Detecting Path Anomalies in Sequential Data on Networks

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In collaboration with





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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

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

Application of methodology to a real system

Intuitive Example: Passenger Flight Data

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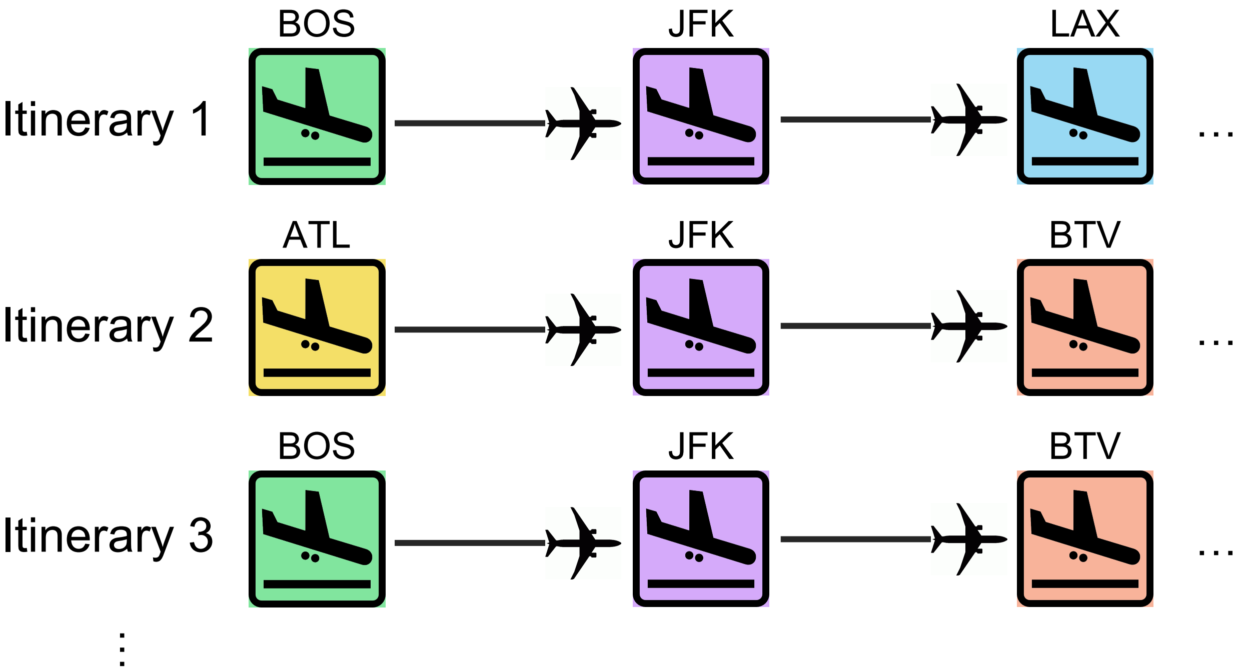
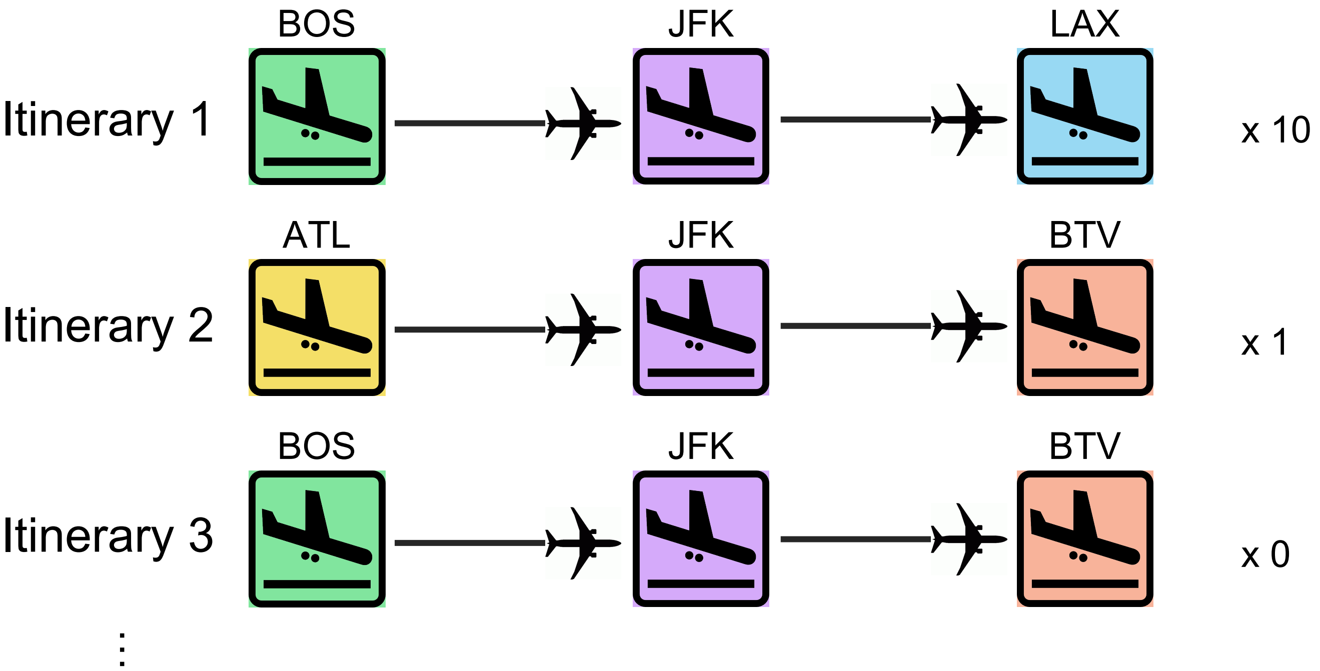


Intuitive Example: Passenger Flight Data



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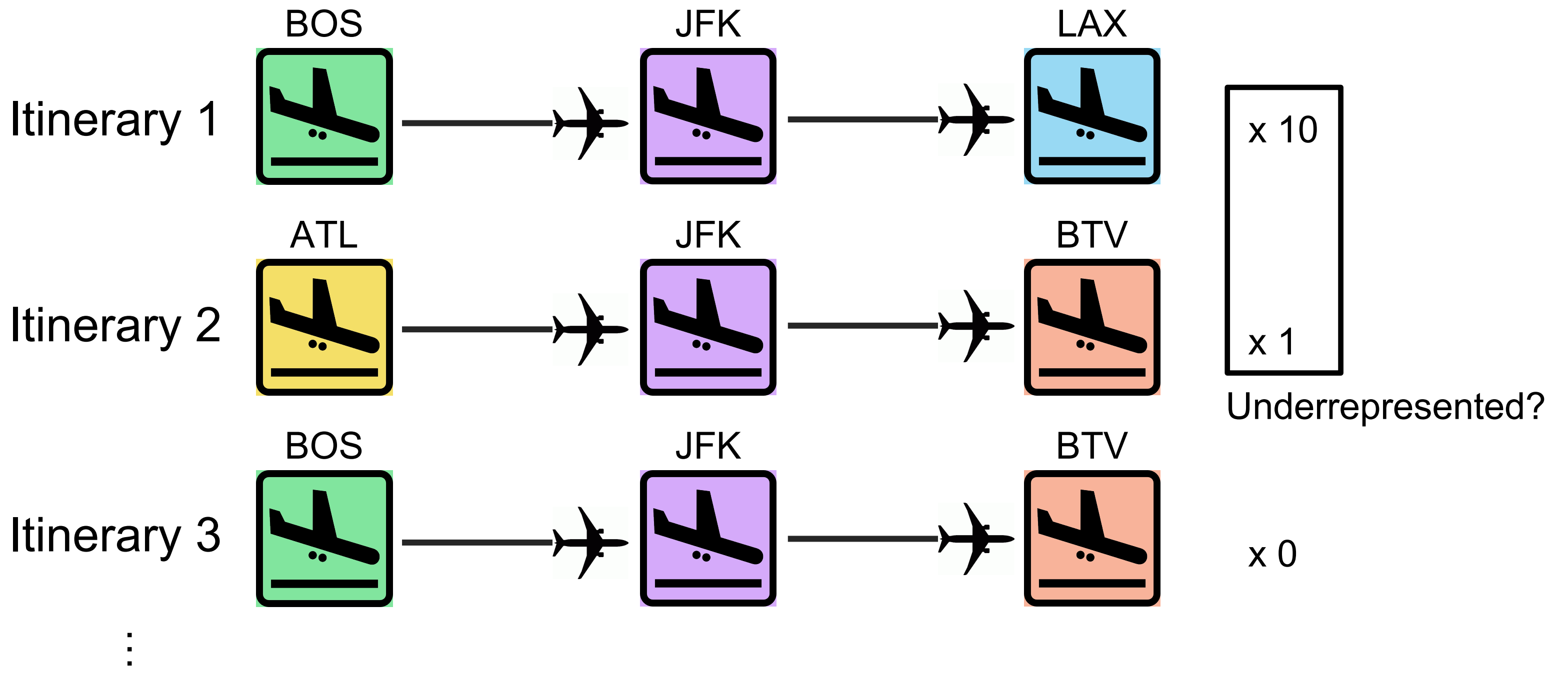

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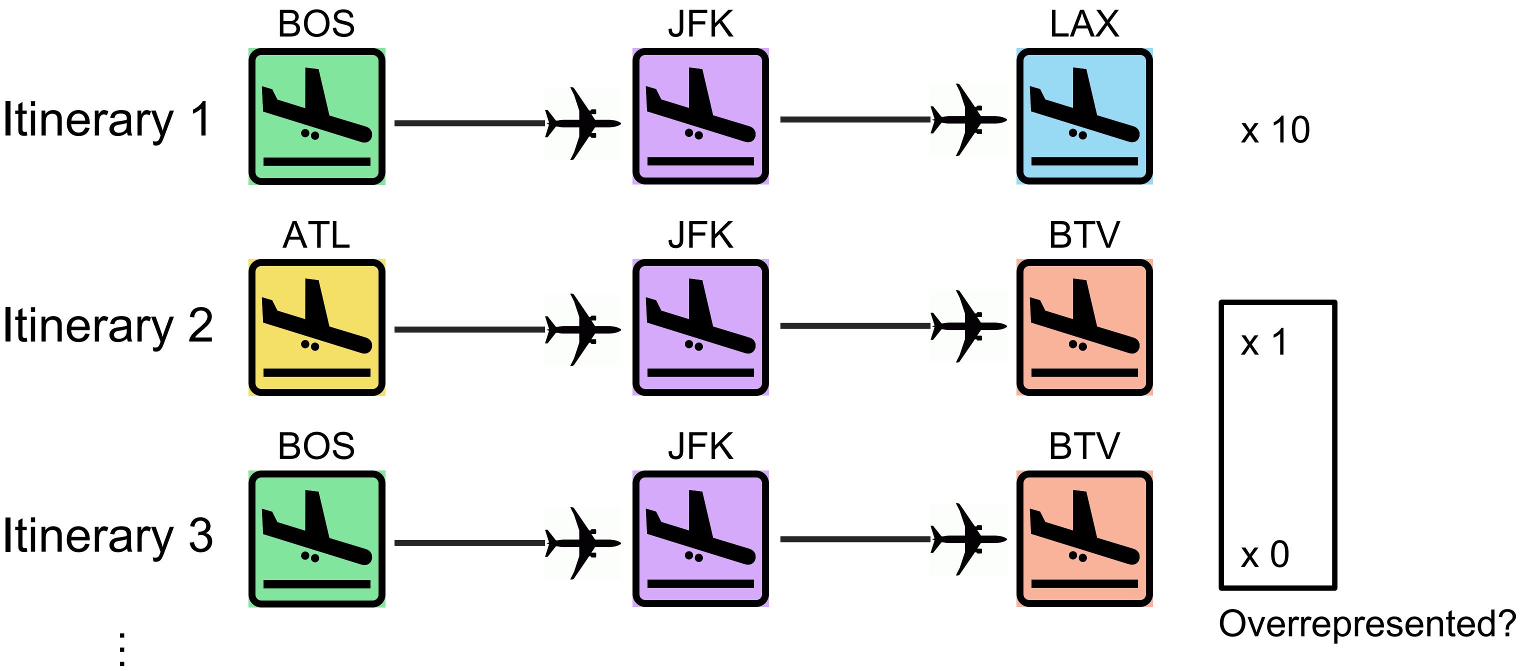
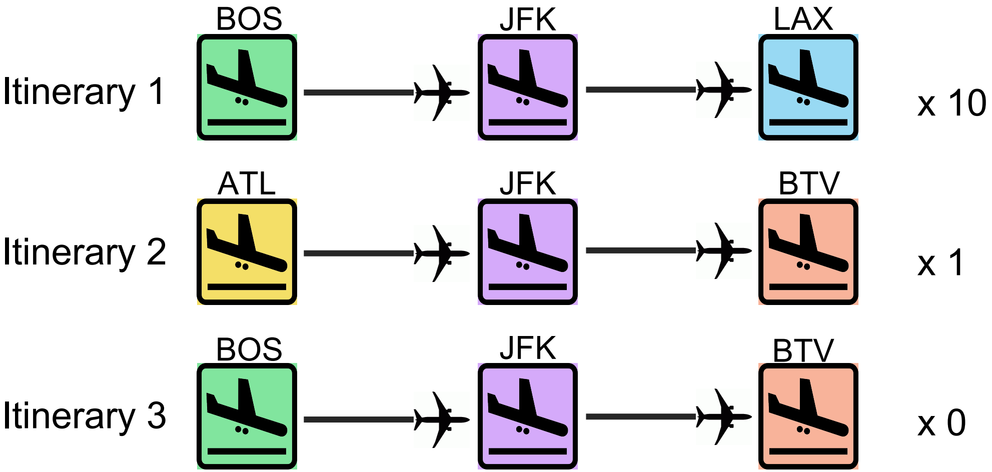


Research Question

Given this pathway dataset, can we determine whether…



is **significantly overrepresented?**

is **significantly underrepresented?**

Problem: Path anomaly detection

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

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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:

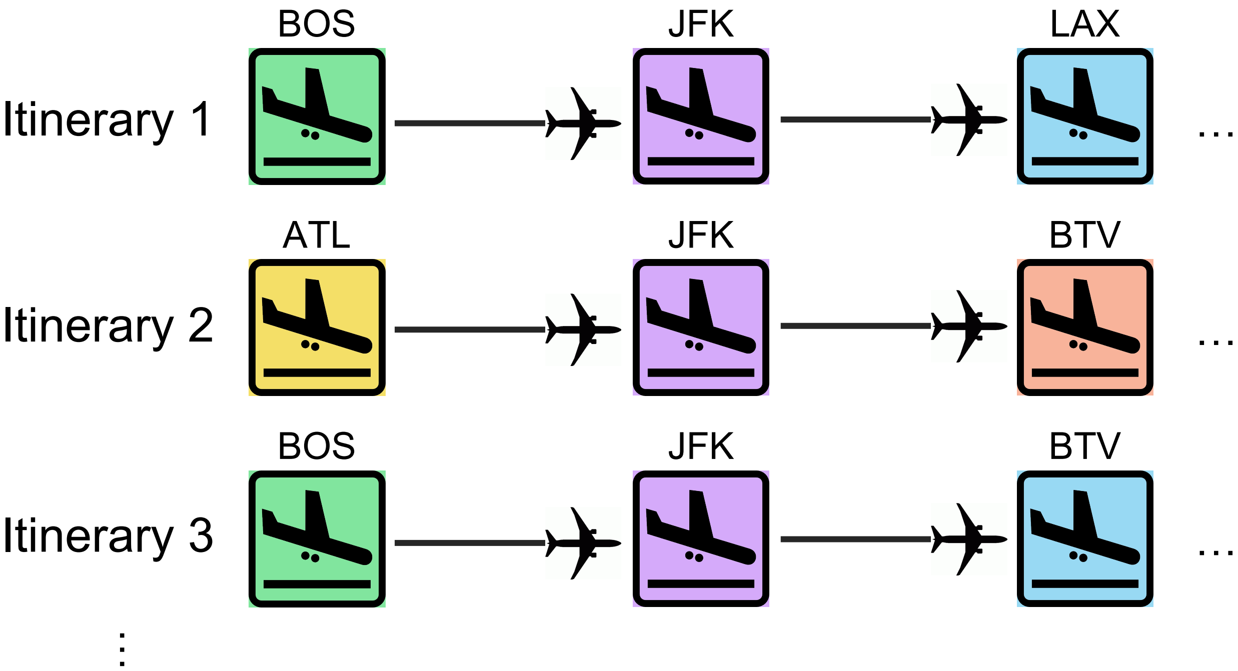
1. Introduce de Bruijn graphs as representations of sequential data

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


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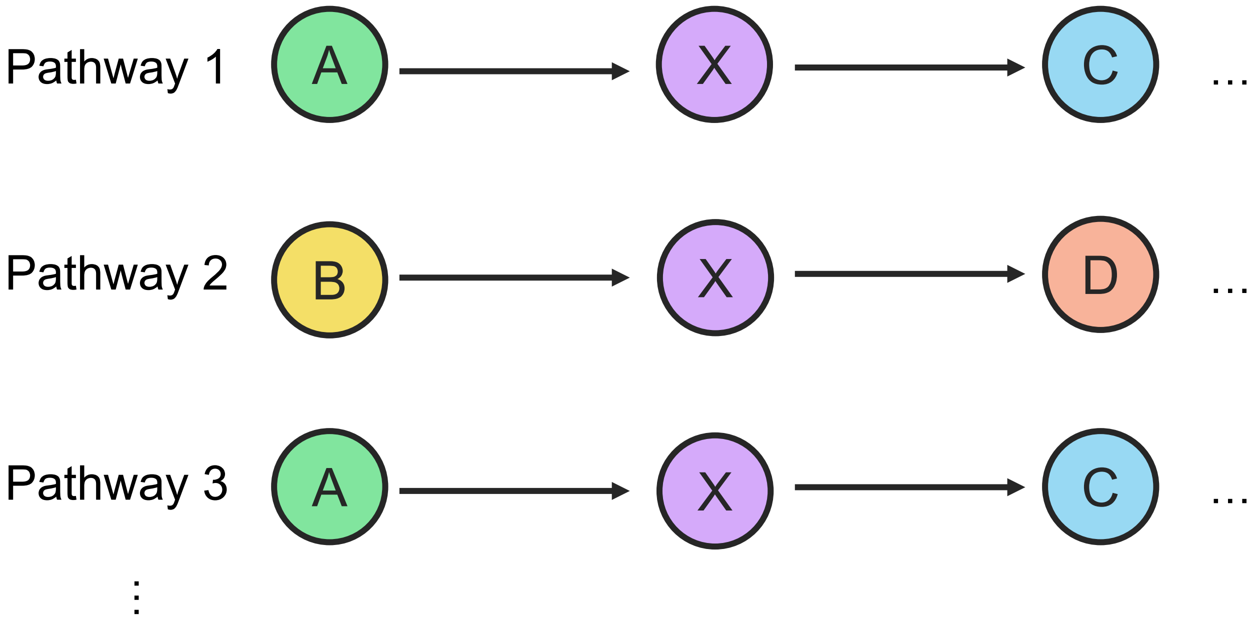
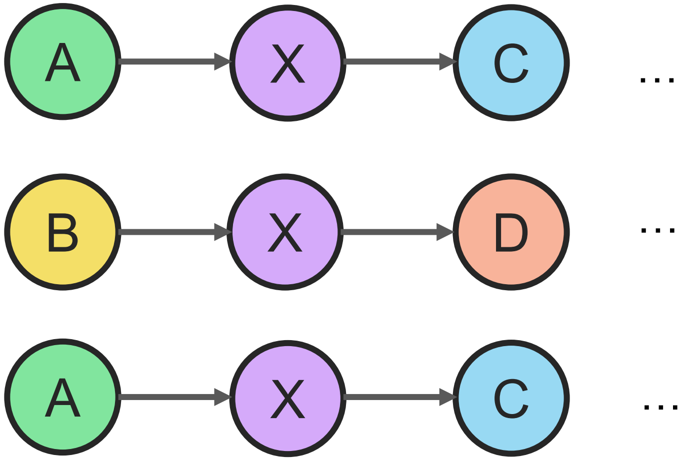
…
Itinerary 2
ATL
JFK
BTV
…
Itinerary 3
BOS
JFK
BTV
…
⋮

Toy Example



Toy Example: Data

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



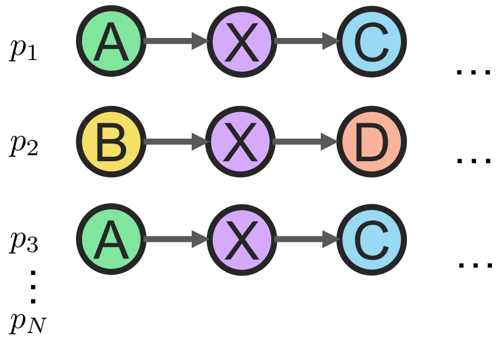
Toy Example: Data

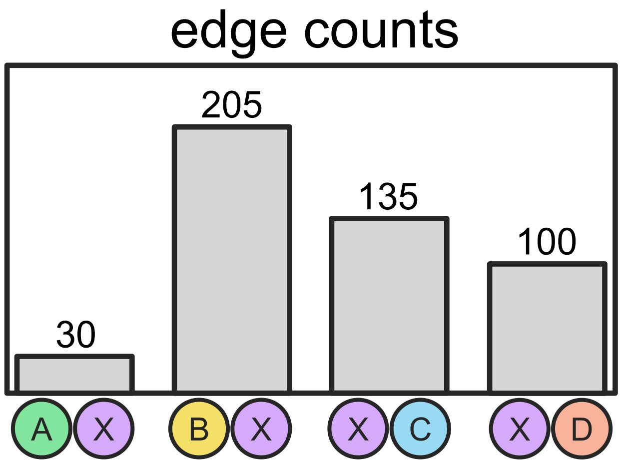
$$S = \left\{ \begin{array}{ll} p_1 & A \rightarrow X \rightarrow C \quad \cdots \\ p_2 & B \rightarrow X \rightarrow D \quad \cdots \\ p_3 & A \rightarrow X \rightarrow C \quad \cdots \\ \vdots & \\ p_N & \end{array} \right.$$

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

Toy Example: Data to (first-order) graph

$$S = \{$$





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

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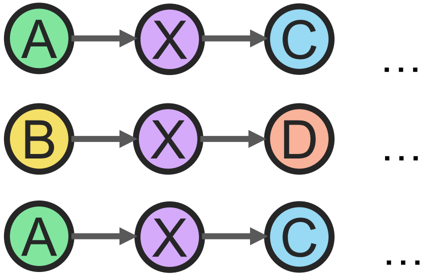
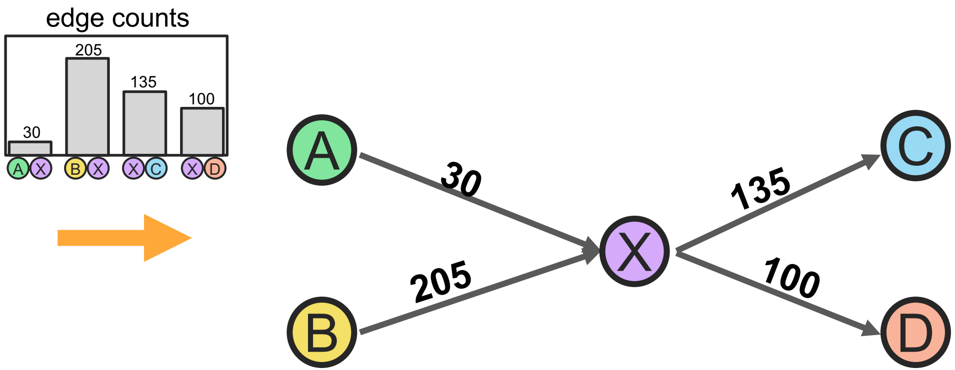
$S = \{$ p_1, p_2, p_3, $\vdots$, p_N





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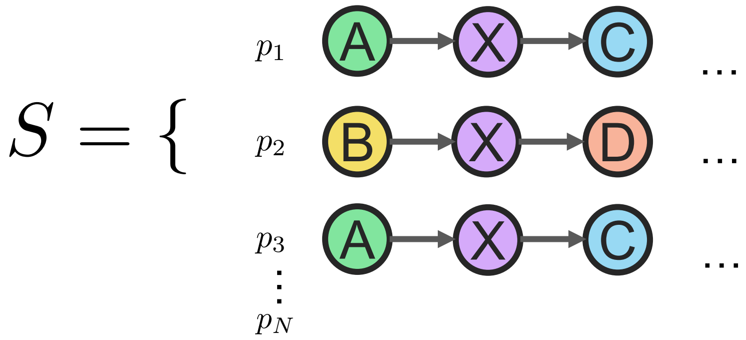
Toy Example: Data to 2nd order de Bruijn graph



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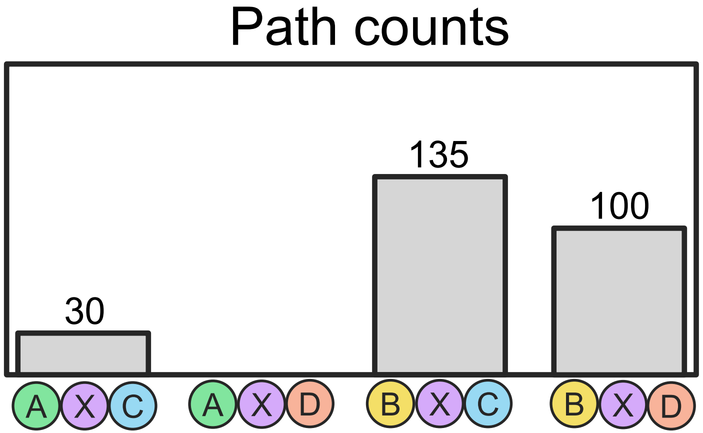

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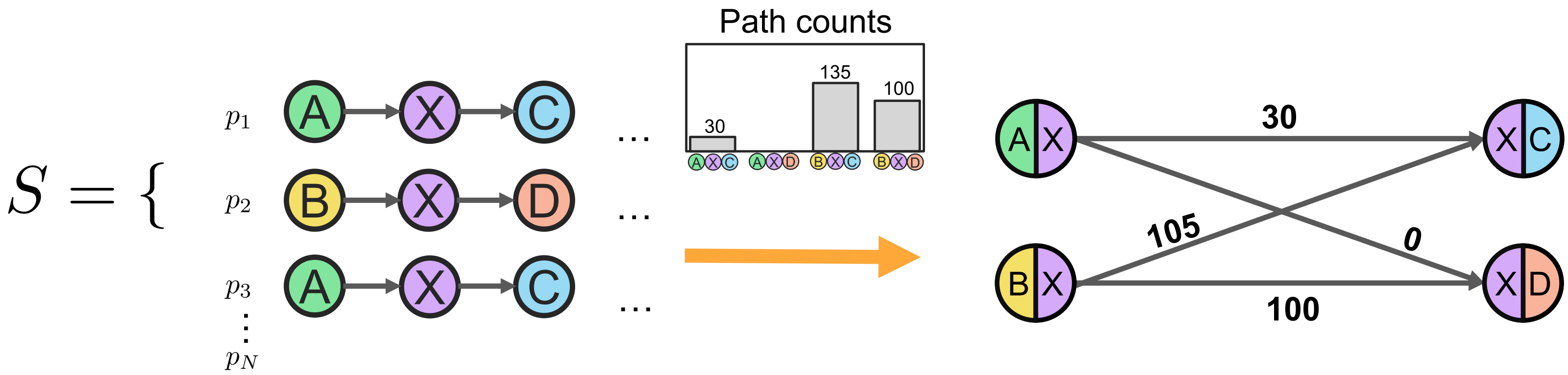

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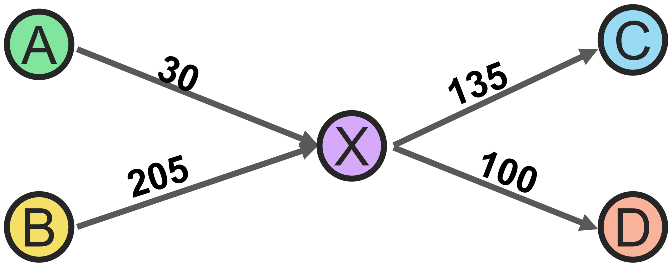
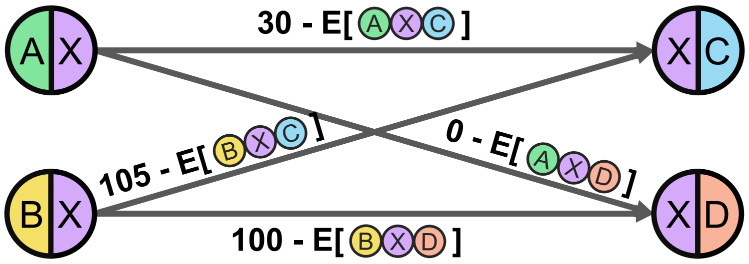
Simulate many random walk datasets



Compute expected frequency of each pathway and subtract from observed value



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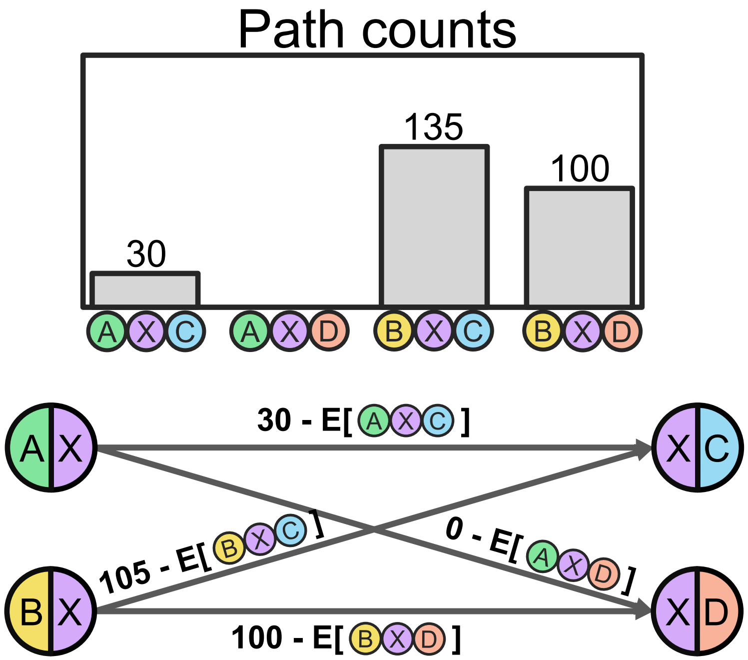

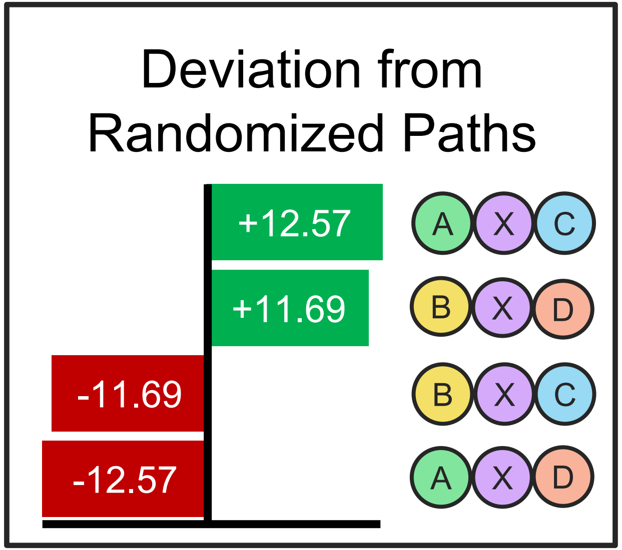

Challenges

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 across whole network (need suffix-prefix 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

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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Intuition: Urn problem where each pair of nodes *i, j* that can possibly connect is assigned a color, and K_{ij} balls are added, where K_{ij} is the total possible multi-edges between the nodes (e.g. $K_{ij} = k_i^{\text{out}} k_j^{\text{in}}$, as in the config model).

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To sample from the ensemble, draw $m = \Sigma_{ij} W_{ij}$ (total observed edges) multi-edges randomly from the urn.

Putting it all together: HYPA scores

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

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

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

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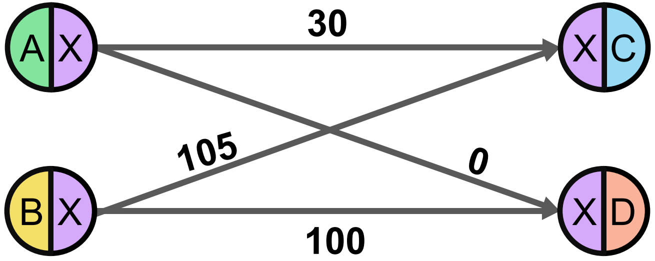
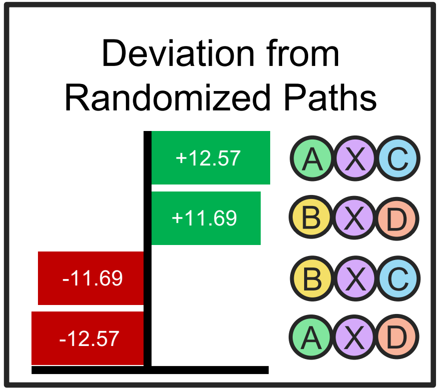
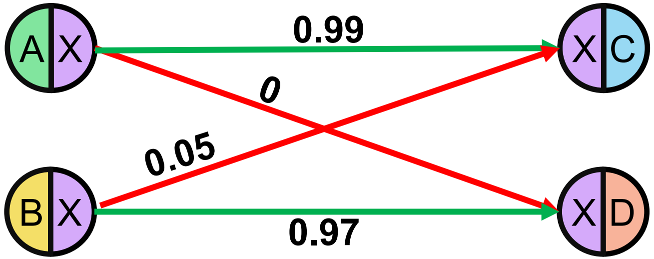
Observed Data



Simulation Result



HYPA Scores



Application to Flight Data

Airlines

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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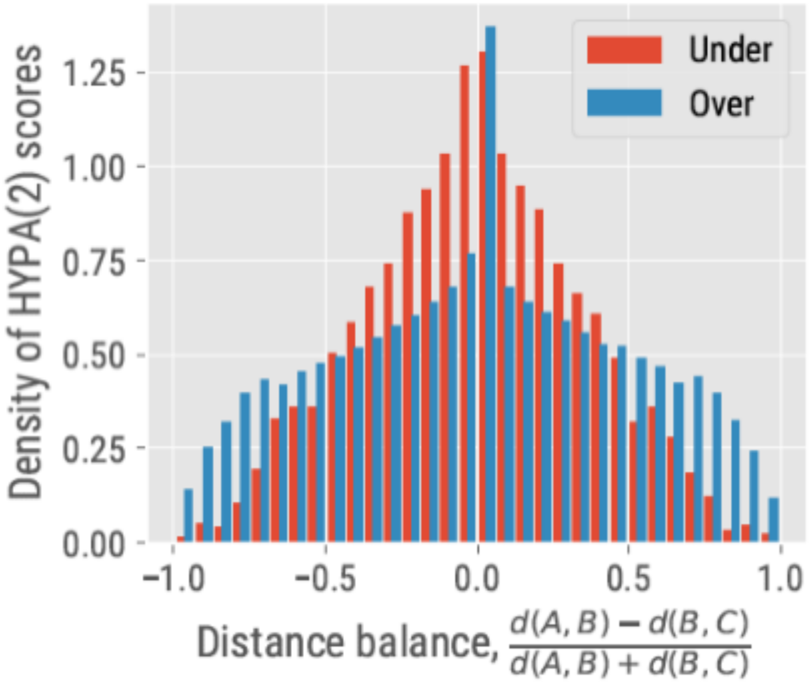
2. Over-represented non-return flights are due to regional/national hubs, since people need to fly from small airports → regional hub → large airport.

Airlines: Trip Balance

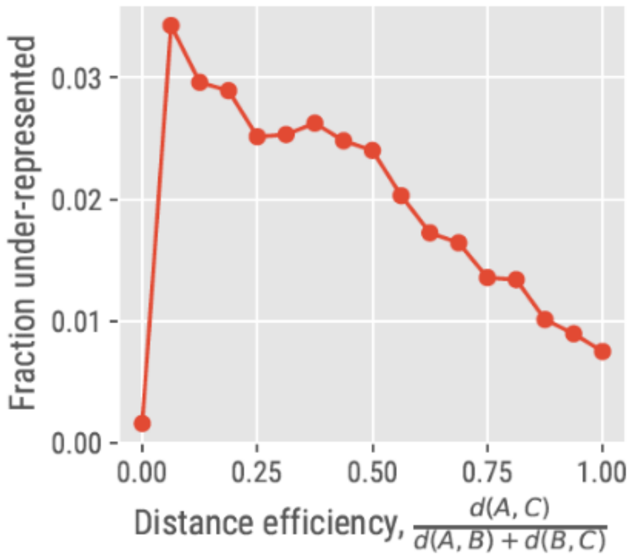


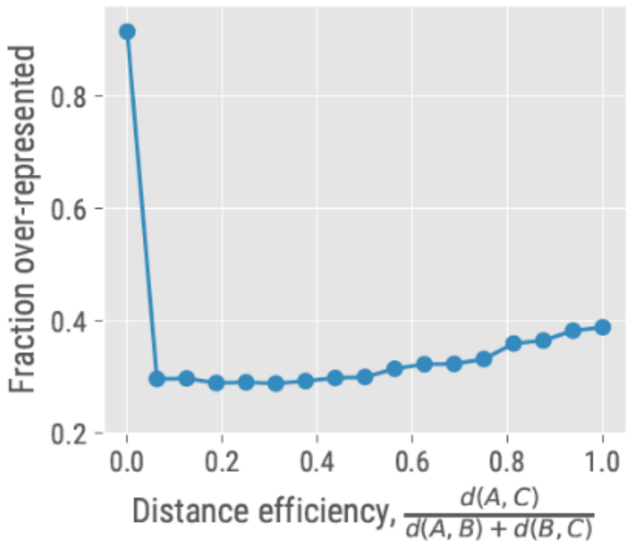
Airlines

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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References

Scholtes, Ingo. "When is a network a network?: Multi-order graphical model selection in pathways and temporal networks." *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. ACM, 2017.

Casiraghi, Giona, et al. "Generalized hypergeometric ensembles: Statistical hypothesis testing in complex networks." *arXiv preprint arXiv:1607.02441* (2016).

Transport for London Open Data: https://tfl.gov.uk/info-for/open-data-users/

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 $\vec{v} := v_0 v_1 \vec{\ldots} v_{k-1} \in V^k$ 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 $i = 0, \ldots, k-2$.

Hypergeometric Ensemble

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

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

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

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Hypergeometric Ensemble

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

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

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

Hypergeometric Ensemble

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

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

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

Hypergeometric Ensemble

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

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

$$Pr(X_{vw} = f(v,w)) \propto \binom{K_{vw}}{f(v,w)} \binom{\sum_{ij} K_{ij} - K_{vw}}{\underbrace{m - f(v,w)}_{\text{Number of ways to pick everything else.}}}$$

Putting it all together: HYPA scores

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

Pseudocode

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

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

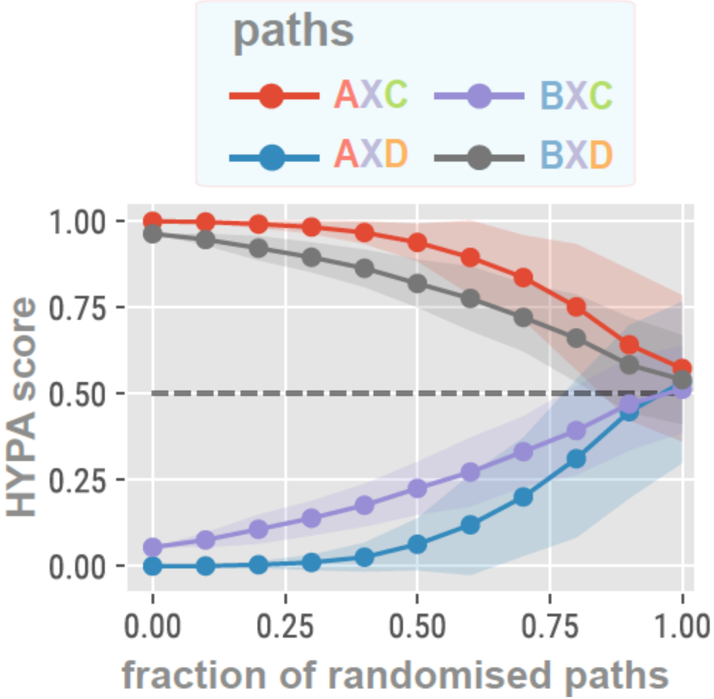
1: $G^k \leftarrow$ DeBruijnGraph(S, k) # Construct kth order graph

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: $\quad \mathrm{HYPA}^{(k)}(\vec{v}, \vec{w}) \leftarrow \Pr(x_{vw} \leq (\vec{v}, \vec{w}) \mid m, \Xi)$
$\quad$ # Compute CDF
5: **return** $\mathrm{HYPA}^{(k)}$

Validation

Noise via Path Randomization



Synthetic Anomalies: Setup

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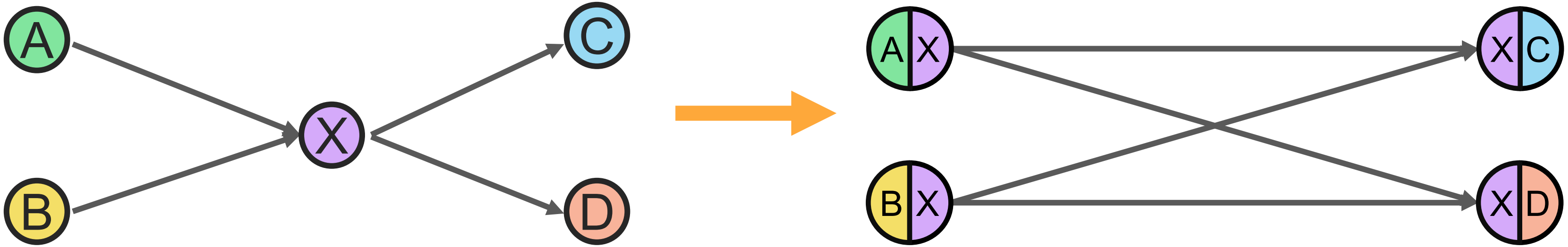
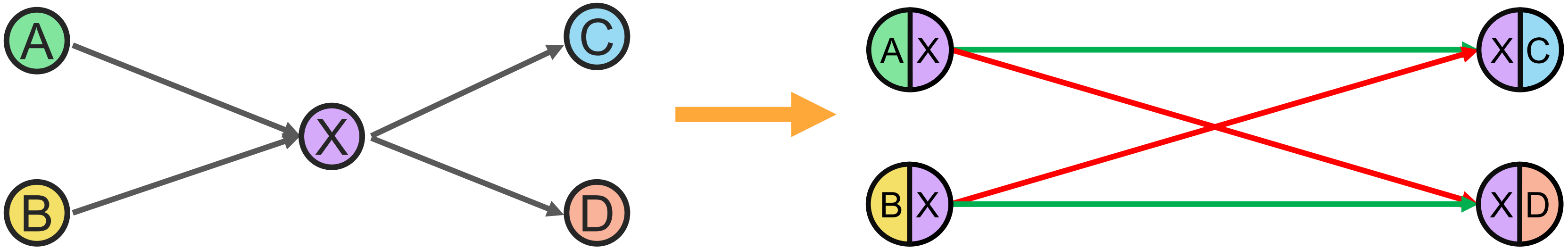
Start with an arbitrary first order topology, then construct the *kth*-order de Bruijn graph



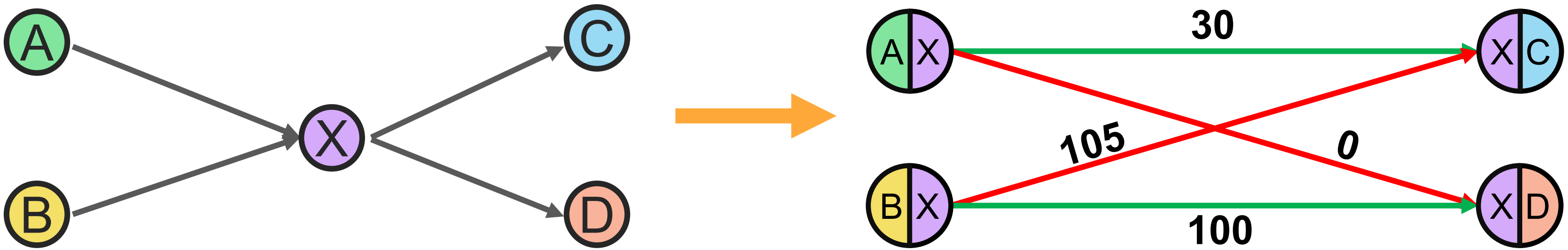
Synthetic Anomalies: Setup

Randomly choose some edges to label over-represented



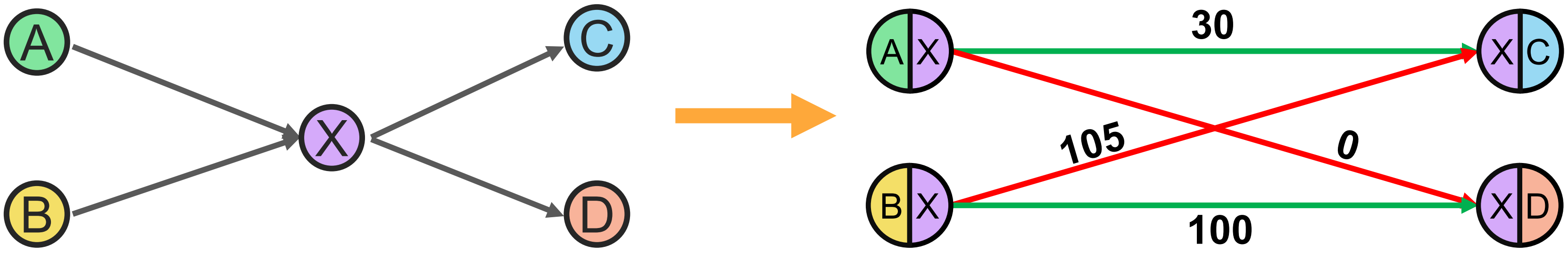
Synthetic Anomalies: Setup

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).



Synthetic Anomalies: ROC Example

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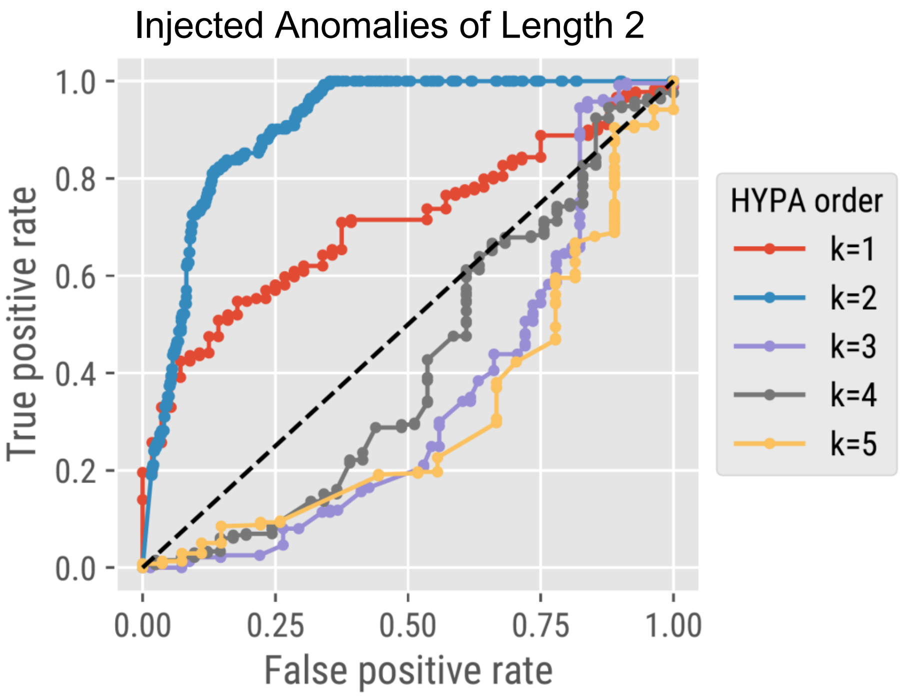

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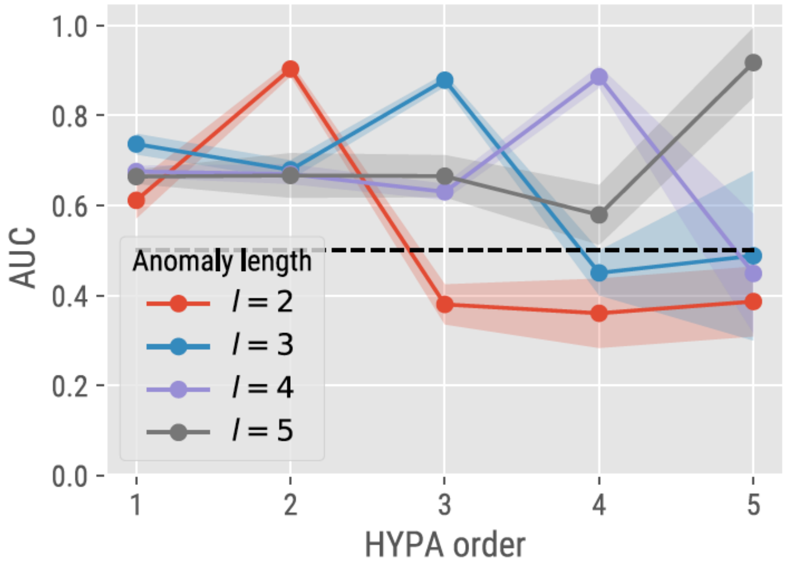
Synthetic Anomalies: AUC Results



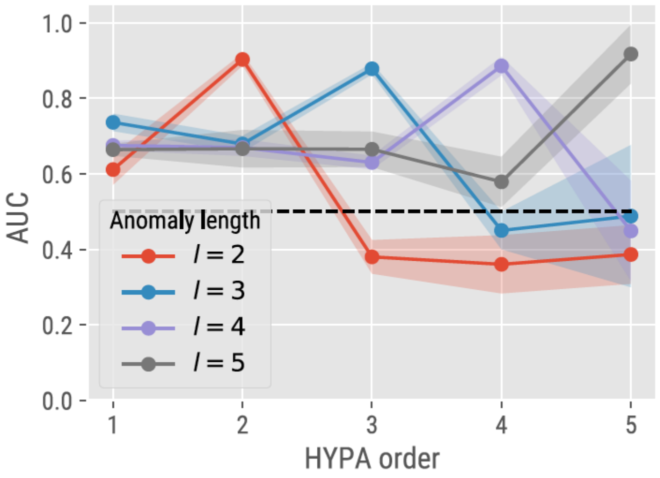
Naïve Baseline Comparison

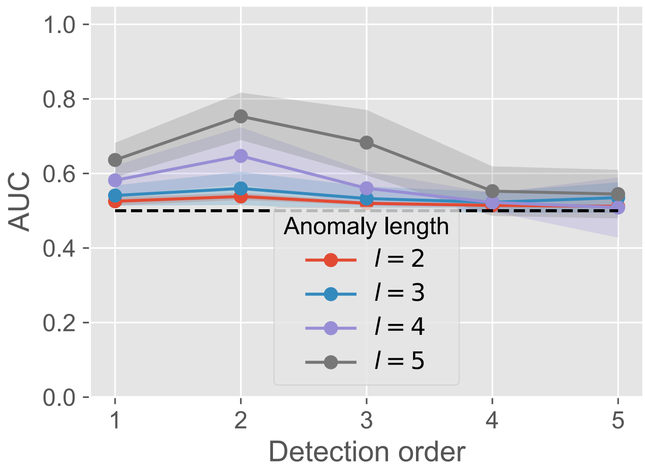
Frequency-Based Anomaly Detection (FBAD)

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

Given scaling factor α, label edges with frequencies larger than $\mu + \sigma\alpha$ over-represented, and smaller than $\mu - \sigma\alpha$ under-represented

Synthetic Anomalies

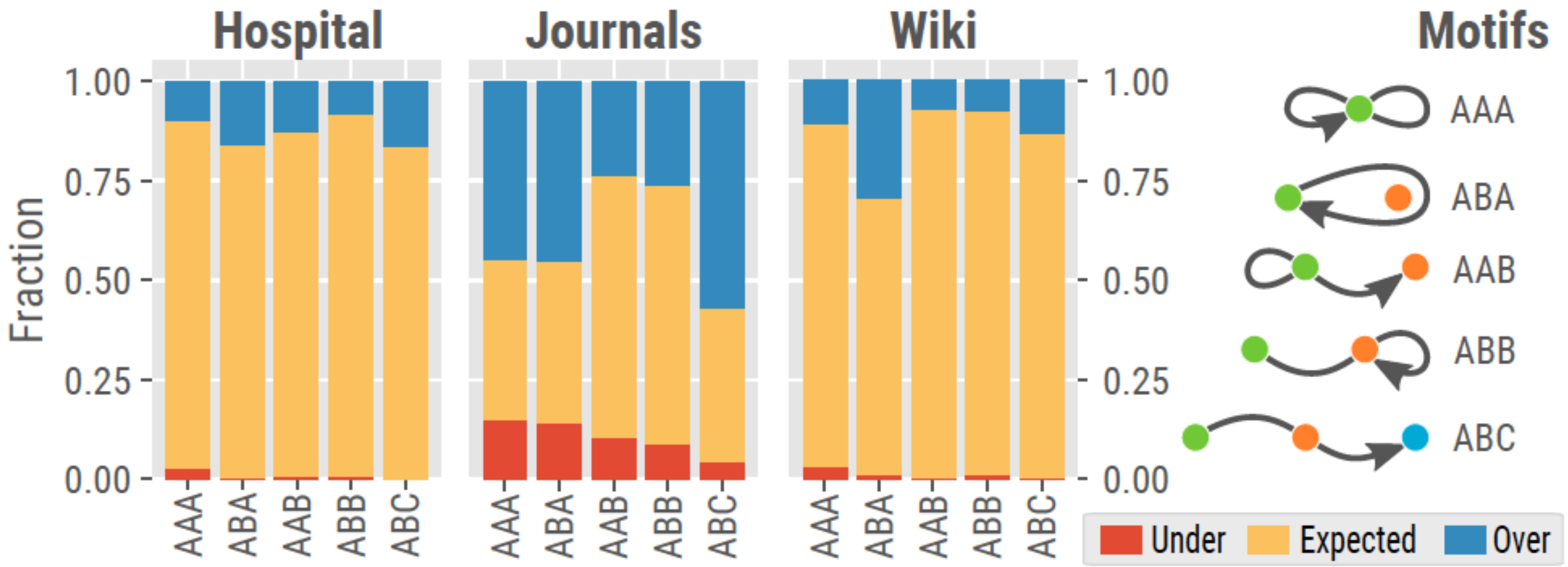




Real Data

	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

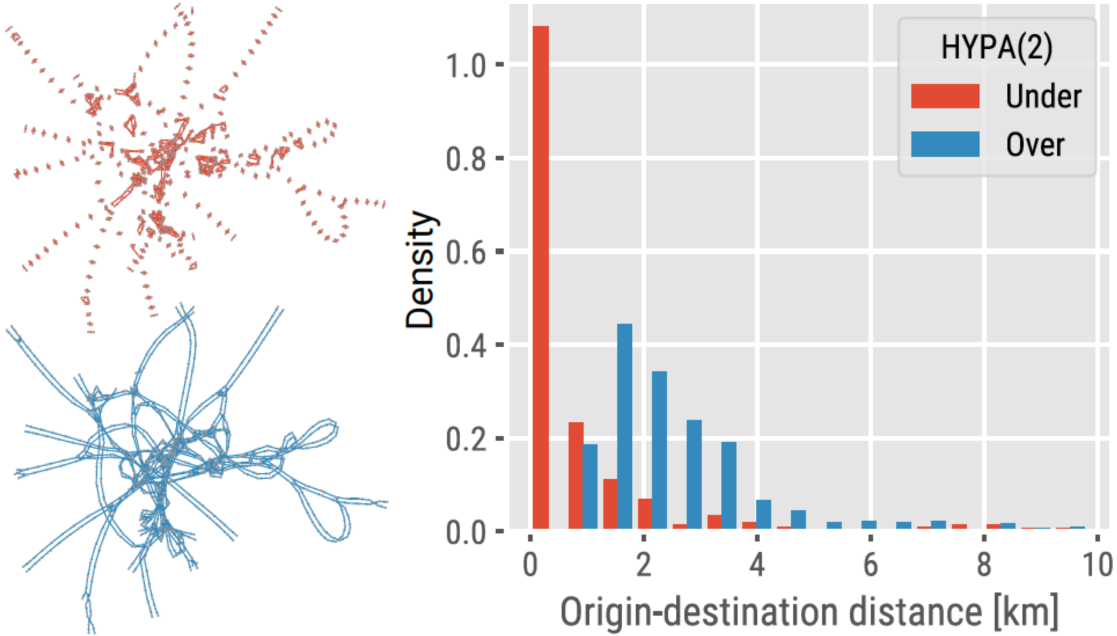
Hypothesis:

- 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


HYPA(2)
Under
Over
Density
Origin-destination distance [km]
0.0
0.2
0.4
0.6
0.8
1.0
0
2
4
6
8
10

London Tube

$\mathrm{HYPA}^{(k)}$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
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

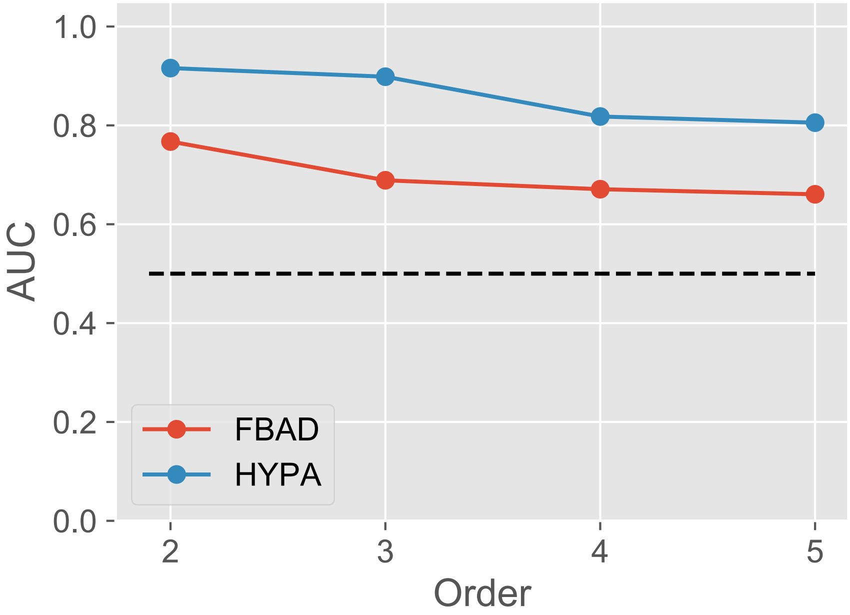
Median distance between source and destination nodes in under/over represented transitions.

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



Hypergeometric Ensemble

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

$$\Xi_{ij} = k_i^{out} k_j^{in}$$

$$\Pr\left(X_{\vec{v}\vec{w}} = f(\vec{v},\vec{w})\right) = \binom{\sum_{ij}\Xi_{ij}}{m}^{-1} \binom{\Xi_{vw}}{f(\vec{v},\vec{w})} \binom{\sum_{ij}\Xi_{ij} - \Xi_{vw}}{m - f(\vec{v},\vec{w})}$$

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

Hypergeometric Ensemble

$$\Xi_{ij} = k_i^{out} k_j^{in}$$

$$\Pr(X_{\vec{v}\vec{w}} = f(\vec{v}, \vec{w})) = \binom{\sum_{ij} \Xi_{ij}}{m}^{-1} \binom{\Xi_{vw}}{f(\vec{v}, \vec{w})} \binom{\sum_{ij} \Xi_{ij} - \Xi_{vw}}{m - f(\vec{v}, \vec{w})}$$

Probability of observing frequency $f(\vec{v}, \vec{w})$ given the entire weighted network structure.

Hypergeometric Ensemble

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

$$\Xi_{ij} = k_i^{out} k_j^{in}$$

$$\Pr\left(X_{\vec{v}\vec{w}} = f(\vec{v}, \vec{w})\right) = \underbrace{\binom{\sum_{ij} \Xi_{ij}}{m}^{-1}}_{} \binom{\Xi_{vw}}{f(\vec{v}, \vec{w})} \binom{\sum_{ij} \Xi_{ij} - \Xi_{vw}}{m - f(\vec{v}, \vec{w})}$$

Normalization. Total number of ways to pick m multiedges from total possible.

Hypergeometric Ensemble

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

$$\Xi_{ij} = k_i^{out} k_j^{in}$$

$$\Pr\left(X_{\vec{v}\vec{w}} = f(\vec{v},\vec{w})\right) = \binom{\sum_{ij}\Xi_{ij}}{m}^{-1} \binom{\Xi_{vw}}{f(\vec{v},\vec{w})} \binom{\sum_{ij}\Xi_{ij} - \Xi_{vw}}{m - f(\vec{v},\vec{w})}$$

Number of ways to pick $f(\vec{v},\vec{w})$ multiedges from $\Xi_{\vec{v}\vec{w}}$ possible.

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

Hypergeometric Ensemble

$$\Xi_{ij} = k_i^{out} k_j^{in}$$

$$\Pr\left(X_{\vec{v}\,\vec{w}} = f(\vec{v}, \vec{w})\right) = \binom{\sum_{ij} \Xi_{ij}}{m}^{-1} \binom{\Xi_{vw}}{f(\vec{v}, \vec{w})} \underbrace{\binom{\sum_{ij} \Xi_{ij} - \Xi_{vw}}{m - f(\vec{v}, \vec{w})}}_{\text{Number of ways to pick everything else.}}$$