ANOMALYMAXQ: Anomaly-Structured Maximization to Query in Attributed Networks

Xinyue Zhang\textsuperscript{1,2}, Nannan Wu\textsuperscript{*1,2}, Zixu Zhen\textsuperscript{2} and Wenjun Wang\textsuperscript{1,2}

\textsuperscript{1}State Key Laboratory of Communication Content Cognition, China
\textsuperscript{2}College of Intelligence and Computing, Tianjin University, China
zhang_xinyue@tju.edu.cn, wunannan@act.buaa.edu.cn, zxzhen@tju.edu.cn, wwj@pku.org.cn

Abstract

The detection of anomaly subgraphs naturally appears in various real-life tasks, yet label noise seriously interferes with the result. As a motivation for our work, we focus on inaccurate supervision and use prior knowledge to reduce effects of noise, like query graphs. Anomalies in attributed networks exhibit structured-properties, e.g., anomaly in money laundering with “ring structure” property. It is the main challenge to fast and approximate query anomaly in attributed networks. We propose a novel search method: 1) decomposing a query graph into stars; 2) sorting attributed vertices; and 3) assembling anomaly stars under the root vertex sequence into near query. We present ANOMALYMAXQ and perform on 68,411 company network (Tianyancha dataset), 7.72m patent networks (Company patents) and so on. Extensive experiments show that our method has high robustness and fast response time. When running the patent dataset, the average running time to query the graph once is about 252 seconds.

1 Introduction

In recent years, high-impact applications, e.g., business investment activities, patent co-author relationships [Sun and Luo, 2020], cheminformatics [Han et al., 2019], and complex network [Willett et al., 1998; Yang and Sze, 2007], are naturally represented as attributed networks [Rivero and Jamil, 2017]. Anomaly detection in attributed networks has attracted much more attention among users in research and industry fields. In supervised learning scenarios, deep learning typically requires a vast number of training data with accurate labels to obtain good performance [Goodfellow et al., 2016]. Nonetheless, for a company, such data is barely acquirable due to artificial compilation. Users usually have the prior knowledge to anomalies, e.g., anomaly in money laundering exhibiting with “ring structure”. Given the ring-query graph, users aim to identify the most anomaly subgraph with the ring structure in attributed networks. In this paper, our target is to present a method that can identify anomaly subgraph isomorphism to the query graph approximately in weak supervision setting using prior knowledge.

Example of investment risk anomaly query. We consider one company as one node and the investment relationship (i.e., the company ca invested in the company cb) as one edge (ca, cb). Each node has the attributes \( \mathbf{W}_{ca} \in \mathbb{R} \) (e.g., investment volume, number of accusations or charges, number of contract disputes). We first build the business attributed networks \( G = (V, E, \mathbf{W}) \) where \( V, E, \mathbf{W} \) represent the node set, edge set, and the attribute set.

Then the user has the prior knowledge to ring anomaly-structured investment relationship. We assume the three unknown companies \( V = \{ca, cb, cc\} \) have the investment relationship \( E = \{(ca, cb), (cb, cc), (cc, ca)\} \). We take \( Q = (V, E) \), and denote \( C(ca) = \mathbf{W}_{ca}^{t} \) as investment volume of the company ca at the time \( t \), and \( B(ca) = 1/|T| \sum_{t \in T} \mathbf{W}_{ca}^{t} \) as the average investment volume of ca over a period of time \( T \). Given the subgraph \( S \) and the function \( F(S) \), we have \( F(S) = C(S) \log C(S)/B(S) + B(S) - C(S) \) if \( C(S) > B(S) \), and \( F(S) = 0 \) otherwise. These investment structures may be money laundering groups. We are target for the investment risk anomaly in the problem (1)

\[
\max_{S \subseteq G} F(S) \quad \text{s.t.} \quad S \sim Q
\]

(1)

where \( S \subseteq G \) represents \( S \) is a subgraph of \( G \), and \( S \sim Q \) represents \( S \) is approximate isomorphic to \( Q \). We can observe that the optimization to \( S \subseteq G \) and \( S \sim Q \) is NP-hard problem. In this paper, we employ two approaches to relax the hard problem: (1) \( S \subseteq G \) is relaxed to \( S \subseteq [V] \) select the top \( k \) vertices from the sorted \([V]\) as the upper bound of anomaly; and (2) \( S \sim Q \) is relaxed to \( \text{star}(S) \sim \text{star}(Q) \) where \( \text{star} \) decomposes \( S \) and \( Q \) as a sequence of “star” like graphs. We assemble stars into \( S \) as the lower bound of anomaly.

For the two approaches, we iteratively update the upper bound and lower bound of the anomaly to achieve the most anomaly-structured maximization to the query graph. We develop the algorithm ANOMALYMAXQ, which can be applied to bioinformatics and cheminformatics fields.

Related work. Anomaly detection assumes that outliers and normal nodes are generated from different distributions. There are two kinds of anomaly detection methods, including parameterized scanning statistics and non-parametric graph scan (NPGS) statistics [Akoglu et al., 2014;
Liu et al., 2018; Wu et al., 2019a; Sun et al., 2020]. Our work on NPGS, which no longer required assumption of specific forms of node distribution. Existing subgraph matching work can be grouped exact matching methods [Yan et al., 2004; He and Singh, 2006; Jiang et al., 2007] and inexact matching methods [Liu et al., 2019]. we propose an algorithm mainly focus on approximate subgraph matching on the large data graph [Bhattarai et al., 2019; Lai et al., 2019].

The main contributions of this paper are summarized as follows:

- **Linear-time algorithm.** A novel algorithm is proposed to fast identify anomaly subgraph isomorphism to the query approximately.
- **Performance.** Extensive experiments on several benchmark datasets demonstrate that the algorithm performs better than the representative methods for this task on both accuracy and run time.
- **Scalability.** Our proposed algorithm is suitable for optimization of a variety of graph scan statistics, which satisfy liner time subset scanning property.

## 2 Methodology

### 2.1 Problem Formulation

**Notation.** First, we briefly review the terminologies that we will use in this paper. Table 1 lists commonly used symbols in this paper. We use italic uppercase letters to denote sets (e.g., $V, E$). The bold uppercase letters are matrices (e.g., $W, X$), and the bold lowercase letters are vectors (e.g., $w, x$).

In this paper, calligraphic letters are networks $^1$. An **attributed network** $\mathcal{G} = (V, E, W)$ consists of: (1) the vertex set $V = [n] = \{1, 2, \ldots, n\}$; (2) the edge set $E \subseteq V \times V$, where

$^1$network and graph can be used interchangeably.

### 2.2 Upper bound $S_{\text{up}}$ & lower bound $S_{\text{low}}$ of anomaly

#### Table 1: Representative symbols

| Symbols | Description |
|---------|-------------|
| $\mathcal{G}$ | an attributed network |
| $\mathcal{Q}$ | a specific shape query graph |
| $\mathcal{S}$ | a subgraph of $\mathcal{G}$ |
| $w$ | the node attributes |
| $\mathcal{M}$ | the graph-structure model |
| $F$ | the differentiable score function |
| $\text{ged}(\mathcal{S}, \mathcal{Q})$ | the minimum graph edit distance between $\mathcal{S}$ and $\mathcal{Q}$ |

$|E| = p$; (3) the vertex attributes $W \in \mathbb{R}^{n \times T}$, where the row vector $w_v \in \mathbb{R}^T$ is the attribute values observed within the time span $T$ for the vertex $v \in V$. For the node subset $S \subseteq V$, $W_S \in \mathbb{R}^{[S] \times T}$ keeps row vectors only in the set $S$. We define subgraph $\mathcal{S}$ of $\mathcal{G}$ as $S \subseteq \mathcal{G}$ if $V_S \subseteq V, E_S \subseteq E$ and $W_S$ is restricted from $W$. Let $\mathcal{Q}$ be a query graph.

We refer to $g$ as a “priority function”. The score function $F(S)$ and priority function $g$ satisfy the Linear Time Subset Scanning (LTSS) property [Neill, 2012] if and only if:

$$\max_{S \subseteq \mathcal{G}} \{F(S)\} = \max_{k=1,\ldots,n} \left[ F \left( \{V(1)\ldots V(k)\} \right) \right]$$ (2)

If $V$ is already sorted by priority with its record data, this property allows us to maximize $F(S)$ in $O(N)$ time. Otherwise, we must first sort the records by priority, which requires $O(N \log N)$ time.

**Problem: Anomaly-Structured Maximization (ASM)**

Given an attributed network $\mathcal{G}$, and the anomaly-structured query graph $\mathcal{Q}$, we maximize the score function over all subgraphs in attributed networks:

$$\max_{S \subseteq \mathcal{G}} F(S) \quad \text{s.t.} \quad S \sim \mathcal{Q}$$ (3)

where $F(S)$ can employ score functions that satisfy the LTSS property, e.g., Kulldorff’s (KULL) original spatial scan statistic, Expectation-based Poisson (EBP) scan statistic.
2.2 AnomalyMaxQ

The overall idea of this method is to iterate the subgraphs of upper and lower bounds in Algorithm 1. First (Root Selection, Line 1), ANOMALYMAXQ evaluates the matching priority of vertices based on their empirical p-values. Second (Upper-Bound Structure Construction, Lines 3-6), a dynamic filtering and refinement strategy is used to maximize the score function of attribute graph $G$. Finally (Lower-Bound Structure Construction, Line 7), ANOMALYMAXQ searches for the lower-bound Graph Structure according to the graph edit distance from the query graph to return the approximate optimal results which have the least loss function cost. In the remaining of this section, we highlight each of these three steps.

**Root selection.** Given an attribute graph $G$, we first select $m$ root vertices to start the matching process, where $m$ is the number of nodes in query graph $Q$. We would choose nodes which (1) have as few candidates as possible, and (2) have most anomaly vertices. For example, in Figure 1, we can choose $\{v_3, v_6, v_8, v_7\}$ as the root. **Upper-bound of anomaly.** It consists of two parts: 1) reserve the previous vertex set $S$, and 2) add next new vertices. We get the vertex set $S_{up}$, which is the upper bound score of anomaly without structure property. We must select vertex not computed to ensure $S_{up}$ will not get stuck in an infinite loop. **Lower-bound of anomaly.** We consider $S_{up}$ as root to select star subgraphs, which are isomorphic to stars in the query graph. The matched stars are assembled into one subgraph which are approximate to the query.

2.3 Theoretical analysis

**Spatial complexity analysis.** In each iteration for numerical conjunctive stars [Zhao et al., 2020a], we only keep $S_{up}$ and $S_{low}$, in step 6 of Algorithm 1. The space complexity of ANOMALYMAXQ is $O(m)$. The size of two subsets is determined by the number of nodes $m$ of query graph $Q$.

**Time complexity analysis.** The time complexity of the algorithm is mainly determined by MAXQ in step 7. MAXQ matches the subgraph of each node and its neighbors in $S_{up}$ with the decomposed query graph to calculate the largest isomorphic part. According to the worst case, the decomposed query graph can have $k$ kinds of neighbors, so each node in $S_{up}$ has $m$ matching methods at most. In general, the time complexity of the algorithm is $O(N \times M)$.

3 Experiments on Real Datasets

3.1 Experiment Design

To verify the performance of ANOMALYMAXQ approach, we conducted experiments on large-scale artificial toy data and real datasets. **Internet Traffic Network.** The real-world *edu.cn* network dataset consists of 8,540,966 web sites browsing logs from May 31, 2014 to May 13, 2015. The network with 31,238 vertices and 118,708 edges was built from the browsing logs (i.e., the edge (IP site A, IP site B) denotes that A visited B). The p-value of vertices are under 0.15 if they were attacked, otherwise were not. For testing the robustness of methods, we flipped p-values of $K \in \{5, 10, 20\}$ percent nodes randomly. **Tianyancha Dataset.** This graph has 68K nodes, each representing an enterprise in Tianjin. An edge represents the investment relationship between two entities. It contains 54 Tags, such as investing information, legal disputes, etc. **Company Patents.** There are 7.72m nodes and 1.87m edges among them. The patent dataset includes the patent information in China from 1990 to 2020. We consider each inventor and company as a node. Thus an edge represents connection between the inventor and his company. **Respiratory Emergency Department (ED) Dataset.** We simulate respiratory medical record data sets with different numbers of nodes, which is $10^2, 10^3, 10^4, 10^5, 10^6$ respectively [Wu et al., 2017; Zhao et al., 2020b]. The sparsity setting of the graph is 0.4.

**Query-map Setting.** We set six query graphs in Figure 2 for each group of data through the work of others. Other graphs can be made up of these basic shapes or close to them. These query graphs can be replicated as hundreds of nodes. We use different shape constraint subgraph to try to find out the anomaly form of the dataset. Specifically, Figures 2(1) is a ring-shaped network [Zou et al., 2007; Sun et al., 2012b], which represents a state that anomaly subgraphs are interconnected; Figure 2(2) is a linear network graph [Wu et al., 2019b], representing the incident effect point to point, like Water Pollution Cases; Figure 2(3),(6) are star-shaped

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The company has more than 0.6 billion users.

Downloaded from https://www.tianyancha.com/

Downloaded from http://www.wanfangdata.com.cn/
subgraphs [Wu et al., 2017] denote that a node infects its neighbors, then the infection from one star-shaped area to another neighbor. Figure 2(4) is a bipartite graph [Wu et al., 2017], which means a case of many-to-many communication. And Figure 2(5) is a tree-shaped graph [Taha and Yoo, 2015; Han et al., 2013] for detecting anomaly subgraphs have a superior-subordinate relationship in the group.

### 3.2 Methods

**Our Method.** As mentioned in Section 3, our method performs subgraph matching in three steps: 1) query decomposition, 2) select the candidate nodes and construct upper bound and lower bound structure, and 3) calculate the graph edit distance between the subgraph and the query graph. Query graph employs the nonparametric scan statistic BJ [Berk and Jones, 1979] and HC [Donoho and Jin, 2004] as the objective function to detect specific shape attack subgraphs in the real networks. When the score of upper and lower limits is less than the threshold, the output result finally gets anomaly structured.

**Comparative Methods.** Several different techniques have been developed for anomaly detection in many real world scenarios, including TSPSD [Wu et al., 2016], Graph-TPP [Wu et al., 2017], Query-map [Wu et al., 2019b] and so on. The baselines are designed for specific shape anomaly discovery in attributed graphs. Source codes of the baseline methods are provided by the original authors. We followed strategies recommended by them to adjust the related model parameters. The algorithm TSPSD is designed in a nonparametric statistical framework, and the specification of algorithms are hence relatively straightforward. We set \( a_{max} \) and the number of seed entities \( K \) to 0.15 and 5 respectively. TSPSD chooses Steiner Tree heuristics for output. Because of it consider just the connected subgraph anomaly without the specific shape anomaly prior. Therefore, we find the subgraphs that are most similar to the query graph with comparison with others.

**Performance metrics.** We use the following performance metrics: 1) precision. We compute precision of our result, i.e. the ratio of the number of correct anomalous nodes and the number of nodes. The recall metric is ignored for computing as target subgraphs return fixed size of nodes. 2) running time. The optimization power of our method can be examined in the iteration of graph scan statistics scores. We compare it with baseline methods on running times.

### 3.3 Experiment Results

We tested our method ANOMALYMAXQ on Internet Traffic Dataset for the star and bipartite-shaped attack patterns. Our algorithm often better able to make connections that were hidden in the jumble of information. Although these IP addresses appear in different places and periods, their attack behaviors are similar. ANOMALYMAXQ can obtain some abnormal IP groups by querying specific attack patterns, such as star and bipartite-shaped graph. Our methods successfully discovered the cyber-attack networks without innocent nodes.

**Star-shaped attacks.** As illustrated in Figure 3, we can see clearly that two attack cases were found by star query graph. On March 10, 2015, ANOMALYMAXQ found the client X.X.223.66 attacked the other server sites yysj.*.edu.cn and szb.*.edu.cn; however, the server site www.*.edu.cn was attacked by four clients on March 12, 2015, different from the last one. These network attack patterns are the most common forms in the network.

**Bipartite-shaped attacks.** Figure 3 shows ANOMALYMAXQ detected some cyber-attack networks. Because attackers often do not use only a single IP address for cyber-attacks. Compared with the star subgraph, we can discover attack group in the meantime. By recording these IP addresses, we find that these IP addresses come from multiple fixed network segments, and the attack mode and location remain unchanged, which means that these IP addresses may come from the same attack source. With this information, we can prevent attacks by blocking the IP of these fixed IP segments.

**Precision for target subgraphs detection.** We randomly selected the average accuracy of two days as a result. Table 3 shows the results of subgraph isomorphism search performance using specific shape query graphs for the Internet traffic dataset. We present a comparison of precision for methods under different noise conditions in detail. At 5% noise level, our proposed ANOMALYMAXQ (i.e., \( \phi_{BJ} \) and \( \phi_{HC} \)) achieved higher precision (close to 1) than competitive baselines (close to 0.7). Moreover, even at 20% noise level, it achieved at least 0.70 precision, and baselines achieved the best precision to 0.50.

### 3.4 Case Study

**Investment decision support.** Cross shareholding would inflated capital or evade tax. Figure 4 shows the results on Tianyancha dataset, including five enterprises. According to the dataset, we can see that Taikete was established in August 2000 and invested by Tiandi Weiye; Fuwo established in December 2001 and invested by Taikete and Tiandi Weiye; Xinmao was established in July 2016, then other companies invested in it. We also examined the legal risks of these com-

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| Dataset          | Graph          | size  |
|------------------|----------------|-------|
| Computer Access  | node           | IP Address | 31,238 |
|                  | link           | Attack/Access | 118,708 |
| Tianyancha      | node           | Company     | 68,411 |
|                  | link           | Investment relationship | 151,591 |
| Company Patents  | node           | Inventor/Company | 7,729,373 |
|                  | link           | Coauthor/Affiliation | 1,875,139 |
| ED Dataset       | node           | Address     | 1,000,000 |
|                  | link           | Contiguous area | 3,996,000 |
Table 3: Query graphs from $Q_1$ to $Q_6$. Comparison on the precision of structure-specific anomalous subgraphs discovered by methods, run times and graph edit distance, and we put in parentheses the results for 5%, 10%, and 20% noise.

| Methods          | $Q_1$                | $Q_2$                | $Q_3$                | $Q_4$                | $Q_5$                | $Q_6$                |
|------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| AnomalyMaxQ(BJ)  | (1.00, 0.67, 0.67)   | (1.00, 0.50, 0.75)   | (1.00, 0.80, 0.70)   | ($0.83$, 0.67, 0.67) | (0.71, 0.57, 0.71)  | (1.00, 0.63, 0.72)  |
| AnomalyMaxQ(HC)  | (1.00, 0.67, 0.67)   | (1.00, 0.50, 0.50)   | (1.00, 0.80, 0.70)   | (0.83, 0.67, 0.67)   | (0.71, 0.57, 0.57)  | (1.00, 0.63, 0.72)  |
| TSPSD(BJ)        | (0.33, 0.33, 0.50)   | (0.25, 0.25, 0.25)   | (0.20, 0.20, 0.20)   | (0.17, 0.17, 0.25)   | (0.14, 0.14, 0.21)  | (0.12, 0.12, 0.19)  |
| TSPSD(HC)        | (0.33, 0.67, 0.33)   | (0.25, 0.50, 0.25)   | (0.20, 0.40, 0.20)   | (0.17, 0.33, 0.17)   | (0.14, 0.33, 0.31)  | (0.12, 0.25, 0.25)  |
| Graph-TPP        | (0.50, 0.50, 0.55)   | (0.62, 0.62, 0.41)   | (0.64, 0.20, 0.46)   | (0.58, 0.58, 0.61)   | (0.57, 0.57, 0.47)  | (0.43, 0.50, 0.58)  |
| Query-map        | (0.50, 0.50, 0.33)   | (0.83, 0.75, 0.83)   | (0.27, 0.20, 0.46)   | (0.58, 0.58, 0.46)   | (0.57, 0.57, 0.47)  | (0.43, 0.50, 0.58)  |

Figure 3: The cyber-attacks on March 12, 2015 are detected by our method. Red nodes denote the attacking or attacked IP sites in real-world, and yellow area is the anomaly vertices we calculated.

Figure 4: Calculation results of patent disputes.

Business Competition Forecast. After calculation, we find that Nanjing Melander Medical Technology Company and Nanjing Weisi Medical Technology Company are consistent with our query graph pattern. Melander is prosecuted by Weisi, whose employees hopping to Melander. There is an identified competitive relationship between the two companies. Through China’s judicial document website, we find that there is more than one patent dispute lawsuit between two companies. Melander was sued for its patent content (No.: 201320752362.7) was as same as the research of Weisi.

3.5 Running Time Analysis

In this part, we compare the running time of our algorithm with that of “Graph-TPP” and “Query-Map” [Wu et al., 2017; Wu et al., 2019b]. Although TSPSD runs very fast, the precision is not satisfactory. The dataset is a simulated ED Dataset. We set up two query graphs, $Q_1$ has five nodes, and $Q_2$ has 22 points and 92 edges [Sun et al., 2012a]. The results show that our proposed method always ran faster than all the baseline methods. On the other hand, the number of nodes and edges in the query graph is more influential than attributes graph.

4 Conclusion

In this paper, we introduce ANOMALYMAXQ that is capable of predicting business risks and assisting investment decisions. A large number of experiments show that our algorithm has good scalability and fast computing speed, and it only needs 90 seconds response time to run on 7.72m nodes. In the future work, we will use multi-dimensional data to generate query graphs automatically.
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