Recovery of Vertex Orderings in Dynamic Graphs: Algorithms for a General Solution

Krzysztof Turowski*, Jithin K. Sreedharan*, and Wojciech Szpankowski

Center for Science of Information, Dept. of Computer Science
Purdue University, West Lafayette, IN, USA
{ksturowsk, jithinks, szpan}@purdue.edu
*Authors contributed equally.

Abstract. Dynamic networks model important processes in diverse applications, from spread of infectious diseases to flow of capital in economic systems. The arrival order of nodes in such networks reveals critical insights into their structural and functional organization. In typical applications, the state of a dynamic network is available as a snapshot in time, and one must infer a node arrival order from it. We formulate a more general problem that infers a partial order or clusters of node arrivals. We provide nearly-optimal and approximate solutions to the associated optimization problem that is suitable for any dynamic graph model with only node and edge additions. Finally our methods are validated for a particular graph model through experiments on both synthetic and real-world networks.

1 Introduction

Clustering of nodes is a classic problem in networks. In its typical form, it finds communities in static networks, where methods like modularity maximization, minimum-cut method and hierarchical clustering are commonly used. On the other hand, in dynamic or growing networks clustering must take into account notions of time. One such an approach is labeling nodes according to their arrival order. In many real-world networks and graph models, it is impossible to find a complete order of arrival of nodes due to symmetries inherent in the graph. Figure 1 shows an example of such a situation. In such cases, it is ideal to classify nodes that are indistinguishable themselves in terms of arrival order into temporal clusters.

![Figure 1](image-url)

**Fig. 1:** Example showing how temporal clustering arises: here $u$ and $v$ are indistinguishable as they have the same set of neighbors. Thus a unique total node arrival order is not possible and $u$ and $v$ should end up in the same temporal cluster.
Temporal ordered clustering finds many application in practice. For example, specific information targeted at nodes arrived around the same time could be disseminated in online social networks. In biological networks, it helps to identify the evolution of biomolecules in the network. In rumor or epidemic networks, we can identify the sources and carriers of certain false information.

**Our contributions.** We provide a general framework for solving temporal ordered clustering in growing networks if only one snapshot of the evolution is given. The framework does not make any assumptions about the graph model. With the knowledge of probabilistic evolution of the graph model, one could find the estimator that output the optimal partial order.

In order to solve the optimal temporal ordered clustering problem, we must estimate, for any node pair \((u, v)\), the probability that node \(u\) is older than node \(v\), denoted by \(p_{uv}\). We build a generalized Markov chain based sequential importance sampling Monte Carlo algorithm, and found a low complexity solution with a importance sampling distribution. In case of huge networks, when the complexity for solving the optimization is higher, we make use of the approximate solutions that apply the estimated \(p_{uv}\).

Moreover when the real networks may not fit well within the probabilistic graph model under consideration, we develop supervised techniques along to improve estimation precision. Use of supervised learning techniques by exploiting the graph structure enhances the estimated values of \(p_{uv}\) quickly, with a small percentage of training data unlike the traditional machine learning algorithms.

In the final sections of the paper, as an application of general techniques, we focus on duplication-divergence (vertex copying) growing model in which, informally, a new node copies the edges of a randomly selected existing node and retains them with a certain probability. It also adds random connections from the new node to remaining nodes. We focus on the duplication-divergence mode due to the following reasons:

- **Non-equiprobable permutations:** In many of the graph models including preferential attachment graph model, all the feasible permutations for finding the total order are equally likely [4]. Later in this paper, we show that this is not the case in duplication-divergence model.
- **Large number of symmetry:** We provide evidence of large number of automorphisms in duplication-divergence graph, which is not the case in Erdős-Rényi and preferential attachment graphs for certain set of parameters.
- **Ineffectiveness of degree based techniques:** In some models including preferential attachment graph, the oldest nodes tend to have large degree than the youngest nodes. But for duplication-divergence, we derive that the average degree of a node \(\text{deg}_t(s)\), which arrived at time \(s\), at a later time \(t\) is of order (with known constants) \((t/s)^p s^{2p-1}\). Note that when for \(s = O(1)\) - very old nodes - the degree is of order \(t^p\). And for \(s = t\) we have \(\text{deg}_t(t) = O(t^{2p-1})\) which for \(p > 1/2\) is growing. For example when \(p = 1\) all degrees on average are of order \(O(t)\). Thus any algorithm based on degree is bound to fail in duplication-divergence model, and it leads us to develop efficient algorithms for this model.
Prior related work. Node arrival order in duplication-divergence model has been studied in some of the previous works (see [3] and [5] and the references therein). Most of the prior works focus on getting the complete arrival order of nodes (total order), which we show here that for large graphs with most of the parameter setting total order is not better than a random guessing. Instead in this work we focus on deriving partial order of nodes that provides a clustering structure for the nodes. Our basic methods are general and applicable to any general graph models too. For the preferential attachment model our recent work [7] considers partial order inference, but the methods are specific to preferential attachment and not extendable to a general graph model.

Notation. In the following π always represents a uniform random permutation from \( S_n \), where \( n \) is implied from the context. Let \( G_n, G_n, \overline{G}_n \) be the deterministic graph, random graph from the model under consideration and the set of graphs with \( n \) nodes. Similar definition holds for \( H_n \) and \( \overline{H}_n \), but with \( \overline{H}_n = \pi(G_n) \). We label the vertices in the original graph \( G \) in their arrival order, \([n] = \{1, ..., n\}\), where node \( j \) is the \( j \)th node to arrive. For a Markov chain \( \{X_k\}_{k \geq 0} \) with transition probability matrix \( P \), \( \mathbb{E}_x[\cdot] \) indicate expectation with respect to its sample paths starting from \( X_0 = x \).

2 Problem Formulation

Let \( H_n \) be the observed graph of \( n \) nodes with \( V(H_n) \) as the set of vertices and \( E(H_n) \) as the set of edges. The graph \( H_n \) is assumed to be evolved over time, starting from a seed graph \( H_{n_0} \) of \( n_0 \) nodes. At a time instant \( k \), when a new node appears and a set of new edges are added with one endpoint at the new node, the graph \( H_k \) will evolve into \( H_{k+1} \). Since the change in graph structure occurs only when a new node is added, assuming addition of a node as a time epoch, \( H_n \) also represents graph at time epoch \( n \).

Given only one snapshot of the dynamic graph \( H_n \), we usually do not know the time or order of arrivals of nodes. Our goal is to label each node with a number \( i \), \( 1 \leq i \leq K \), such that all the nodes labeled by \( i \) arrived before nodes with labels \( j \) where \( j > i \). The number of clusters (labels) \( K \) is unknown a priori, and is part of the optimal clustering formulation. Let \( C_i \) denote the set of nodes which carry label \( i \). We note here that unlike the classical clustering, on top of the objective of the clustering, these clusters are ordered such that \( C_1 < C_2 \ldots < C_K \).

The arrival of a new node and the strategy it uses to choose the existing nodes to make connections depend on the graph generation model. We thus express the above formulation in the following way. Let \( G_n \) be a graph drawn from a dynamic random graph model \( G_n \) on \( n \) vertices in which nodes are labeled \( 1, 2, \ldots, n \) according to their arrival, i.e., node \( j \) was the \( j \)th node to arrive. Let \( G_n \) be evolved from the seed graph \( G_{n_0} \). To model the lack of knowledge of the original labels, we subject the nodes to a permutation \( \pi \) drawn uniformly at

\[ \text{The time epoch } t_0 \text{ denotes the creation of } G_{n_0} \text{ or } H_{n_0} \text{ graph} \]
random from the symmetric group on \( n \) letters \( S_n \), and we are given the graph
\( H_n := \pi(G_n) \); that is, the nodes of \( G_n \) are randomly relabeled. Our original goal is to infer the arrival order in \( G_n \) after observing \( H_n \), i.e., to find \( \pi^{-1} \). The permutation \( \pi^{-1} \) gives the true arrival order of the nodes of the given graph.

Instead of putting constraint on recovering total order (i.e., recovery of \( \pi^{-1} \) that requires \( K = n \) in terms of the cluster labeling formulation), we resort to strict partial orders (without reflexive condition). For a partial order set \( \sigma \), a relation \( u \prec_{\sigma} v \) means that \( u \) is less than \( v \) in \( \sigma \), that is, node \( u \) is older than node \( v \). Every partial order \( \sigma \) can be represented by bins (clusters) \( \{C_i\} \) as follows.

A strict partial order set can be represented initially by a directed acyclic graph (DAG) with nodes as the nodes in the graph \( H_n \) and directed edges as given by \( \sigma \), like an edge from \( v \) to \( u \) exists when \( u \prec_{\sigma} v \). Then taking the transitive closure of this DAG will result in the DAG of the partial order set \( \sigma \). Now, all the nodes with in-degree 0 will be part of cluster \( C_K \) and the set of nodes with all the in-edges coming from nodes in \( C_K \) will form cluster \( C_{K-1} \). This process repeats until we get \( C_1 \). The number of clusters \( K \) is not define before, but found from the DAG structure.

We define an estimator \( \phi \) of the node age recovery problem as a function \( \phi : G_n \to S_n \), where \( S_n \) is the set of all partial orders of nodes 1, ..., \( n \).

We consider estimators based on unsupervised and supervised algorithms:

- Unsupervised: In this case the node arrival order estimator does not assume any knowledge of arrival order of some nodes. Since the estimator should designed incorporating intricacies of a graph model, the results of unsupervised estimator will be purely based on the assumption that the graph model fits well the real-world network under consideration.

- Supervised: In some of the real-world networks, partial information of the order of nodes is known. Taking this information into account would help the estimator to more tailor towards the real-data. We call such information as perfect pairs, that exists with probability 1. The estimator learns the partial orders in the data without violating the perfect pairs.

Measures for evaluating partial order. For a partial order \( \sigma \), let \( K(\sigma) \) denote the number of pairs \( (u, v) \) that are comparable under \( \sigma \): i.e., \( K(\sigma) = |\{(u, v) : u \prec_{\sigma} v\}| \), where \( |K(\sigma)| \leq \binom{n}{2} \).

Density: the density of a partial order \( \sigma \) is simply the number of comparable pairs, normalized by the total possible number, \( \binom{n}{2} \). That is, \( \delta(\sigma) = \frac{K(\sigma)}{\binom{n}{2}} \). Note that \( \delta(\sigma) \in [0, 1] \). Then the density of a partial order estimator \( \phi \) is simply its minimum possible density \( \delta(\phi) = \min_H[\delta(\phi(H))] \).

Measure of precision: this measures the expected fraction of correct pairs out of all pairs that are guessed by the partial order. It is given by

\[
\theta(\sigma) = \mathbb{E} \left[ \frac{1}{K(\sigma)} |\{u, v \in [n] : u \prec_{\sigma} v, \pi^{-1}(u) < \pi^{-1}(v)\}| \right].
\]

For an estimator \( \phi \), we also denote by \( \theta(\phi) \) the quantity \( \mathbb{E}[\theta(\phi(\pi(G)))] \).
3 Formulation and Solution of an Optimization Problem

The precision of a given estimator $\phi$ can be written in the form of a sum over all graphs $H$:

$$
\theta(\phi) = \sum_{H} \Pr[\pi(G) = H] \frac{1}{K(\phi(H))} \times \mathbb{E}\left[\left|\{u, v \in [n] : u <_{\phi(H)} v, \pi^{-1}(u) < \pi^{-1}(v)\}\right| \pi(G) = H\right]
$$

Here $\pi$ and $G$ are the random quantities in the conditional expectation. We formulate the optimal estimator as the one that gives maximum precision for a given minimum density. To form the optimal estimator, it is then sufficient to choose, for each $H$, a partial order $\phi(H)$ that maximizes the expression

$$
J_\varepsilon(\phi) := K(\phi(H))^{-1} \mathbb{E}\left[\left|\{u, v \in [n] : u <_{\phi(H)} v, \pi^{-1}(u) < \pi^{-1}(v)\}\right| \pi(G) = H\right]
$$

subject to the density constraint that $K(\phi(H)) \geq \varepsilon^{(n)}_2$.

3.1 Integer programming formulation

In this subsection we recall and extend some results from our recent work in [7]. We now represent the optimization problem with $J_\varepsilon(\phi)$ as an integer program (IP). For an estimator $\phi$, we define a binary variable $x_{u,v}$ for each ordered pair $(u,v)$ as $x_{u,v} = 1$ when $u <_{\phi(H)} v$. Note that $x_{u,v} = 0$ means either $u <_{\phi(H)} v$ or the pair $(u,v)$ is incomparable in the partial order $\phi(H)$. Let $p_{u,v}(H) = \Pr[\pi^{-1}(u) < \pi^{-1}(v)|\pi(G) = H]$ be the probability that $u$ arrived before $v$ given the relabeled graph $H$.

In the following, we write the optimization in two forms: the original integer program (left) and the linear programming approximation (right). The objective functions of both the formulations are equivalent to $J_\varepsilon(\phi)$. The constraints of the optimizations correspond to domain restriction, minimum density and partial order constraints - antisymmetry and transitivity respectively. To use a linear programming (LP) approximation, we first convert the rational integer program into an equivalent truly integer program. With the substitution $s = 1/\sum_{1 \leq u < v \leq n} x_{u,v}$, and $y_{u,v} = sx_{u,v}$, the objective function rewritten as a linear function of the normalized variables. The new variables $y_{u,v}$ takes values from $\{0, s\}$. In fact, taking $s = \frac{1}{\varepsilon^{(n)}_2}$ is enough for the equivalence. For the LP relaxation, we assume the domain of $y_{u,v}$ as $\left[0, 1/\varepsilon^{(n)}_2\right]$. 
Original integer program

\[
\max \sum_{1 \leq u \neq v \leq n} p_{u,v}(H)x_{u,v}
\]
subject to
\[
x_{u,v} \in \{0, 1\}, \forall u, v \in [n]
\]
\[
\sum_{1 \leq u \neq v \leq n} x_{u,v} \geq \binom{n}{2}
\]
\[
x_{u,v} + x_{v,u} \leq 1, \forall u, v \in [n]
\]
\[
x_{u,w} \geq x_{u,v} + x_{v,w} - 1, \forall u, v, w \in [n].
\]

The next lemma bounds the effect of approximating the coefficients \(p_{uv}\) on the optimal value of the integer program.

**Lemma 1.** Consider the integer program whose objective function is given by \(\hat{J}_{\epsilon,\lambda}(\phi) = \sum_{1 \leq u \neq v \leq n} \hat{p}_{u,v}(H)x_{u,v} / \sum_{1 \leq u \neq v \leq n} x_{u,v}\), with the same constraints as in the original IP. Assume \(p_{u,v}(H)\) can be approximated with \(|\hat{p}_{u,v}(H) - p_{u,v}(H)| \leq \lambda\) uniformly for all \(u, v\). Let \(\hat{\phi}_1\) and \(\hat{\phi}_2\) denote optimal points for the original and modified integer programs, respectively. Then \(|\hat{J}_{\epsilon,\lambda}(\hat{\phi}_1) - \hat{J}_{\epsilon,\lambda}(\hat{\phi}_2)| \leq 3\lambda\), for arbitrary \(\lambda > 0\).

The proof of the above lemma is an extension of a similar lemma in [7]. But in [7], we assume \(|\hat{p}_{uv}/p_{uv} - 1| \leq \lambda\), which is a stronger condition than our present assumption \(|\hat{p}_{uv} - p_{uv}| \leq \lambda\).

### 3.2 Estimating coefficients of optimal precision integer program

Let \(\Gamma(H_t)\) be the set of all permutations \(\sigma\) which has a positive probability for \(\sigma(H_t)\) under the graph generation model. We have, for \(p_{uv} := \P(\pi^{-1}(u) \leq \pi^{-1}(v)|\pi(G_t) = H_t, i)\),

\[
p_{uv} = \sum_{\sigma : \sigma^{-1}(\Gamma(H))} \P(\pi = \sigma|\pi(G_t) = H_t) = \sum_{\sigma : \sigma^{-1}(\Gamma(H))} \frac{\P[\pi = \sigma, \pi(G_t) = H_t]}{\P[\pi(G_t) = H_t]}
\]

\[
= \sum_{\sigma : \sigma^{-1}(\Gamma(H))} \frac{\P[\pi = \sigma^{-1}(H_t)]}{\P[\pi(G_t) = \sigma^{-1}(H_t)]},
\]

when we assume \(\P[\pi = \sigma]\) independent of \(H_t\) as \(1/n!\) (or any other distribution).

**A Markov chain approach to approximate** \(p_{uv}\). Let \(R_{H_t} \subset V(H_t)\) be the set of possible candidates for youngest nodes at time \(t\), and let \(R_{H_t}(v)\), represents possible parents of \(v\) in \(H_t\), i.e., the nodes \(v\) selects for duplication.
The set $\mathcal{R}_{H_t} \subset V(H_t)$ depends on the graph model. For e.g., in case of preferential attachment model, in which a new node attaches $m$ edges to the existing nodes with a probability distribution proportional to the degree of the existing node, $\mathcal{R}_{H_t}$ is the set of $m$-degree nodes. We consider only permutations that do not change the initial graph $G_{t_0}$ labels. For example, if $G_{t_0}$ has three nodes and $G_t$ has 6 nodes, we consider the following permutations (represented in cyclic notation): $(1)(2)(3)(456)$, $(1)(2)(3)(45)(6)$, $(1)(2)(3)(46)(5)$, $(1)(2)(3)(4)(56)$, $(1)(2)(3)(4)(5)(6)$. Thus we define $H_{t_0}$ as $G_{t_0}$ itself.

Let $\delta(H_t, v_t)$ represent the graph in which node $v_t$ is deleted from $H_t$, where $v_t \in \mathcal{R}_{H_t}$. Then the graph sequence $\mathcal{H}_t = H_t, \mathcal{H}_{t-1} = \delta(H_t, v_t), \ldots, \mathcal{H}_{t_0} = H_{t_0}$ forms a nonhomogeneous Markov chain – nonhomogeneous because the state space $\{\mathcal{H}_s\}_{s \leq t}$ changes with $s$ and thus the transition probabilities too. Similarly $\mathcal{G}_t, \mathcal{G}_{t-1}, \mathcal{G}_{t_0}$ also make a Markov chain, and for a fixed permutation $\sigma$, $\sigma(G) = H$, both the above Markov chains have same transition probabilities.

Note that the posterior probability of producing $H_t$ from $\delta(H_t, v_t)$ is given by

$$w(\delta(H_t, v_t), H_t) := \mathbb{P}[\mathcal{H}_t = H_t | \mathcal{H}_{t-1} = \delta(H_t, v_t)]$$

The following theorem characterizes our estimator.

**Theorem 1.** Consider a time-nonhomogeneous Markov chain $\mathcal{H}_t = H_t, \mathcal{H}_{t-1} = \delta(H_t, v_t), \ldots$, where $v_t \in \mathcal{R}_{H_t}, v_{t-1} \in \mathcal{R}_{H_{t-1}}, \ldots$ be the nodes removed randomly by the Markov chain and let its transition probability matrices be $\{q_s = [q_{s}(\mathcal{H}_t, \mathcal{H}_j)]\}_{s \leq t}$ with $\mathcal{H}_t \in \mathcal{G}_s$ and $\mathcal{H}_j \in \mathcal{G}_{s-1}$. Then we have

$$\sum_{\sigma^{-1} \in \Pi(H_t)} \mathbb{P}[\mathcal{G}_t = \sigma^{-1}(H_t) | H_0] = \mathbb{E}_{\mathcal{H}_t = H_t} \left[ \prod_{s \leq t} \frac{w(\delta(H_s, v_s), H_s)}{q_s(\mathcal{H}_s, \delta(H_s, v_s))} \right].$$

The proof of the theorem is given in Appendix A. Note that unlike $q_t(H_s, \delta(H_t, v_t))$, which is under our control to design a Markov chain, $w(\delta(H_t, v_t), H_t)$ is well defined fixed quantity (see (3)). The only constraint for the transition probability matrices $\{q_s\}_{s \leq t}$ is that it should be chosen to be in agreement with the graph evolution such that the choices of jumps from $H_s$ to $H_{s-1}$ restricts to removing nodes from $\mathcal{R}_{H_s}$. In other words, the Theorem 1 gives a sequential importance sampling strategy with normalized terms.

Now we can form the estimator for $p_{st}$ for a node pair $(s, t)$ as follows. Let $v^{(k)}$ be the vector denoting the sampled node sequence of the $k$th run of the Markov chain. It can either represent a vector notation as $v^{(k)} = (v^{(k)}_t, v^{(k)}_{t-1}, \ldots, v^{(k)}_{t_0})$ or take a function form $v^{(k)}(s)$ denoting the new label of a vertex $s$ in $H$. The estimator $\hat{p}_{st}^{(k)}$ is now, for all $s, t \in H$

$$\hat{p}_{st}^{(k)} = \frac{\sum_{i=1}^{k} 1_{v^{(i)}(s) < v^{(i)}(t)} \prod_{s \leq t} w(\delta(H_s, v^{(i)}), H_s)}{\sum_{i=1}^{k} \prod_{s \leq t} w(\delta(H_s, v^{(i)}), H_s)}$$

(2)
4 Approximating optimal solution

In this section, we describe our main algorithms for node arrival order recovery of a general graph model.

**Algorithms for sampling the Markov chain.** Finding the whole set of permutations and calculating the exact $p_{uv}$ according to (1) is of exponential complexity. With Theorem 1, we approximate $p_{uv}$ using the empirical average of two Markov chain based sampling schemes. We try two different importance sampling distributions $\{Q_s\}_{s \leq t}$.

- **local-unif-sampling**: This algorithm has the transition probabilities

$$q_s(H_s, \delta(H_s, v_s)) = \frac{1}{|R_{H_s}|}.$$ 

- **high-prob-sampling**: This technique forms the Markov chain with

$$q_s(H_s, \delta(H_s, v_s)) = \frac{w(\delta(H_s, v_s), H_s)}{\sum_{u \in R_{H_s}} w(\delta(H_s, u), H_s)}.$$

The above transition probability corresponds to choosing the high probability paths.

Though **high-prob-sampling** is right approach to follow in theoretical terms, as we show later in Section 6.1, it has much lower rate of convergence than **local-unif-sampling**. Moreover at each step $s$, **high-prob-sampling** requires $O(n^2)$ computations, while **local-unif-sampling** requires only $O(n)$.

The **local-unif-sampling** can be further improved with acceptance-rejection sampling: at a step $t$, randomly sample a node $u$ from $V(H_t)$ (instead of sampling from $R_{H_t}$). Then calculate the probability that the node $u$ be the youngest node in the graph. If this probability is positive, we accept $u$ as $V_t$ and if it is zero, we randomly sample again from $V(H_t)$.

Now we assume that $p_{uv}$ are estimated for all $u$ and $v$ to propose algorithms for temporal clustering. In fact, according to Lemma 1, we only need to have $\max_{u,v} |\hat{p}_{uv} - p_{uv}| \leq \lambda$ for a small $\lambda > 0$. Thus for small $p_{uv}$, $\hat{p}_{uv}$ can be assumed to be zero. We propose the following supervised and unsupervised algorithms based on the estimates of $p_{uv}$.

4.1 Unsupervised solution

**sort-by-$p_{uv}$-sum algorithm.** Using the estimated $p_{uv}$, we assume a new complete graph with nodes same as that of $H_n$ and edge weights as $p_{uv}$. A metric $p_u := \sum_{v \in V} p_{uv}$ is defined for all nodes $u$ of $H_n$. Since $p_{uv}$ denotes the probability that node $u$ is older than node $v$, $p_u$ would give a high score when a node $u$ becomes the oldest node. Our ranking is then sorted order of the $p_u$ values.

Instead of a total order, a partial order can be found by a simple binning over $p_u$ values: fix the bin size $|C|$ and group $|C|$ nodes in the sorted $p_u$ values into a cluster, and the process repeats for other clusters.
Here, each of the estimated $p_{uv}$’s is compared against a threshold $\tau$. Only the node pairs that are strictly greater than this condition are put into the estimator output partial order. Note that if $\tau = 0.5$, we get a total order in virtually all relevant cases.

### 4.2 Supervised solution

Suppose we have partial true data available. Let it be ordered in partial order as $\sigma_{\text{orig}} = \{(u,v)\}$, in which for the pair $(u,v)$, $u$ is the older than $v$. Let $\sigma_{\text{train}} \subset \sigma_{\text{orig}}$ be the training set and the let the test set be $\sigma_{\text{test}} := \sigma_{\text{orig}} \setminus \sigma_{\text{train}}$. Let $|\sigma_{\text{train}}| = \alpha |\sigma_{\text{orig}}|$ for some $0 < \alpha < 1$. With the knowledge of $\sigma_{\text{train}}$, we modify the the estimation of $p_{uv}$ as follows. The set of removable nodes $R_H$ at each instant is modified to $R_H \setminus N \cap R_H$, where $N \cap R_H$ is the set of nodes that cannot be included in the removable nodes as it would violate the partial order of $\sigma_{\text{train}}$. It is defined as follows:

$$N \cap R_H := \{u : (u,v) \in \sigma_{\text{train}}, u, v \in V(H_i)\}.$$  

After estimating $p_{uv}$ with the redefined $R_H$, we employ sort-by-$p_{uv}$-sum algorithm and $p_{uv}$-threshold algorithms to find partial order. An example of $R_H$ construction is shown in Figure 2.

![Fig. 2: Supervised learning example DAG for $\sigma_{\text{train}} = \{(u,v),(v,w),(w,x),(y,w)\}$: $N \cap R_H = \{v,w,x\}$ and $R_H = \{u,y,z\}$.](image)

### 5 Node Arrival Order Recovery in Duplication-Divergence Model

#### 5.1 Duplication-divergence model

We consider Pastor-Satorras et al. version of duplication-divergence model [6]. It proceeds as follows. Given an undirected, simple, seed graph $G_{n_0}$ on $n_0$ nodes and target number of nodes $n$, the graph $G_{k+1}$ with $k + 1$ nodes evolves from the graph $G_k$ as follows: first, a new vertex $v$ is added to $G_k$. Then the following steps are carried out:

- **Duplication**: Select an node $u$ from $G_k$ uniformly at random. The node $v$ then makes connections to $\mathcal{N}(u)$, the set of neighbors of $u$.
- **Divergence**: Each of the newly made connections from $v$ to $\mathcal{N}(u)$ are deleted with probability $1 - p$. Furthermore, for all the nodes in $G_k$ to which $v$ is not connected, create an edge from it to $v$ independently with probability $\frac{r}{k}$.

---

2 The subscript $k$ with $G_k$ can also be interpreted as time instant $k$. 
The above process is repeated until the number of nodes in the graph is equal to \( n \). We denote the graph \( G_n \) generated from the DD-model with parameters \( p \) and \( r \), starting from seed graph \( G_{n_0} \), by \( G_n \sim \text{DD-model}(n, p, r, G_{n_0}) \).

For a node \( v_t \in V(H_t) \), the probability of having the node \( u \) as its parent in the above model is defined as

\[
 w(\delta(H_t, v_t), u, H_t) = \frac{1}{t-1}p^{\lvert \mathcal{N}(v_t) \cap \mathcal{N}(u) \rvert} (1 - p)^{\lvert \mathcal{N}(u) \setminus \mathcal{N}(v_t) \rvert} \left( \frac{r}{t-1} \right)^{\lvert \mathcal{N}(v_t) \setminus \mathcal{N}(u) \rvert} \left( 1 - \frac{r}{t-1} \right)^{t-1 - \lvert \mathcal{N}(v_t) \setminus \mathcal{N}(u) \rvert - \lvert \mathcal{N}(u) \setminus \mathcal{N}(v_t) \rvert + \lvert \mathcal{N}(v_t) \cap \mathcal{N}(u) \rvert}
\]

(3)

Then \( w(\delta(H_t, v_t), u, H_t) = \sum_{u \in \mathcal{R}_{H_t}(v_t)} w(\delta(H_t, v_t), u, H_t) \).

Since all permutations have positive probability in this version of the model, we have \( \mathcal{R}_{H_t} = V(H_t) \) and \( \Gamma(H_t) = t! \).

5.2 Greedy algorithms

To form a comparison with algorithms proposed in Section 4, we propose the following greedy algorithms that are suited for duplication-divergence model.

**sort-by-degree.** The nodes are ordered according to their degree and arrange into clusters. Cluster \( C_0 \) contains nodes with largest degree.

**peel-by-degree.** The nodes with lowest degree are first collected and put in the highest cluster. Then they are removed from the graph, and the nodes with lowest degree in the remaining graph are found and the process repeats.

**sort-by-neighborhood.** This algorithm will output a partial order with all ordered pairs \((u, v)\) \((u \) is older than \( v)\) such that \( \mathcal{N}(u) \) contains \( \mathcal{N}(v) \). Such a condition is true when \( r = 0 \). When \( r > 0 \), we consider \( \lvert \mathcal{N}(v) \setminus \mathcal{N}(u) \rvert \leq r \) as \( r \) is the average number of extra connections a node makes apart from duplication process. In most real-world data, we estimate \( r \) as smaller than 1, and hence the original check is sufficient.

**peel-by-neighborhood.** Here, we first find the set \( \{u : \mathcal{N}(u) \cap \mathcal{N}(v) \leq r\} \) (as mentioned before, it is sufficient to check \( \mathcal{N}(u) \subset \mathcal{N}(v) \) in many practical cases) and put them as the youngest cluster. These nodes are removed from the graph, and the process repeats until it hits \( G_0 \). This algorithm make use of the DAG of the neighborhood relationship and includes isolated nodes into the bins.

5.3 Comparison with other graph models

The node arrival order recovery problem in duplication-divergence model is different from that in other graph models like Erdős-Renyi graphs and preferential attachment graphs.

Firstly, for a fixed graph \( H_n \) on \( n \) vertices let us consider a set of graphs \( \Gamma(H) = \{\sigma(H) : \sigma \in S_n\} \). It is obvious that for the Erdős-Renyi model, any
graph in $\Gamma(H)$ is generated equally likely with a given seed graph $G_{n_0}$. Such a property was also proved for the preferential attachment model in [4]. However, this does not hold for duplication-divergence graphs as shown in the following example.

For the graph $G_n$ presented in Fig. 3a, let $G_{n_0}$ consists of vertices 1, 2, 3, and let the parameters of the duplication-divergence model be $p = 0.2$ and $r = 0$. The total probability of generating a structure (ignoring labels) identical to $G_t$ is equal to 0.224. Therefore, from eq. 3, the probability of adding vertices in a sequence $(1, 2, 3, 4, 5)$ is equal to 0.7714, but the probability of adding vertices in a sequence $(1, 2, 3, 5, 4)$ is equal to 0.2285.

(a) Example asymmetric graph  
(b) $E \log |\text{Aut}(G_t)|, G_t' \sim \text{DD-model}(500, p, r, K_{20})$.

Fig. 3: Auxiliary figures for comparison duplication-divergence with other models.

Secondly, it is well-known that both the Erdős-Renyi graphs and preferential attachment graphs are asymmetric with high probability [2,4]. On the other hand, the graphs generated from duplication-divergence model for a certain range of parameters also show a significant amount of symmetry, as shown in Fig. 3b. This is in accordance with the reality of many networks (for example social and biological), which exhibit lots of symmetries as shown later in Table 2.

Lastly, the behavior of the average degree at time $t$ of the node arrived at an earlier time $s$ is completely different for all three models. For Erdős-Renyi graph it is known that $\mathbb{E}[\deg_s(t)] = p(t - 1)$. For the preferential attachment graphs $\mathbb{E}[\deg_s(t)] = \Theta \left( \sqrt{\frac{t}{2}} \right)$ ([9], Theorem 8.2). However, for the duplication-divergence model we can show that $\mathbb{E}[\deg_s(t)] = \Theta \left( \left( \frac{t}{s} \right)^p s^{2p-1} \right)$ for $p > 0.5$ and for any $t \geq s$ (see Appendix B).

6 Experiments

In this section, we evaluate our methods on synthetic and real-world data. We made publicly available all the code and data of this project at https://github.com/krzysztof-turowski/duplication-divergence

We now revise the definitions of precision $\theta$ and density $\delta$ when the original ranking is not a total order. Let $\mathcal{K}(\sigma)$ be the set of comparable unordered pairs
of partial order \( \sigma \). Then precision and density can be redefined as follows:

\[
\delta(\sigma) = \frac{|K(\sigma) \cap K(\sigma_{\text{orig}})|}{|K(\sigma_{\text{orig}})|}
\]

\[
\theta(\sigma) = \frac{1}{|K(\sigma) \cap K(\sigma_{\text{orig}})|} |\{u, v \in [n] : u <_{\sigma} v, \pi^{-1}(u) < \pi^{-1}(v)\}|
\]

If the original order is a total order \( |K(\sigma_{\text{orig}})| \).

### 6.1 Synthetic data

In Figures 4 and 5, we provide the optimal curve or an approximation to it by sampling. The optimal curve is the optimal precision for a given density lower bound of \( \varepsilon \binom{n}{2} \) (see Section 3.1 for more details). In all the figures \( \sigma_{\text{tries}} \) denote the number of Markov chain sample paths considered for sampling.

Figure 4 shows the convergence of the optimal curve obtained through different sampling methods to the exact optimal curve. We observe that the convergence of the estimated curve is highly dependent on the method of estimation: local-unif-sampling method requires only 100 samples, but high-prob-sampling is still visibly far away even for 1000 samples. We consider a small size example here since it becomes infeasible \( (O(n!)) \) to compute the exact curve for larger values Therefore (and also for the computational reasons stated in Section 4) we use local-unif-sampling in the subsequent experiments.

In Figure 5, we present the results of the unsupervised algorithms and its comparison with the estimated optimal curve. We observe that greedy algorithms perform close to optimal for small \( p \), but their performance deteriorates for higher values of \( p \). On the other hand, \( p_{uv} \)-based algorithms offer consistent, close to the theoretical bound, behavior for the whole range of \( p \). Moreover, both bin size in sort-by-\( p_{uv} \)-sum and threshold in \( p_{uv} \)-threshold algorithm offer a trade off between higher precision and higher density.

Table 1 contains the results of supervised learning for \( p_{uv} \)-based algorithms. It is worth noting that a small increase in the percentage of training set \( \alpha \) produces a large increase in the precision of the algorithms for all sets of parameters. Moreover, for larger bin size in sort-by-\( p_{uv} \)-sum algorithm we observe mainly only an increase in precision with \( \alpha \), but for \( p_{uv} \)-threshold algorithm both \( \delta \) and \( \theta \) grow visibly with \( \alpha \), especially for large \( \tau \).

### 6.2 Real-world networks

We consider three real-world networks with ground truth (temporal information) available. The directed networks are treated as undirected networks and hides the edge direction for testing our algorithms.

**The ArXiv network**: It is a directed network with 7,464 nodes and 116,268 edges. Here the nodes are the publications and the edges are formed when a publication cite another. The original ranking has 1,457 bins.

**The Simple English Wikipedia dynamic network**: A directed network with 10,000
results on synthetic networks with exact curve: $G_n \sim \text{DD-model}(13, 0.6, p, G_{n_0})$ for $p = 0.3$ (left) and 0.6 (right), averaged over 100 graphs. $G_{n_0}$ is generated from Erdős-Renyi graph with $n_0 = 4$ and $p_0 = 0.6$.

Fig. 5: Results on synthetic networks with greedy and unsupervised learning $p_{uv}$-based algorithms: $G_n \sim \text{DD-model}(50, p, 1.0, G_{n_0})$ for $p = 0.3$ (left) and 0.6 (right), averaged over 100 graphs. $p_{uv}$-based algorithms use $\sigma_{tries} = 100000$. $G_{n_0}$ is generated from Erdős-Renyi graph with $n_0 = 10$ and $p_0 = 0.6$.

nodes and 169,894 edges. Nodes represent articles and an edge indicates that a hyperlink was added or removed. It shows the evolution of hyperlinks between articles of the Simple English Wikipedia.

CollegeMsg network: In this dataset of private message sent on an online social platform at University of California, Irvine, nodes represent users and an edge from $u$ to $v$ indicates user $u$ sent a private message to user $v$ at time $t$. Number of nodes is 1,899 and number of edges is 59,835. Figures 6-8 show the result of supervised learning and the greedy algorithms. We note here that a small increase in the percentage of training set ($\alpha$) leads to a huge change in the precision. This happens also in synthetic data, and is caused by the large structural dependency within graphs, unlike in classical machine learning data where often the data is assumed to be independent. It helps us to obtain a significant improvement over greedy algorithms.
Algorithm & $p = 0.3$ & $p = 0.6$ \\
\hline
sort-by-$p_{uv}$-sum, $|C| = 1$ & 0.001 & 1.0 & 0.598 & 1.0 & 0.613 \\
sort-by-$p_{uv}$-sum, $|C| = 1$ & 0.01 & 1.0 & 0.643 & 1.0 & 0.650 \\
sort-by-$p_{uv}$-sum, $|C| = 1$ & 0.1 & 1.0 & 0.836 & 1.0 & 0.832 \\
sort-by-$p_{uv}$-sum, $|C| = 5$ & 0.001 & 0.897 & 0.603 & 0.897 & 0.624 \\
sort-by-$p_{uv}$-sum, $|C| = 5$ & 0.01 & 0.897 & 0.656 & 0.897 & 0.651 \\
sort-by-$p_{uv}$-sum, $|C| = 5$ & 0.1 & 0.889 & 0.857 & 0.889 & 0.864 \\
sort-by-$p_{uv}$-sum, $|C| = 10$ & 0.001 & 0.769 & 0.605 & 0.769 & 0.626 \\
sort-by-$p_{uv}$-sum, $|C| = 10$ & 0.01 & 0.768 & 0.661 & 0.767 & 0.660 \\
sort-by-$p_{uv}$-sum, $|C| = 10$ & 0.1 & 0.758 & 0.864 & 0.759 & 0.859 \\
$p_{uv}$-threshold, $\tau = 0.5$ & 0.001 & 1.0 & 0.604 & 1.0 & 0.617 \\
$p_{uv}$-threshold, $\tau = 0.5$ & 0.01 & 1.0 & 0.637 & 1.0 & 0.649 \\
$p_{uv}$-threshold, $\tau = 0.5$ & 0.1 & 1.0 & 0.829 & 1.0 & 0.823 \\
$p_{uv}$-threshold, $\tau = 0.7$ & 0.001 & 0.120 & 0.754 & 0.219 & 0.755 \\
$p_{uv}$-threshold, $\tau = 0.7$ & 0.01 & 0.287 & 0.791 & 0.382 & 0.770 \\
$p_{uv}$-threshold, $\tau = 0.7$ & 0.1 & 0.778 & 0.899 & 0.800 & 0.888 \\
$p_{uv}$-threshold, $\tau = 0.9$ & 0.001 & 0.010 & 0.906 & 0.028 & 0.871 \\
$p_{uv}$-threshold, $\tau = 0.9$ & 0.01 & 0.020 & 0.951 & 0.090 & 0.907 \\
$p_{uv}$-threshold, $\tau = 0.9$ & 0.1 & 0.521 & 0.966 & 0.559 & 0.960 \\
\hline
\end{tabular}

Table 1: Results on synthetic networks with supervised learning $p_{uv}$-based algorithms: $G_n \sim \text{DD-model}(50, p, 1.0, G_{n_0})$, averaged over 100 graphs. $p_{uv}$-based algorithms use $\sigma_{trials} = 100000$. $G_{n_0}$ is Erdős-Renyi graph with $n_0 = 10$ and $p_0 = 0.6$.

| Network ($G_{\text{obs}}$) | $\log |\text{Aut}(G_{\text{obs}})|$ | $\hat{p}$ | $\hat{r}$ | p-value for $\mathbb{E}[\log |\text{Aut}(G)|]$ |
|---------------------------|-------------------------------|-------|-----|---------------------------------|
| ArXiv hep                 | 12.594                        | 0.72  | 1.0 | 0.56                           |
| Wikipedia                 | 1018.939                      | 0.66  | 0.5 | 0.88                           |
| College messages          | 231.540                       | 0.65  | 0.45| 0.64                           |

Table 2: Parameters of the real-world networks estimated using recurrence-based method in [8]

| Greedy algorithm | $\delta$ | $\theta$ |
|------------------|----------|----------|
| sort-by-degree   | 0.983    | 0.477    |
| peel-by-degree   | 0.989    | 0.469    |
| sort-by-neighborhood | 0.0001 | 0.514 |
| peel-by-neighborhood | 0.131  | 0.509 |

Fig. 6: ArXiv: $p_{uv}$-based (left) and greedy (right) algorithms

References

1. Bebek, G., Berenbrink, P., Cooper, C., Friedetzky, T., Nadeau, J., Sahinalp, S.C.: The degree distribution of the generalized duplication model. Theoretical Computer Science 369(1-3), 239–249 (2006) 17
2. Kim, J.H., Sudakov, B., Vu, V.: On the asymmetry of random regular graphs and random graphs. Random Structures & Algorithms 21(3-4), 216–224 (2002) 11
A Proof of Theorem 1

Now we have the following iterative expression for the denominator of $p_{uv}$.

$$p_{uv}^{\text{denom}}(H_t, H_{t_0}) := \sum_{\sigma^{-1} \in \Gamma(H_t)} \mathbb{P} [\mathcal{G}_t = \sigma^{-1}(H_t) | H_{t_0}]$$

$$= \sum_{v_t \in R_{H_t}} \sum_{\sigma^{-1} \in \Gamma(H_t)} \mathbb{P} [\mathcal{G}_t = \sigma^{-1}(H_t), \mathcal{G}_{t-1} = \sigma_1^{-1}(\delta(H_t, v_t)) | H_{t_0}]$$

### Greedy algorithm

|    | $\delta$   | $\theta$   |
|----|------------|------------|
| sort-by-degree | 0.962      | 0.594      |
| peel-by-degree  | 0.963      | 0.593      |
| sort-by-neighborhood | 0.036      | 0.603      |
| peel-by-neighborhood  | 0.807      | 0.593      |

Fig. 7: Simple English Wikipedia: $p_{uv}$-based (left) and greedy (right) algorithms

Fig. 8: CollegeMsg: $p_{uv}$-based algorithms (left), greedy algorithms (right)
where $\sigma_1 \in S_{n-1}$ is the permutation $\sigma$ with “$v$ maps to $n$” removed. Now we can rewrite above expression as

$$\sum_{v_t \in R_{H_t}} \sum_{\sigma^{-1} \in \Gamma(H_t)} \mathbb{P}[G_t = \sigma^{-1}(H_t) | G_{t-1} = \sigma^{-1}_1(H_t, v_t)] \mathbb{P}[G_{t-1} = \sigma^{-1}_1(H_t, v_t)] | H_{t_0}].$$

Note that $\mathbb{P}[G_t = \sigma^{-1}(H_t) | G_{t-1} = \sigma^{-1}_1(H_t, v_t)]$ is equivalent to $w(\delta(H_t, v_t), H_t)$. Now introducing a transition probability $\{Q_s = \{q_s(i, j)\}_{s \leq t}\}$ for the Markov chain $\{H_s\}_{s \leq t}$, and using importance sampling,

$$p_{uv}^{\text{denom}}(H_t, H_{t_0}) = \sum_{v_t \in R_{H_t}} \frac{w(\delta(H_t, v_t), H_t)}{q_t(H_t, \delta(H_t, v_t))} q_t(H_t, \delta(H_t, v_t))
\times \sum_{\sigma^{-1} \in \Gamma(H_t, v_t)} \mathbb{P}[G_{t-1} = \sigma^{-1}_1(H_t, v_t)] | H_{t_0}].
= \sum_{v_t \in R_{H_t}} \frac{w(\delta(H_t, v_t), H_t)}{q_t(H_t, \delta(H_t, v_t))} q_t(H_t, \delta(H_t, v_t)) p_{uv}^{\text{denom}}(\delta(H_t, v_t), H_{t_0}), \quad (4)$$

with $p_{uv}^{\text{denom}}(H_{t_0}, H_{t_0}) = 1$. Here $q_t(H_t, \delta(H_t, v_t))$ is the transition probability to jump from $H_t = H_t$ to $H_{t-1} = \delta(H_t, v_t)$.

Now let $\mu(H_t, H_{t_0}) = \mathbb{E}_{H_{t} = H_t} \left[ \prod_{s \leq t} \frac{w(\delta(H_s, v_s), H_s)}{q_s(H_s, \delta(H_s, v_s))} \right]$.

Then we have,

$$\mu(H_t, H_{t_0}) = \sum_{v_t \in R_{H_t}} \frac{w(\delta(H_t, v_t), H_t)}{q_t(H_t, \delta(H_t, v_t))} q_t(H_t, \delta(H_t, v_t))
\times \mathbb{E}_{H_{t-1} = \delta(H_t, v_t)} \left[ \prod_{s \leq t} \frac{w(\delta(H_s, v_s), H_s)}{q_s(H_s, \delta(H_s, v_s))} \right] \quad (5)$$

$$= \sum_{v_t \in R_{H_t}} \frac{w(\delta(H_t, v_t), H_t)}{q_t(H_t, \delta(H_t, v_t))} q_t(H_t, \delta(H_t, v_t)) \mu(H_t, v_t), \quad (6)$$

where (5) follows from the Markov property.

Defining the function at $t_0$ as

$$\frac{w(\delta(H_{t_0}, v_{t_0}), H_{t_0+1})}{q_{t_0}(H_{t_0+1}, \delta(H_{t_0}, v_{t_0}))} = 1, \text{ for any } v_{t_0}$$

we note here that the iteration (6) of $\mu(H_t, H_{t_0})$ is identical to that of $p_{uv}^{\text{denom}}$ in (4). This completes the proof. $\square$
B Average degree at time $t$ of a node arrived in time $s$ in duplication-divergence model.

Lemma 2. For the duplication-divergence model it holds that if $p > 0.5$, then for any $t \geq s$:

$$E[\deg_s(t)] = \Theta \left( \left( \frac{t}{s} \right)^p s^{2p-1} \right).$$

Proof. From the definition of the model it follows that

$$E[\deg_{t+1}(s)|G_t] = \left( \frac{\deg_s(s)}{t} - \frac{t - \deg_s(s)}{t} \right) (\deg_s(s) + 1)$$

$$+ \left( \frac{\deg_s(s)}{t} (1 - p) + \frac{t - \deg_s(s)}{t} \left( 1 - \frac{r}{t} \right) \right) \deg_s(s)$$

$$= \deg_s(s) \left( 1 + \frac{p}{t} - \frac{r}{t^2} \right) + \frac{r}{t}$$

therefore

$$E[\deg_s(s)] = E[\deg_s(s)] \prod_{k=s}^{t-1} \left( 1 + \frac{p}{k} - \frac{r}{k^2} \right) + \sum_{j=s}^{t-1} \sum_{j+1}^{t-1} \left( 1 + \frac{p}{k} - \frac{r}{k^2} \right).$$

Now, $\deg_{t+1}(t+1)$ is a sum of two binomial processes: one with probability $p$ on the neighbors of parent of $t+1$, the other with probability $\frac{r}{n}$ on all other vertices. Therefore

$$E[\deg_{t+1}(t+1)|G_t] = \sum_{k=0}^{t} \sum_{\binom{k}{a}}^{} P(\deg_s(\text{parent}(t + 1)) = k) \sum_{b=0}^{a} \binom{k}{b} p^a (1 - p)^{k-a}$$

$$\times \sum_{b=0}^{t-k} \binom{t-k}{b} \left( \frac{r}{t} \right)^b \left( 1 - \frac{r}{t} \right)^{t-k-b} (a+b)$$

$$= \sum_{k=0}^{t} P(\deg_s(\text{parent}(t + 1)) = k) \left( pk + \frac{r}{t} (t-k) \right)$$

$$= \left( p - \frac{r}{t} \right) \frac{2}{t} E(G_t) + r,$$

where $E(G_t)$ is the number of edges in $G_t$.

Finally, from [1] it is known that for $p > 0.5$ and any $r$ (which covers the case of all real-world networks considered here) it holds that $\mathbb{E}E(G_t) = \Theta \left( t^{2p} \right)$. Therefore, after all substitutions we obtain $E[\deg_s(s)] = \Theta \left( \left( \frac{t}{s} \right)^p s^{2p-1} \right)$. 