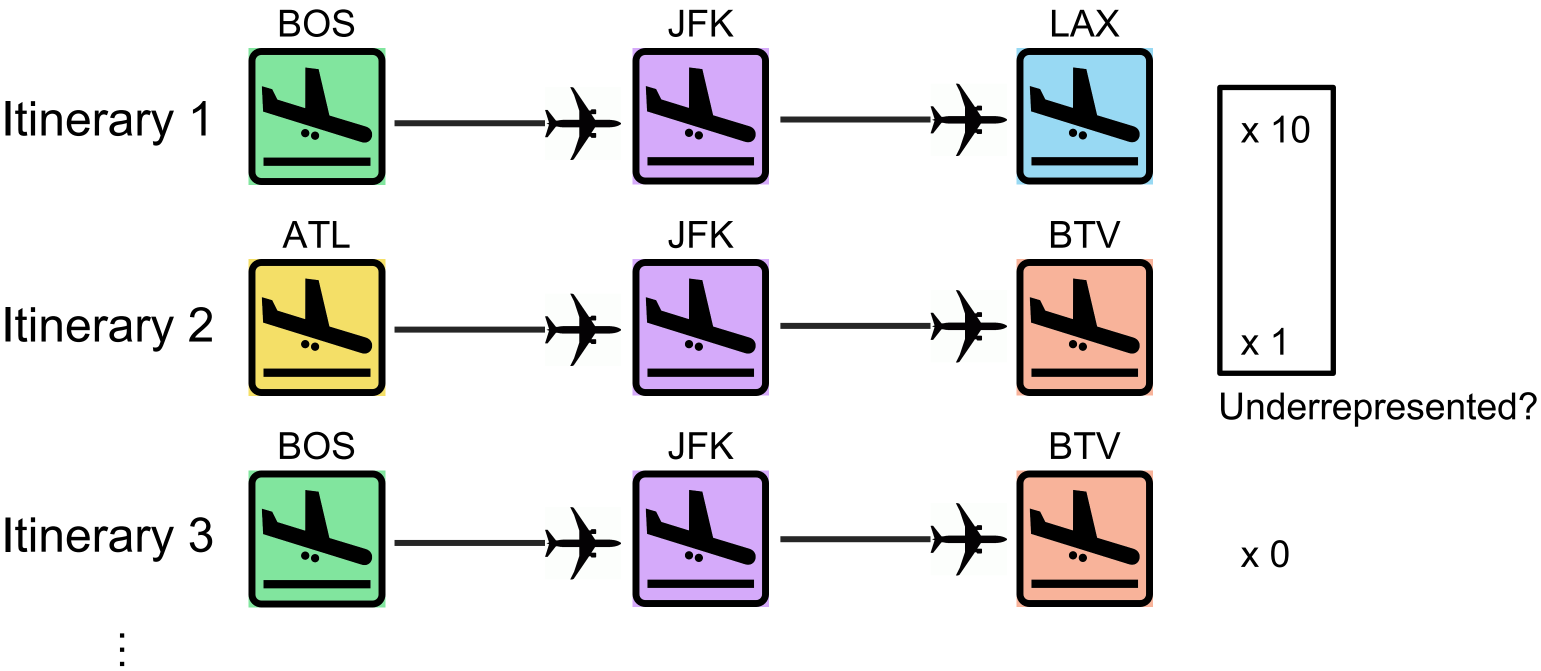

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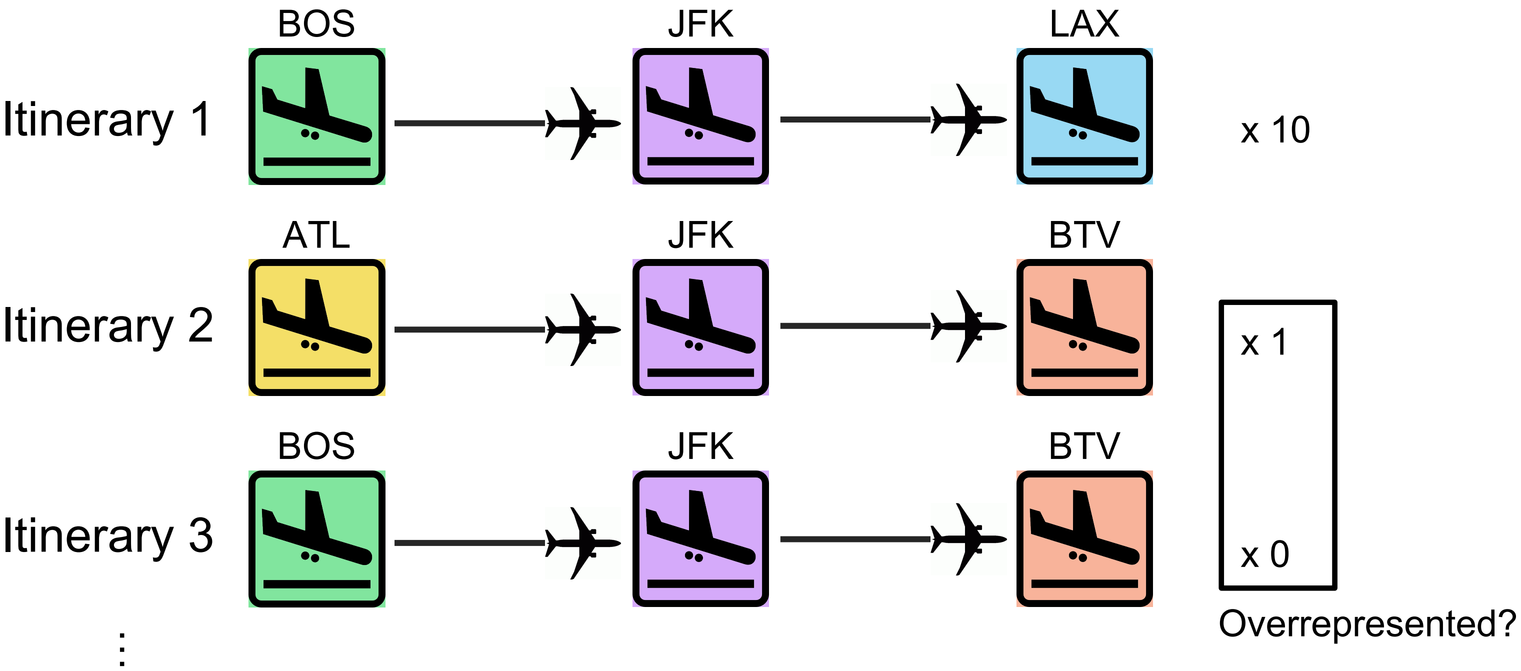
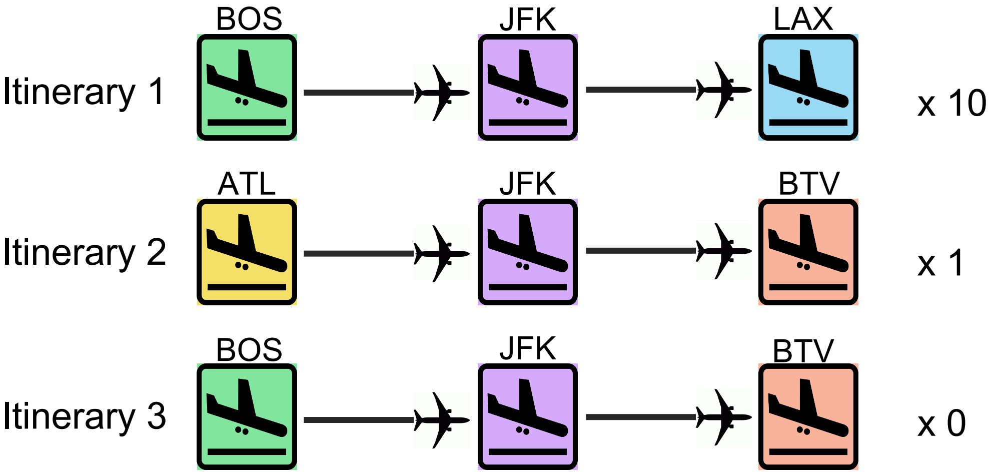


Research Question

Given this pathway dataset, can we determine whether…



is **significantly overrepresented?**

is **significantly underrepresented?**

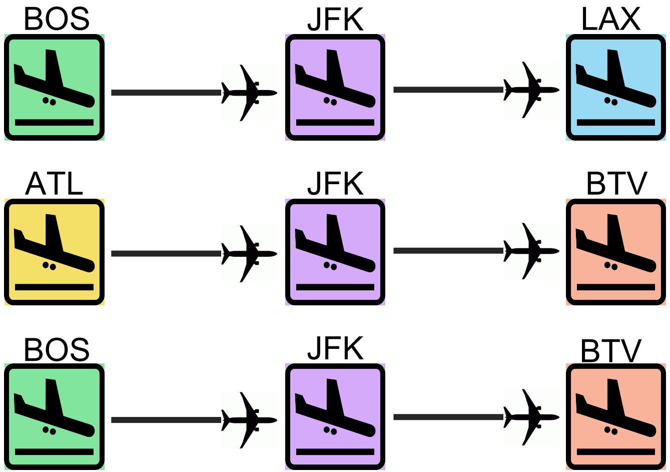
Research Question

Given this pathway dataset, can we determine whether…

Itinerary 1

Itinerary 2

Itinerary 3



x 10

x 1 is **significantly overrepresented?**

x 0 is **significantly underrepresented?**

In other words: Which **paths** are **anomalous**?

Problem: Path anomaly detection

For a given pathway dataset S, graph G, and integer k, identify paths of length k through G whose observed frequencies in S deviate significantly from random expectation in a $(k\text{-}1)$-order model of paths through G.

Problem: Path anomaly detection

For a given pathway dataset *S*, graph *G*, and integer *k*, identify paths of length *k* through *G* whose observed frequencies in *S* deviate significantly from random expectation in a (*k-1*)-order model of paths through *G*.

When *k=2*, this corresponds to comparing a random walk with a single step of memory to a memoryless (Markovian) random walk on *G*.

Toy Example

Three Goals:

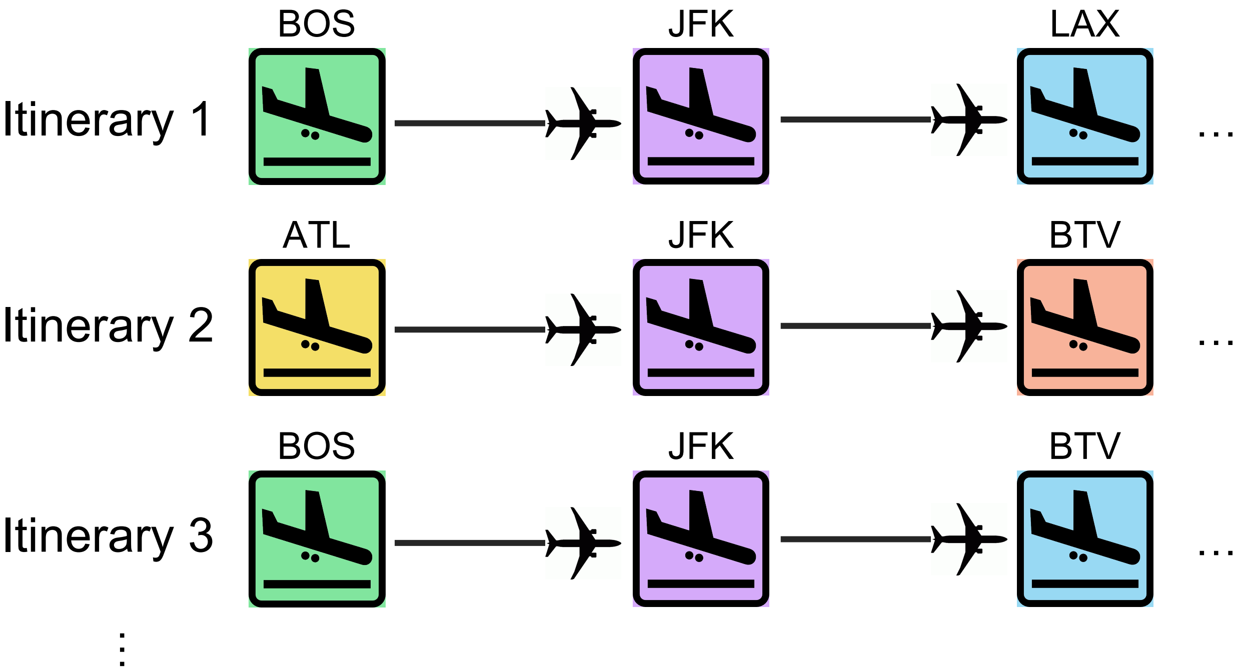
1. Introduce de Bruijn graphs as representations of sequential data

2. Show how path anomalies emerge in a simple setting

3. Show how path anomalies can be detected through a random walk simulation approach

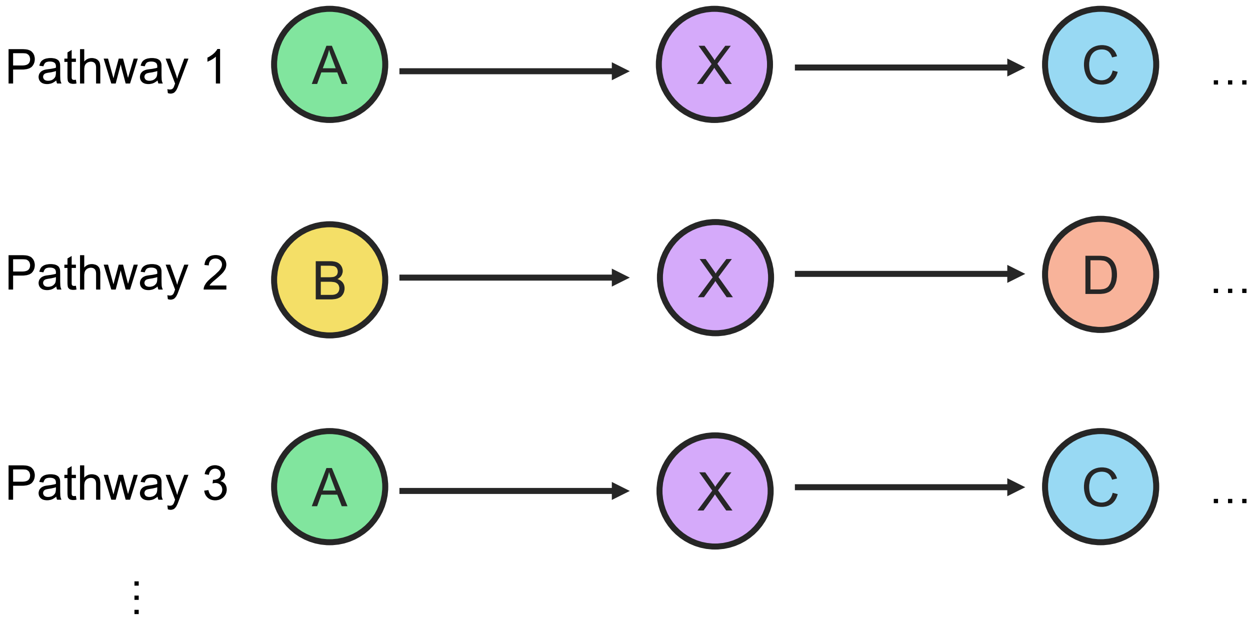
(Spoiler: Simulation approach is infeasible for real world datasets!)

Toy Example



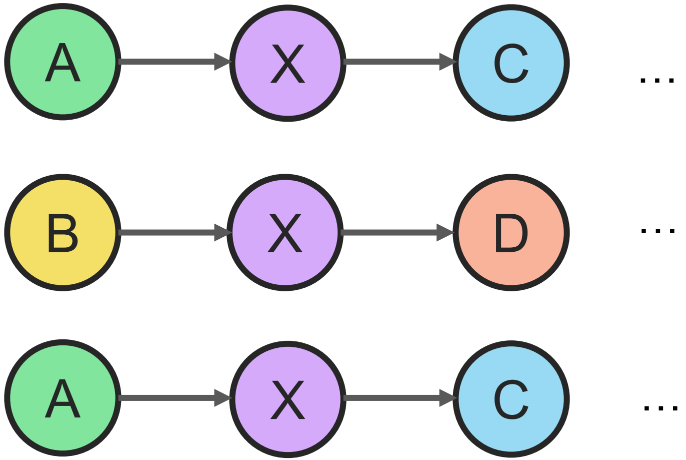
BOS
JFK
LAX
Itinerary 1
…
ATL
JFK
BTV
Itinerary 2
…
BOS
JFK
BTV
Itinerary 3
…
⋮

Toy Example



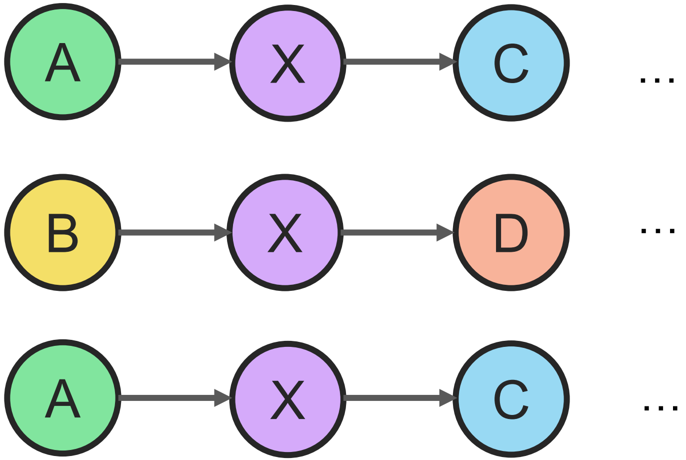
Toy Example: Data

$$S = \{ \quad \begin{matrix} p_1 \\ p_2 \\ p_3 \\ \vdots \\ p_N \end{matrix}$$



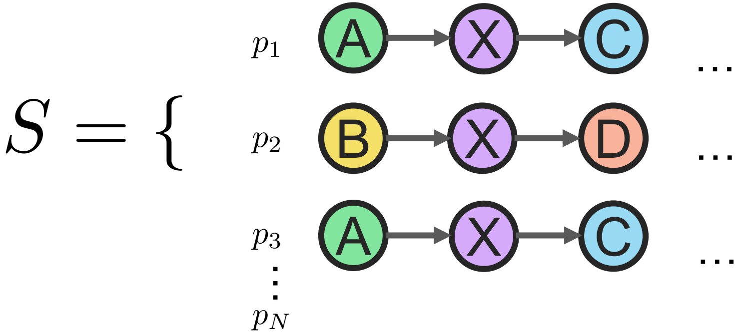
Toy Example: Data

$$S = \{ \quad p_1, p_2, p_3, \ldots, p_N$$

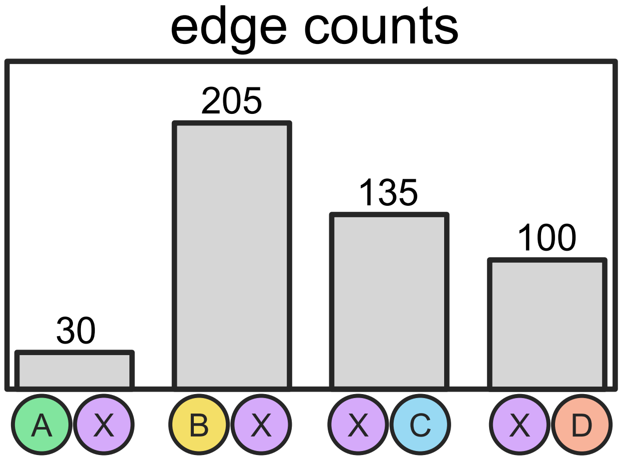


$$\text{Total number of paths } N = |S| = 235$$

Toy Example: Data to (first-order) graph

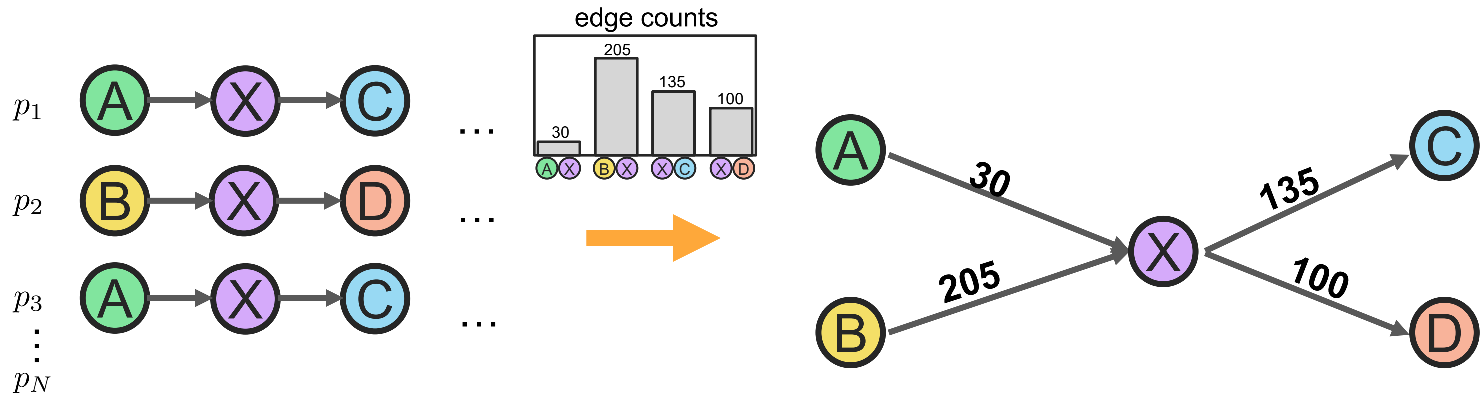


Total number of paths $N = |S| = 235$



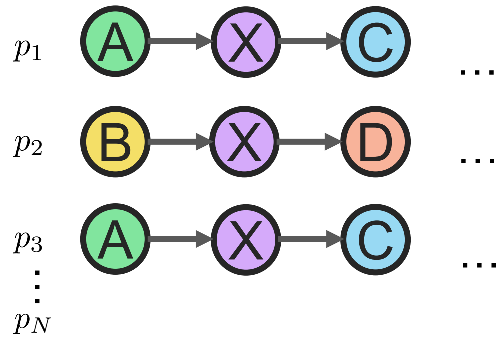
Toy Example: Data to (first-order) graph

$S = \{$



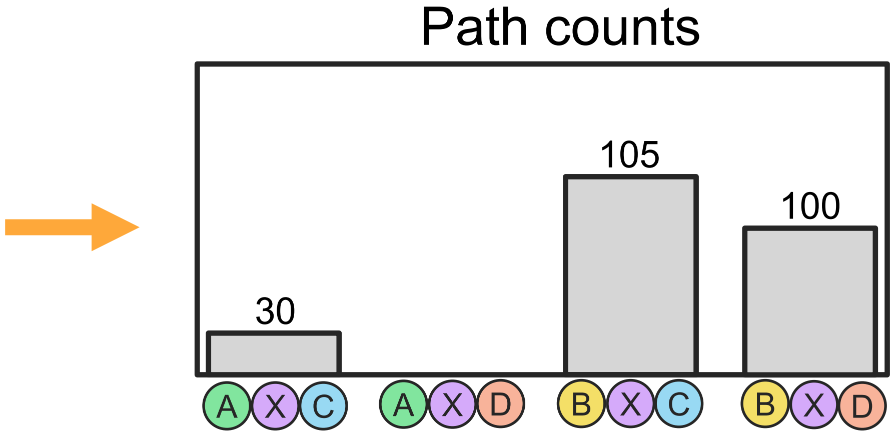
Total number of paths $N = |S| = 235$

Toy Example: Data to 2nd order de Bruijn graph



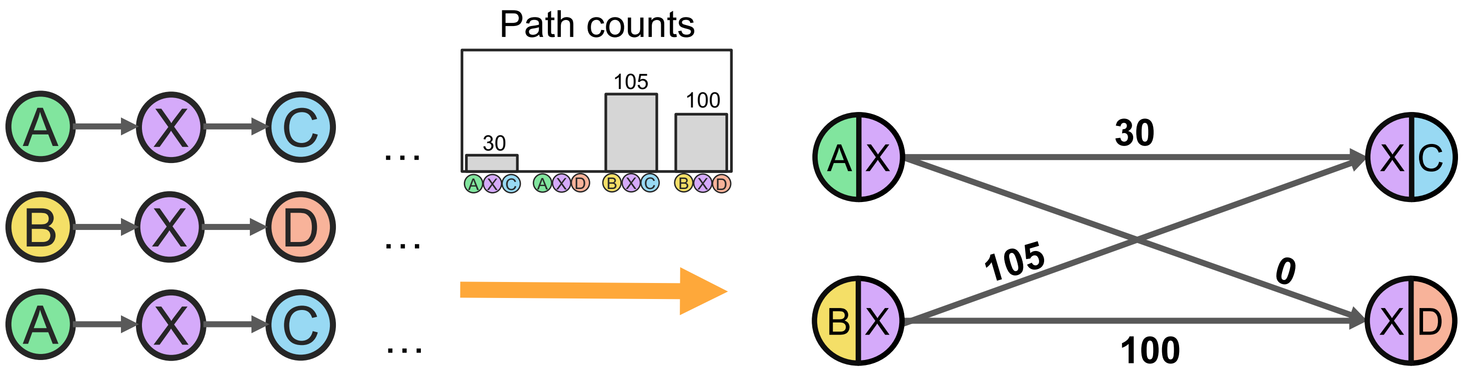
$$S = \{$$

Total number of paths $N = |S| = 235$



Toy Example: Data to 2nd order de Bruijn graph

$S = \{ \; p_1, p_2, p_3, \vdots, p_N$



Total number of paths $N = |S| = 235$

Toy Example: Path Anomalies via Simulations

For a given pathway dataset *S*, graph *G*, and integer *k*, identify paths of length *k* through *G* whose observed frequencies in *S* deviate significantly from random expectation in a *(k-1)*-order model of paths through *G*.

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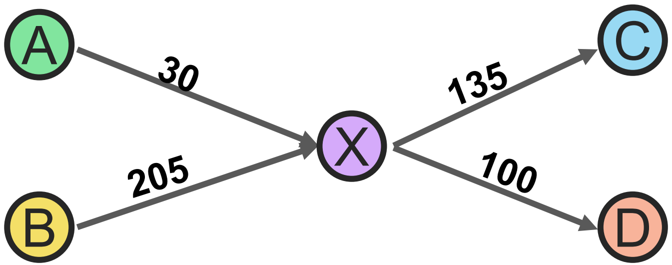
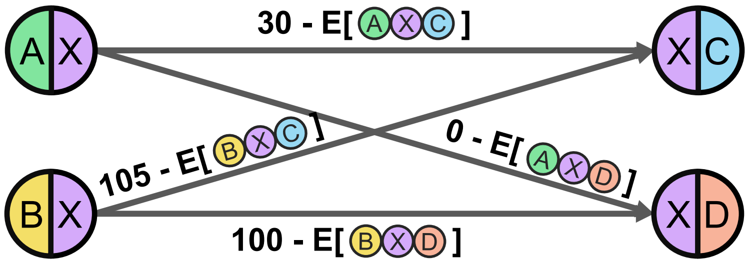
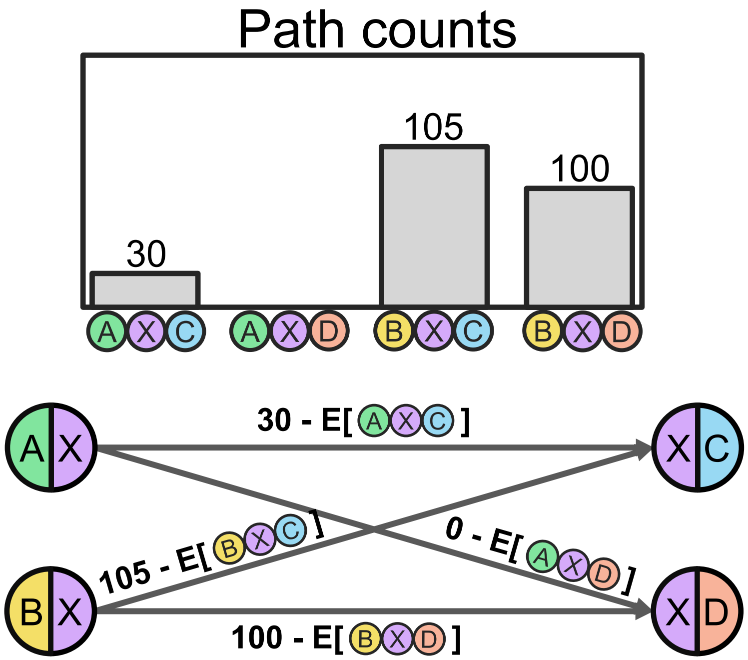
Simulate many random walk datasets

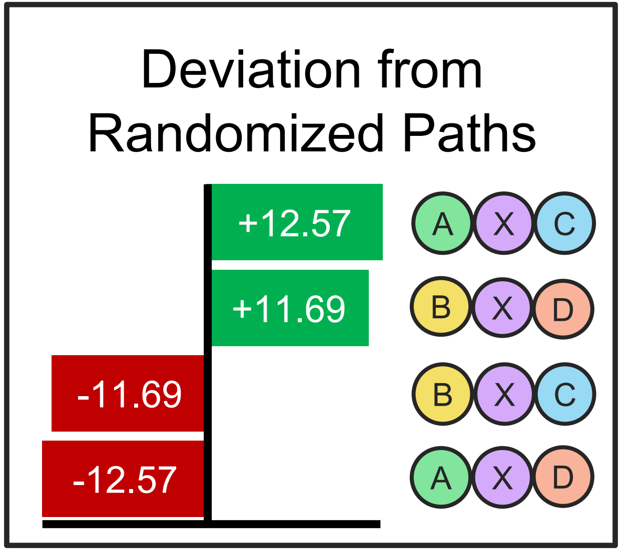


Compute expected frequency of each pathway and subtract from observed value



Toy Example: Path Anomalies via Simulations





Challenges

Path Anomaly Detection: Challenges

Detecting path anomalies via simulations → computationally intensive

Result is expected value, no concrete notion of significance

Alternative: detect path anomalies analytically by developing a tractable null model

Null Model: Challenges

Traditional null models (e.g. configuration model) cannot be applied directly

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Edges between higher-order nodes can not be randomized by stub-matching

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Edges between higher-order nodes can not be randomized by stub-matching

Need to randomize *edge weight distribution* in de Bruijn graph models, since connectivity structure is fixed by 1st-order topology

HYPA: Efficient Detection of Path Anomalies

Generalized Hypergeometric Ensemble

Generalized Hypergeometric Ensembles:
Statistical Hypothesis Testing in Complex Networks

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[2]*AIFB, Karlsruhe Institute of Technology, Karlsruhe, Germany*
(Dated: 5th August 2016)

Statistical ensembles of networks, i.e., probability spaces of all networks that are consistent with given aggregate statistics, have become instrumental in the analysis of complex networks. Their numerical and analytical study provides the foundation for the inference of topological patterns, the definition of network-analytic measures, as well as for model selection and statistical hypothesis testing. Contributing to the foundation of these data analysis techniques, in this Letter we introduce *generalized hypergeometric ensembles*, a broad class of analytically tractable statistical ensembles of finite, directed and weighted networks. This framework can be interpreted as a generalization of the classical configuration model, which is commonly used to randomly generate networks with a given degree sequence or distribution. Our generalization rests on the introduction of *dyadic link propensities*, which capture the *degree-corrected* tendencies of pairs of nodes to form edges between each other. Studying empirical and synthetic data, we show that our approach provides broad perspectives for model selection and statistical hypothesis testing in data on complex networks.

PACS numbers: 89.75.Hc, 02.50.Sk, 89.75.Kd

Generalised hypergeometric ensembles of random graphs:
the configuration model as an urn problem

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Abstract

We introduce a broad class of random graph models: the generalised hypergeometric ensemble (GHypEG). This class enables to solve some long standing problems in random graph theory. First, GHypEG provides an elegant and compact formulation of the well-known configuration model in terms of an urn problem. Second, GHypEG allows to incorporate arbitrary tendencies to connect different vertex pairs. Third, we present the closed-form expressions of the associated probability distribution ensures the analytical tractability of our formulation. This is in stark contrast with the previous state-of-the-art, which is to implement the configuration model by means of computationally expensive procedures.

Casiraghi et al. (2016, 2018)

Generalized Hypergeometric Ensemble

Generalization of the configuration model to weighted, directed networks.

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Fixes the *expected* weight of every node, rather than the *exact* degree sequence.

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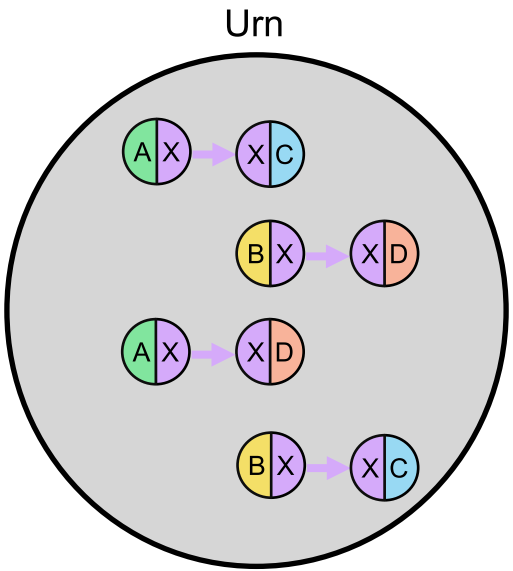
Urn Problem Intuition:

- Each pair of nodes that can possibly connect is assigned a color



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Generalization of the configuration model to weighted, directed networks.

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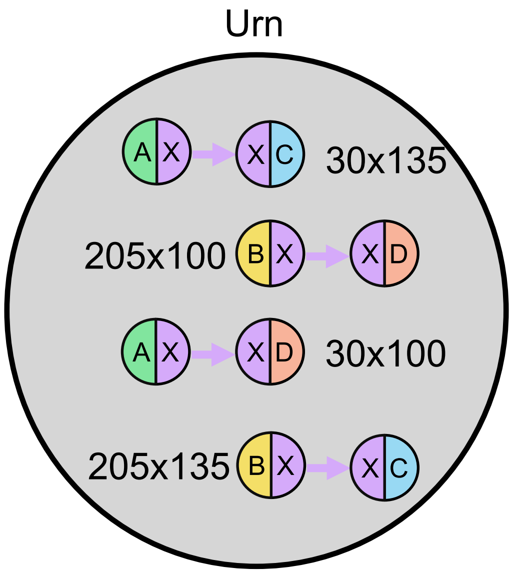
Urn Problem Intuition:

- Each pair of nodes that can possibly connect is assigned a color
- Add K_{ij} balls, where $K_{ij} = k_i^{\text{out}} k_j^{\text{in}}$



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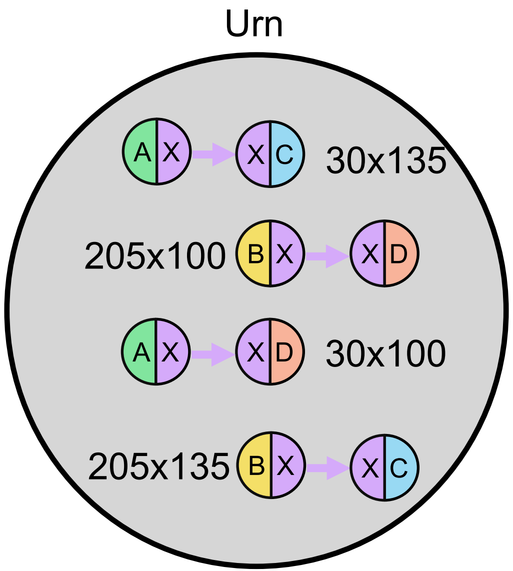
Urn Problem Intuition:

- Each pair of nodes that can possibly connect is assigned a color
- Add K_{ij} balls, where $K_{ij} = k_i^{\text{out}} k_j^{\text{in}}$
- Draw m edges to sample a network from the urn, where $m = \Sigma_{ij} W_{ij}$



$$m = \Sigma_{ij} W_{ij}$$

Hypergeometric Ensemble

$$K_{ij} = k_i^{\text{out}} k_j^{\text{in}}$$

$$Pr(X_{vw} = f(v,w)) \propto \binom{K_{vw}}{f(v,w)} \binom{\sum_{ij} K_{ij} - K_{vw}}{m - f(v,w)}$$

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Probability of observing frequency *f(v,w)* given the entire weighted network structure.

$$m = \Sigma_{ij} W_{ij}$$

Hypergeometric Ensemble

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$$Pr(X_{vw} = f(v,w)) \propto \binom{K_{vw}}{f(v,w)} \binom{\sum_{ij} K_{ij} - K_{vw}}{m - f(v,w)}$$

Number of ways to pick *f(v,w)* multiedges from K_{vw} possible.

$$m = \Sigma_{ij} W_{ij}$$

$$K_{ij} = k_i^{\text{out}} k_j^{\text{in}}$$

Hypergeometric Ensemble

$$Pr(X_{vw} = f(v,w)) \propto \binom{K_{vw}}{f(v,w)} \binom{\sum_{ij} K_{ij} - K_{vw}}{m - f(v,w)}$$

Number of ways to pick everything else.

Putting it all together: HYPA scores

$$\mathrm{HYPA}^{(k)}(\vec{v}, \vec{w}) := \Pr\left(X_{\vec{v}\vec{w}} \leq f(\vec{v}, \vec{w})\right)$$

Putting it all together: HYPA scores

$$\text{HYPA}^{(k)}(\vec{v}, \vec{w}) := \Pr(X_{\vec{v}\vec{w}} \leq f(\vec{v}, \vec{w}))$$

If "close" to **0**, then the pathway is **underrepresented**.

If "close" to **1**, then pathway is **overrepresented**.

Putting it all together: HYPA scores

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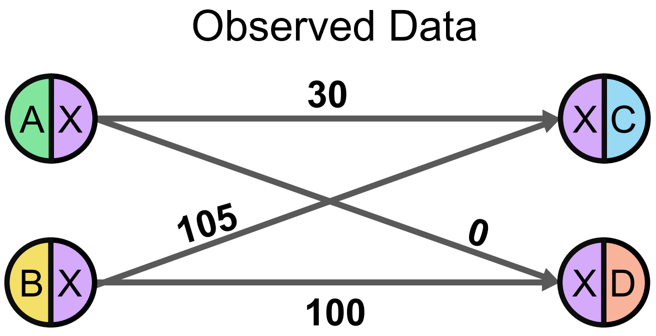
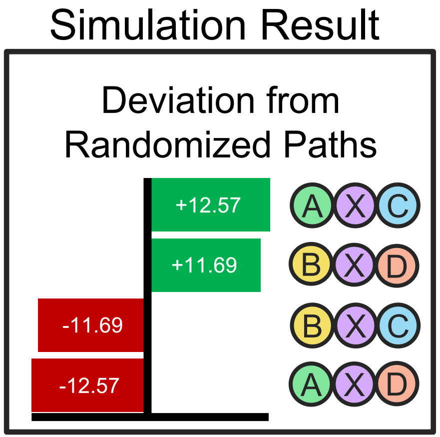
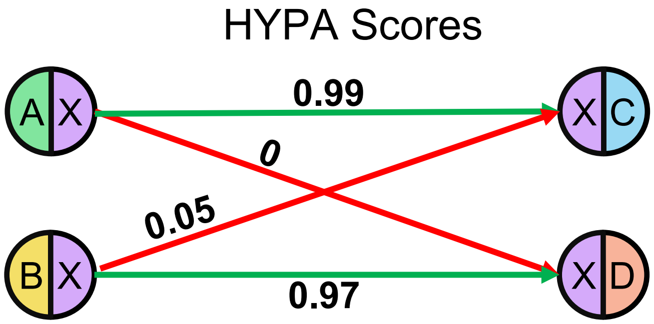
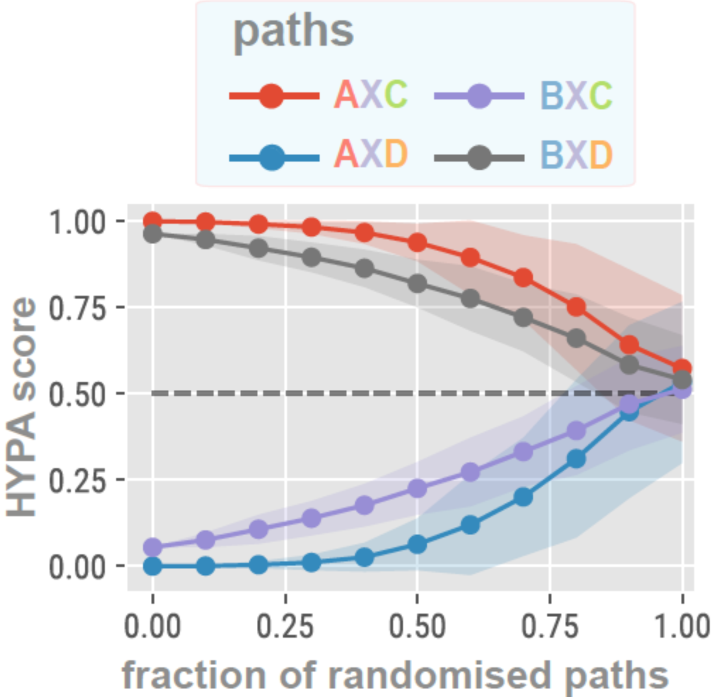






Validation

Noise via Path Randomization



Synthetic Anomalies: Setup

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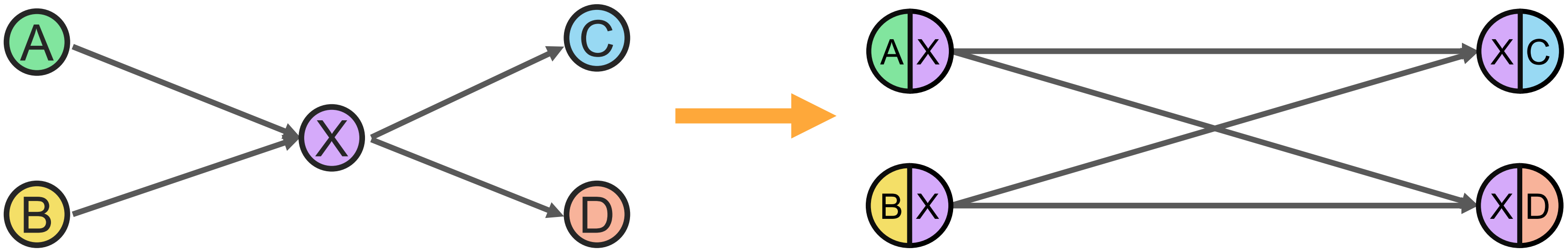
Start with an arbitrary first order topology, then construct the *kth*-order de Bruijn graph

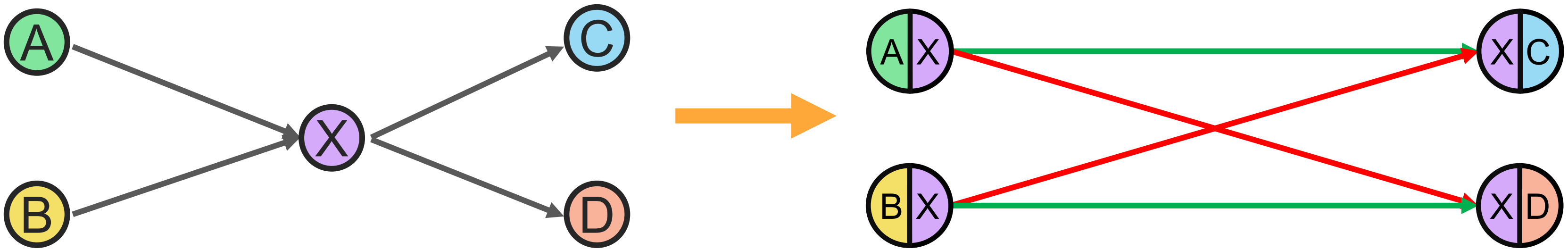
$k = 2$



Synthetic Anomalies: Setup

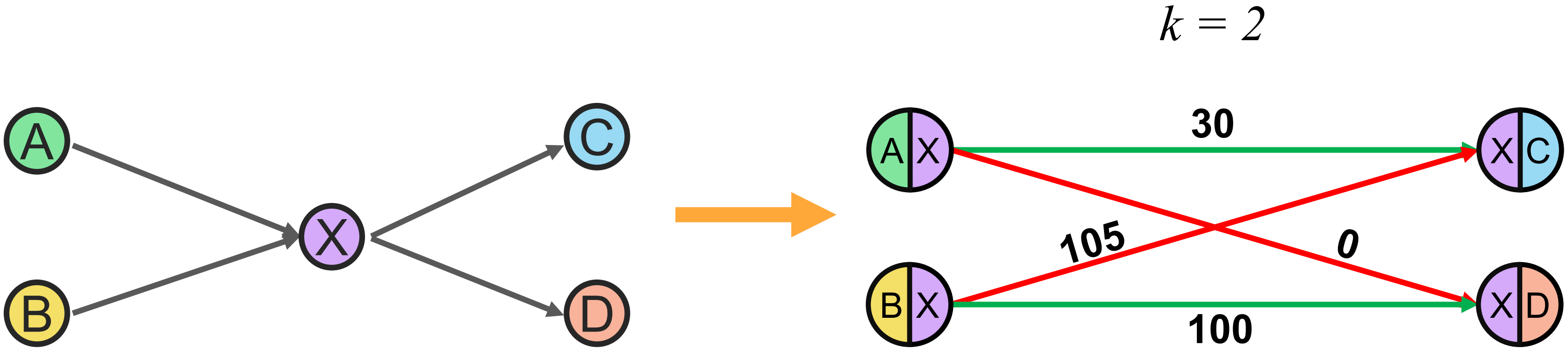
Randomly choose some edges to label over-represented

$k = 2$



Synthetic Anomalies: Setup

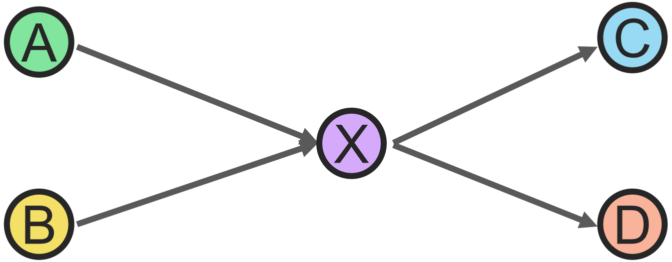
Assign heterogeneous weights based on label

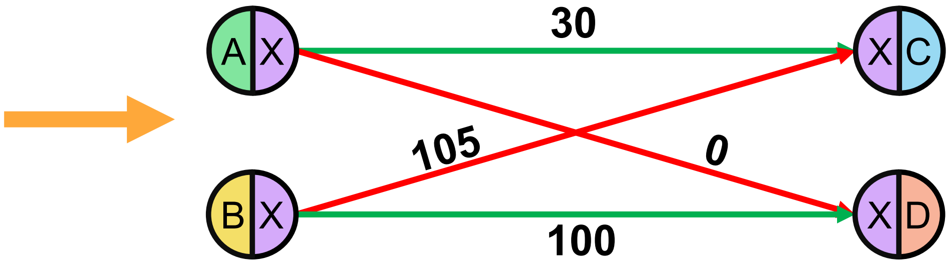


Synthetic Anomalies: Setup

Generate paths via random walks on this model, then evaluate ability of HYPA to detect injected anomalies (binary classifier).

$k = 2$





Synthetic Anomalies: ROC Example

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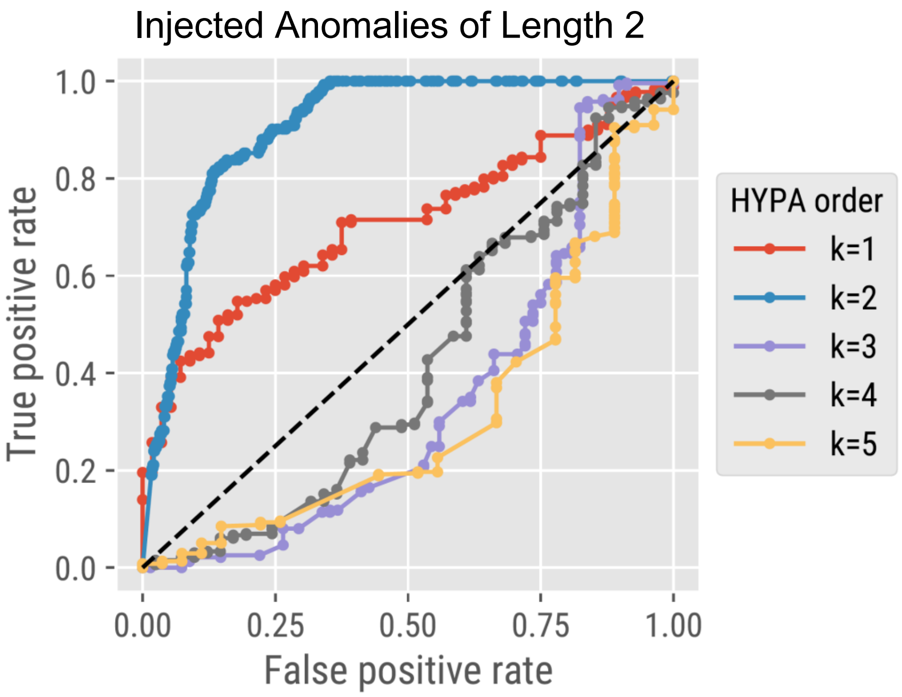

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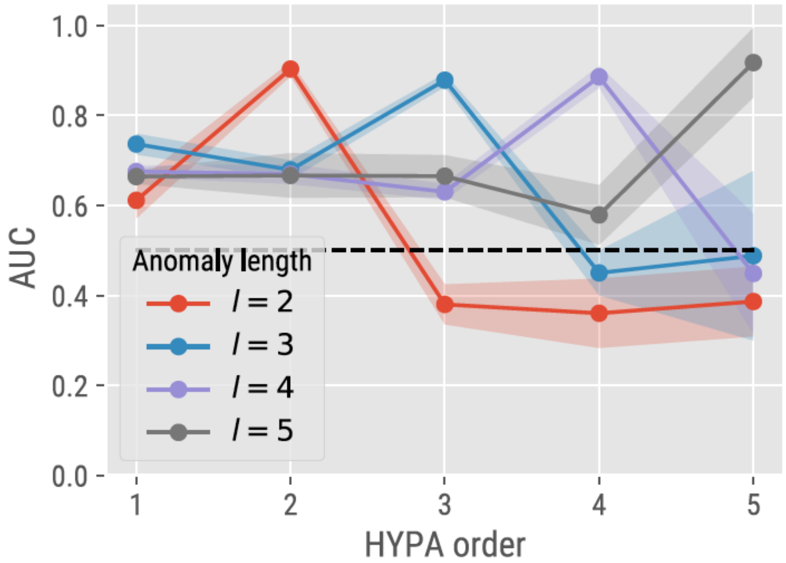
Synthetic Anomalies: AUC Results



Application to Flight Data

Airlines

5% sample of all US domestic flights in 2018

	Topology		**Sequences**			
Data	Nodes	Edges	Total	Unique	$l^{\max}$	$\langle l \rangle$
Flights	382	6933	185871	88539	10	2.48

Data from: http://www.transtats.bts.gov/Tables.asp?DB_ID=125

Airlines

Hypotheses:

1. Return flights should be over-represented, since people most often travel round trip.

Airlines: Return trips are over-represented

α	**Return**	**Non-return**
0.05	0.915	0.340
0.01	0.851	0.130
0.001	0.760	0.023
0.0001	0.688	0.004
0.00001	0.628	0.001

Fraction of over-represented return/non-return flights for various discrimination thresholds.

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1. Return flights should be over-represented, since people most often travel round trip.
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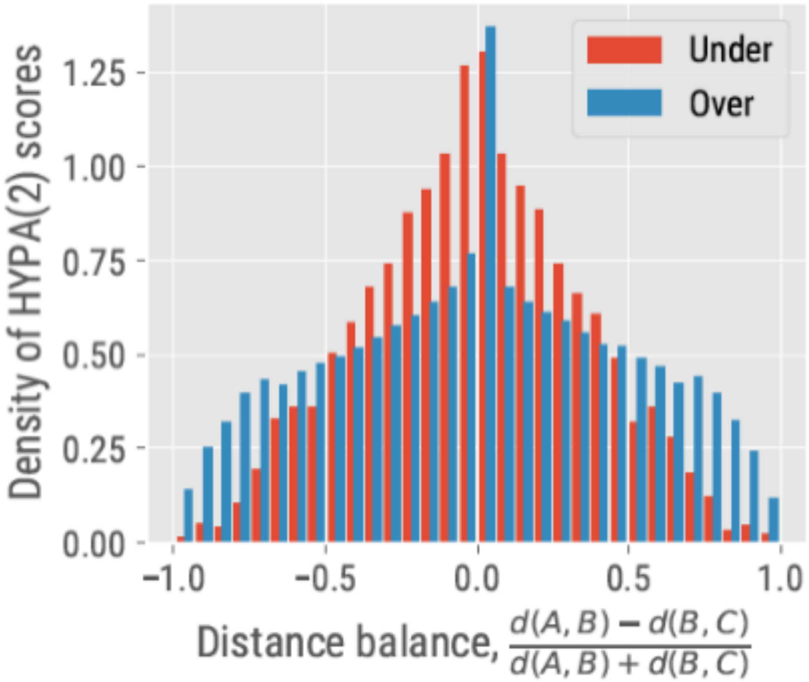
Airlines: Trip Balance

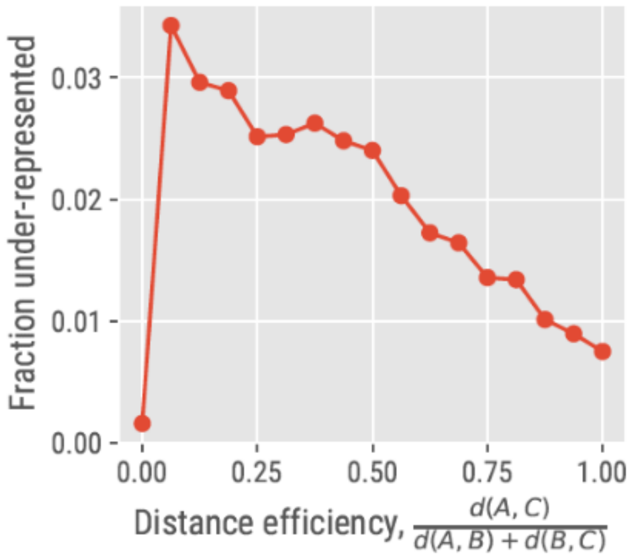


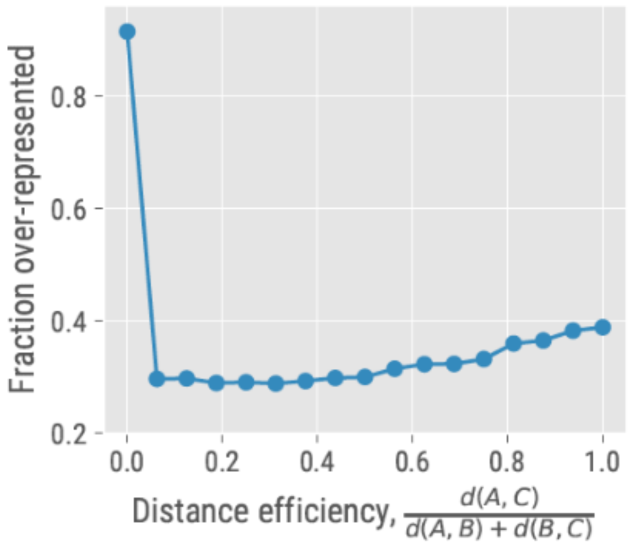
Airlines

Hypotheses:

1. Return flights should be over-represented, since people most often travel round trip.
2. Over-represented non-return flights are due to regional/national hubs, since people need to fly from small airports → regional hub → large airport.
3. “Efficient” paths are more likely to be over-represented.

Airlines: Efficiency





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Thanks!

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https://arxiv.org/abs/1905.10580

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Detecting Path Anomalies in Time Series Data on Networks

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https://arxiv.org/abs/1905.10580

Definition: kth-order de Bruijn Graph

For a given graph $G = (V, E)$ and positive integer k we define a k-th order De Bruijn graph of paths in G as a graph $G^k = (V^k, E^k)$, where (i) each node $\vec{v} := v_0 v_1 \overset{\rightarrow}{\ldots} v_{k-1} \in V^k$ is a path of length $k-1$ in G, and (ii) $(\vec{v}, \vec{w}) \in E^k$ iff $v_{i+1} = w_i$ for $i = 0, \ldots, k-2$.

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Pseudocode

Algorithm 1 ComputeHYPA(S, k): *Compute* k*th order HYPA scores for sequence dataset* S*.*

Input: S (sequences), k (desired order)
Output: $\text{HYPA}^{(k)}$ score for all k-th order paths

1: $G^k \leftarrow$ DeBruijnGraph(S, k) # Construct kth order graph

2: $\Xi \leftarrow$ fitXi(G^k, tolerance) # Optimization (Algorithm 2 in Appendix A.1)

3: **for** $(\vec{v}, \vec{w}) \in G^k$ **do**
4: $\quad \text{HYPA}^{(k)}(\vec{v}, \vec{w}) \leftarrow \Pr(x_{vw} \leq (\vec{v}, \vec{w}) \mid m, \Xi)$
$\quad$ # Compute CDF
5: **return** $\text{HYPA}^{(k)}$

Naïve Baseline Comparison

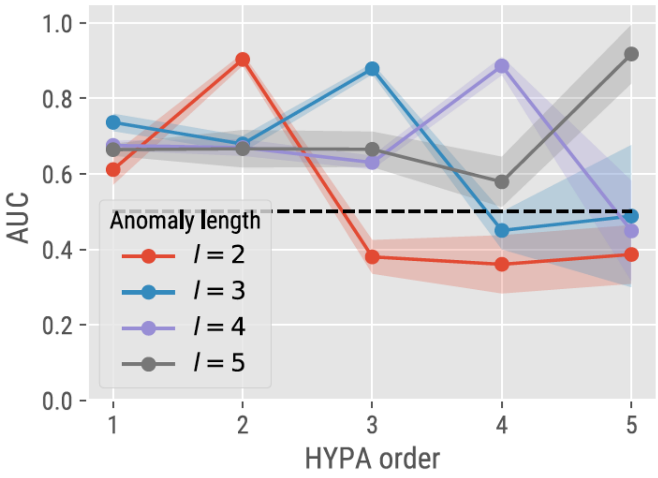
Frequency-Based Anomaly Detection (FBAD)

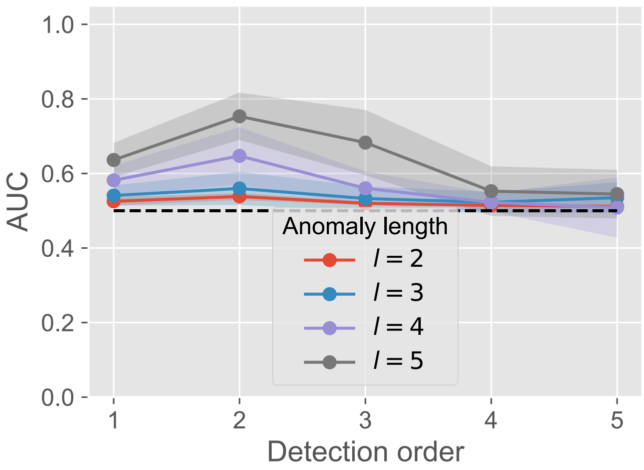
Compute mean, μ, and standard deviation, σ, of kth order edge weights

Given scaling factor α, label edges as

- Overrepresented if frequency is larger than $\mu + \sigma\alpha$
- Underrepresented if frequency is smaller than $\mu - \sigma\alpha$

Synthetic Anomalies

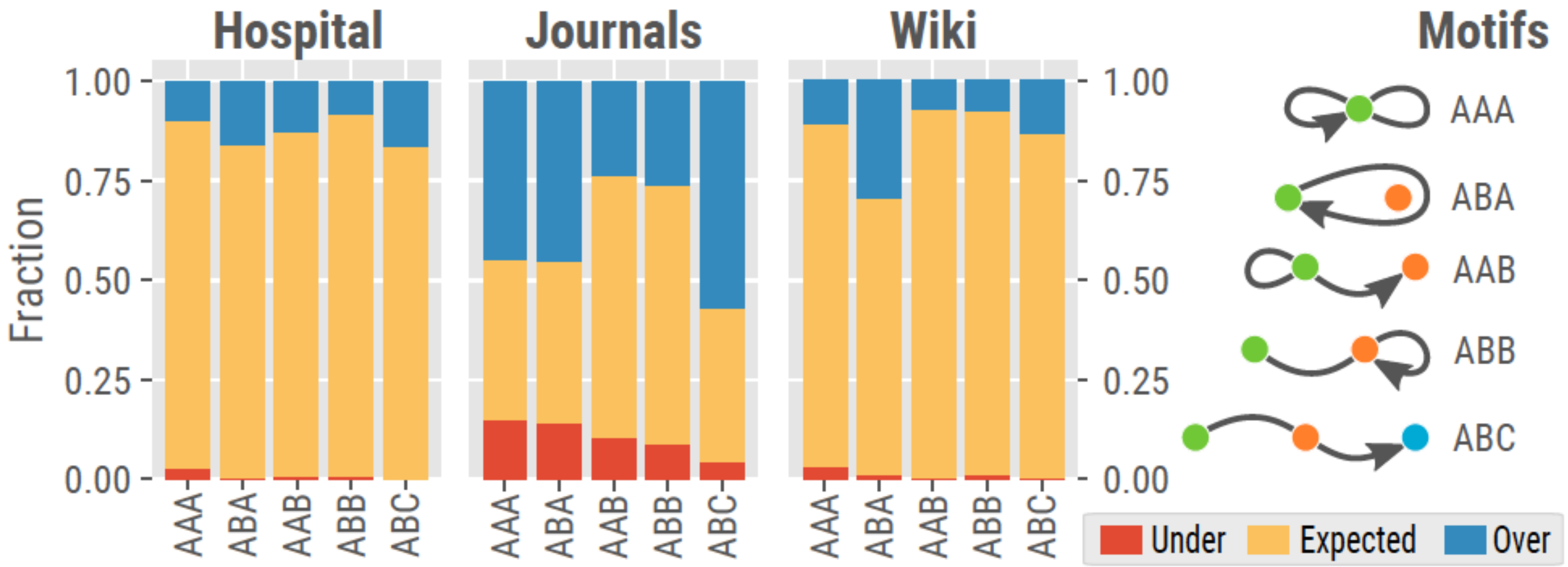




Real Data

	Topology		Sequences			
Data	Nodes	Edges	Total	Unique	$l^{\max}$	$\langle l \rangle$
Tube	268	646	4295731	67015	35	6.75
Flights	382	6933	185871	88539	10	2.48
Journals	283	1743	480496	309565	35	14.8
Hospital	75	1138	28422	2561	5	1.19
Wiki	100	1598	29682	7431	21	1.64

Exploring Motifs



Case Study: London Tube

Data:

- Origin → destination statistics between London Tube stations
  - (origin, destination, #observations)
- Shortest paths between stations
  - Assume people follow shortest paths

London Tube

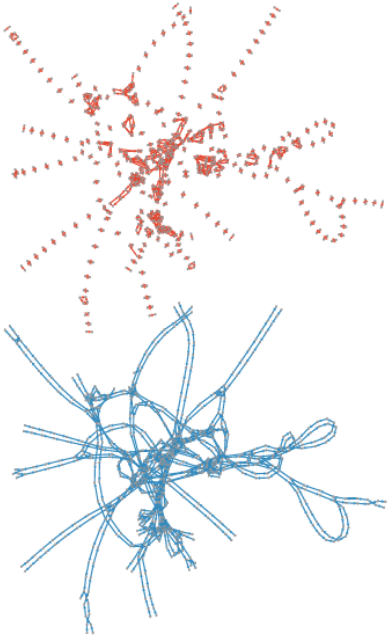
Hypothesis:

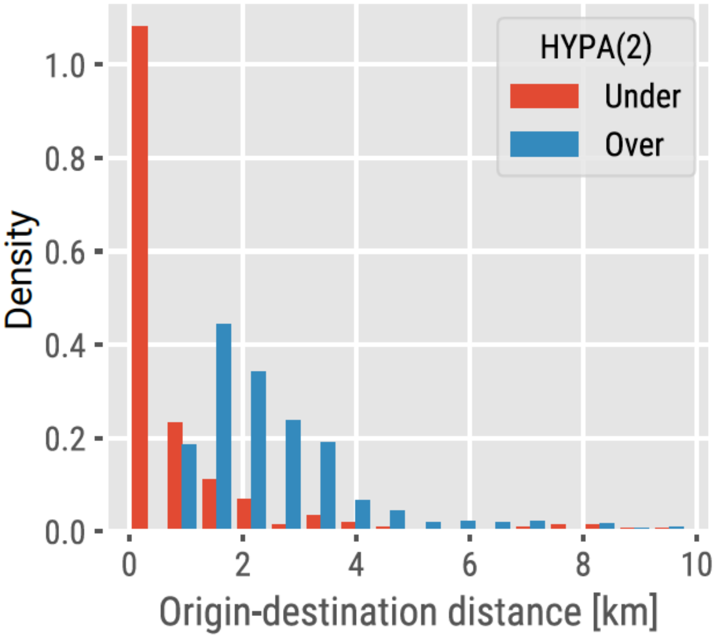
- People typically use public transportation to travel large geographic distances
- *Overrepresented* pathways should cover *larger* distances

Test:

- Measure distance between every station
- For 2nd order transitions A-B-C, compute distance between nodes A and C
- Analyze distributions of distance in over vs. under represented transitions
    - Expect to see distribution shifted towards higher values for over-represented transitions

London Tube





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London Tube

$\text{HYPA}^{(k)}$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
Under [km]	0.00	2.38	3.29	4.60	5.43
Over [km]	2.20	2.93	3.79	5.21	5.63
***p*-value**	$< 10^{-170}$	$< 10^{-7}$	$< 10^{-4}$	0.006	0.08

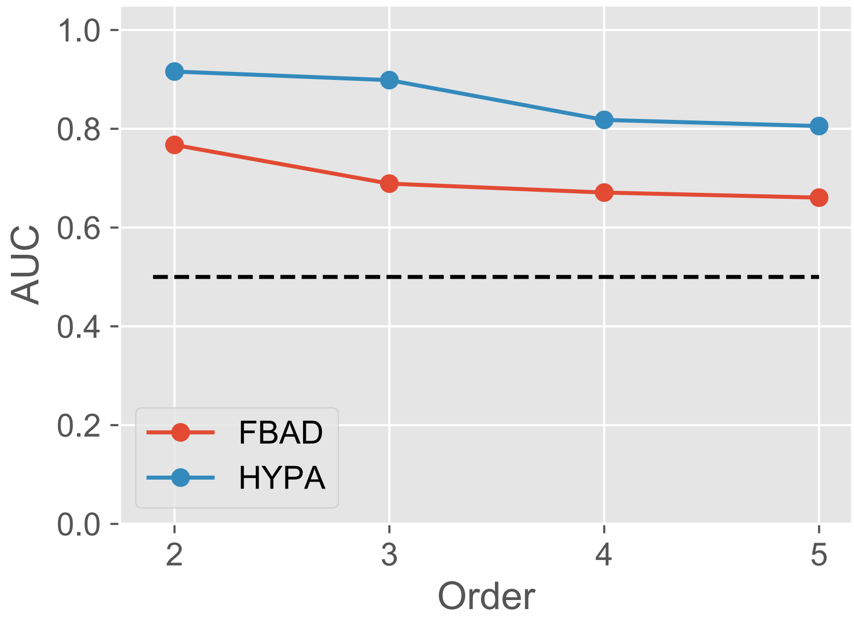
Median distance between source and destination nodes in under/over represented transitions.

Constructing Ground Truth

Construct ground truth based on the method discussed earlier:

- Randomize path data using k-1st order random walks
- Compute kth-order path statistics
- Repeat m times, noting the frequency of each path
- Estimate multinomial distribution and its CDF from these statistics
- If CDF(path) > threshold, label over-represented

Tube Data - Ground Truth



Computational complexity

$$O(N + |V|^2 \lambda_1^k)$$

Scalability

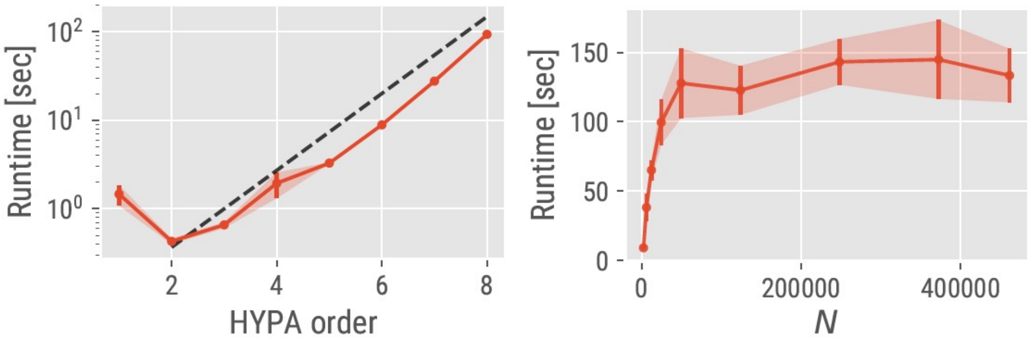


Figure 8: Empirical scalability of HYPA. Left: Required time to detect path anomalies of length k for the Tube data. Right: Runtime in Flights data for detection order $k = 1$ and varying data size N randomly sampled from the data. All data points correspond to the mean of ten repeated measurements, with the standard deviations shown as bars.