





## **Anomalies in labeled graphs**

#### Problem:

# Q1. Given a graph in which nodes and edges contain (non-unique) labels, what are unusual substructures?





## Background

- Subdue\*: An algorithm for detecting repetitive patterns (substructures) within graphs.
- Substructure: A connected subgraph of the overall graph.
- Compressing a graph: Replacing each instance of the substructure with a new vertex representing that substructure.
- Description Length (DL): Number of bits needed to encode a piece of data

<sup>\*</sup> http://ailab.wsu.edu/subdue/



## Background

#### Subdue uses the following heuristic:

- The best substructure is the one that minimizes
   F1(S,G) = DL(G | S) + DL(S)
  - G: Entire graph, S: The substructure,
  - DL(G|S) is the DL of G after compressing it using S,
  - DL(S) is the description length of the substructure.



Iterations after compressing at each step



## Background

Given database D and set of models for D, Minimum Description Length selects model M that minimizes

<u>L(M)</u> +











 $a_9 x^9 + ... + a_1 x + a_0$ 

VS.

 $a_1x+a_0$ 

deltas



## 1) Anomalous Substructures

- Main idea: anomalies (by def.) occur infrequently, they are roughly opposite to "best substructures"
  - Find substructures S that maximize F1(S,G)?
    - Nope, it flags all single nodes as anomalies!
  - Instead, find those that minimize

F2(S, G) = Size(S) \* Instances(S,G)

Approximate inverse of F1(S,G)

Intuition: Larger substructures are <u>expected</u> to occur few times; the smaller the substructure, the less likely it is rare



#### Example

#### F2(S, G) = Size(S) \* Instances(S,G)

- □ For node D, F2 = 1 \* 1 = 1
- For A→C and D→A, it is 2 \* 1 = 2
- For G (whole graph), it is 9 \* 1 = 9
- Hence D is considered the most anomalous.



 Note: Usually a threshold for F2 is used and anomalies are ranked by their scores.



## **Anomalies in labeled graphs**

#### Problem:

# Q1. Given a graph in which nodes and edges contain (non-unique) labels, what are unusual substructures?

Q2. Given a set of subgraphs, what are the unusual subgraphs?



Note: assumption is anomalies are connected



## 2) Anomalous Subgraphs

- Main idea: subgraphs containing few common substructures are generally more anomalous
  - Define anomaly score A in [0,1]



#### Experiments

- Data: 1999 KDD Cup Network Intrusion (
  - Ground truth: connection records, "normal" or attack (37 types), 41 features of connection (duration, protocol type, number of bytes, etc.)
  - Each individual test involved 50 records of which only one is of a particular attack type.
- Use Subdue to find anomalous substructures
   Prune all subgraphs with size>3, F2>6 (arbitrary)

## **Anomalies with numeric labels**

- How about numeric labels?
  - Noble & Cook work with categorical labels
  - (1) unusual substructures



Davis et al. '11



## **Anomalies with numeric labels**

- How about numeric labels?
  - Noble & Cook work with categorical labels





### **Anomalies with numeric labels**

- Main idea (discretization):
  - $\square$  assign categoric label  $q_0$  to "normal" values, and
  - "outlierness" score  $q_i$  to all others i
- Example: empirical distribution of a label



 Several "outlierness" scores (pdf-fitting, kNN, LOF, clustering-based)



### Discretization







kNN distance







#### distance to closest "large" (k-means) cluster centroid



#### Discretization

- Other possible discretization techniques
  - SAX (Symbolic Aggregate approXimation)
    - <u>http://www.cs.ucr.edu/~eamonn/SAX.htm</u>
  - MDL-binning
    - P. Kontkanen and P. Myllymäki. *MDL histogram density estimation*. In AISTAT, 2007.
  - Minimum entropy discretization
    - U.M. Fayyad and K.B. Irani. Multi-interval discretization of continuous-valued attributes for classification learning. In Proc. IJCAI, 1989.
  - Logarithmic binning
    - especially for skewed distributions



#### Experiment

#### Data: Access card transaction graphs

node: door sensor, edge (u,w): movement u→w, weight(u,w): time u→w (only numeric attribute)



Eberle and Holder. '07

# **Anomalies in labeled graphs**

#### Problem:

Q1. Given a graph in which nodes and edges contain (non-unique) labels, how to find substructures that are very similar to, though not the same as, a normative substructure? ("best substructure" as for Subdue)\*

#### Intuition:

"The more successful money-laundering apparatus is in imitating the patterns and behavior of legitimate transactions, the less the likelihood of it being exposed."

- United Nations Office on Drugs and Crime



## **Formal definition**

Given graph G with a normative substructure S, a substructure S' is anomalous if difference d between S and S' satisfies 0 < d <= X, where X is a (user-defined) threshold and d is a measure of the unexpected structural difference.

#### Assumptions

- Majority of G consists of a normative pattern, and no more than X% of it is altered in an anomaly.
- Anomalies consist of one or more modifications, insertions or deletions.
- Normative pattern is connected.



## **Three Types of Anomalies**

- 1) GBAD-MDL (Minimum Descriptive Length): anomalous modifications
- 2) GBAD-P (Probability): anomalous insertions
- 3) GBAD-MPS (Maximum Partial Substructure): anomalous deletions

#### Note: prone to miss more than one type of anomaly • e.g., a deletion followed by modification



## 1) Information Theoretic Approach

- Find normative substructure S that minimizes
  F(S,G) = DL(G | S) + DL(S)
- For each instance I<sub>k</sub> of S
- anomalyScore( $I_k$ ) = freq( $I_k$ ) \* matchcost( $I_k$ ,S) the lower, the more anomalous cost to modify  $I_k$  into S Example:





## 2) Probabilistic Approach

- Find normative substructure S
- Find extensions to **S** with lowest probability
- For each extension I<sub>k</sub> of S

anomalyScore( $I_k$ ) =  $\frac{\text{number of instances of } I_k}{\text{all instances } I_n \text{ with a unique extension}}$ 

Example:





#### 3) Maximum Partial Substructure Approach

- Find normative substructure S
- Find "ancestral" substructures  $S_n \subseteq S$  that are missing various edges and vertices.
- For each instance  $I_k$  of  $S_n$

anomalyScore( $I_k$ ) =  $|I_n| * \text{matchcost}(I_k,S)$ # instances of  $I_k$ 

Example:





# **Experiments (Cargo shipments)**

 Data: obtained from Customs and Borders Protection (CBP)

#### Scenario:



- Marijuana seized at Florida port [press release by U.S. Customs Service, 2000].
- Smuggler did not disclose some financial information, and ship traversed extra port.
- GBAD-P discovers the extra traversed port;
- GBAD-MPS discovers the missing financial info.

# **Experiments (Network intrusion)**

Data: 1999 KDD Cup Network Intrusion

- 100% of attacks were discovered with GBAD-MDL
- 55.8% for GBAD-P and 47.8% for GBAD-MPS

#### Note

- Data consists of TCP packets that have fixed size
- Thus, the inclusion of additional structure, or the removal of structure, is not relevant here.
- Modification is the only relevant one, at which GBAD-MDL performs well

#### High (unreported) false positive rate!

# **Community Outliers**

#### Definition



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Gao et al. '10

- Two information sources: links, node features
- Communities based on both links and node features
- Objects with features deviating from other community members defined as community outliers



## **Other network outliers**

 $\left( \mathbf{V}_{7}\right)$ 

 $|\mathbf{V_8}\rangle$ 

1) Global outlier: only considers node features

 $(\mathbf{V}_9)$  $V_3$ V<sub>10</sub>) 10 30 40 70 100 110 140 **Salary (in \$1000)** structural outlier local outlier 2) Structural outlier: only consider links  $(V_7)$ 10K 70K 160K **30K**  $\mathbf{V}_2$  $V_8$ 10K 140K(V Vg 100K **40K 110K 30K** 

**Global Outlier** 

 $\left( V_{2}\right)$ 

160

90

3) Local outlier: only consider the feature values of direct neighbors

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Gao+KDD'10 Anomaly detection in graph data (WSDM'13) modified with permission

# A unified probabilistic model



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# **Optimization formulation**



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- Maximize  $P(X) \propto P(X|Z) P(Z)$ 
  - P(X|Z) depends on community label and model param.s
    - e.g., salaries in the high or low-income communities follow Gaussian distributions defined by mean and std

$$P(x_i = s_i | z_i = k) = P(x_i = s_i | \theta_k)$$
  
Normal with  $\{\mu_k, \sigma_k^2\}$   
$$P(x_i = s_i | z_i = 0) = \rho_0 \checkmark$$
 Uniform for outliers

- P(Z) is higher if neighboring nodes from normal communities share the same community label
  - e.g., two linked nodes are likely to be in the same community
  - outliers are isolated—does not depend on the labels of neighbors

$$P(Z) \propto \sum_{w_{ij}>0, z_i\neq 0, z_j\neq 0} w_{ij}\delta(z_i-z_j)$$



### Algorithm



- Initialization is very important (by clustering)
- Convergence/correctness not guaranteed

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# **Algorithm: parameter estimation**

- Calculate model parameters Θ
  - maximum likelihood estimation
- Continuous:  $\{\mu_k, \sigma_k^2\}$ 
  - mean: sample mean of the community
  - std: square root of sample variance of community



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Anomaly detection in graph data (WSDM'13) Gao+KDD'10



# **Algorithm: inference**

#### Calculate label assignments Z

- Model parameters are known
- Iteratively update the community labels of nodes
- For each node: select label that maximizes:



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Anomaly detection in graph data (WSDM'13) modified with permission



## **Experiments: Simulations**

#### Data

- Generate continuous data based on Gaussian distributions and generate labels according to the model
- **r**: percentage of outliers, K: number of communities
- Baseline models
  - GLODA: global outlier detection (based on node features only)
  - DNODA: local outlier detection (check the feature values of direct neighbors)
  - CNA: partition data into communities based on links and then conduct outlier detection in each community



## **Experiments: Simulations**





### Case study on DBLP

- Conferences graph
  - Links: % common authors among two
  - Node features: publication titles in the conference

#### Communities:

- Database: ICDE, VLDB, SIGMOD, PODS, EDBT
- Artificial Intelligence: IJCAI, AAAI, ICML, ECML
- Data Mining: KDD, PAKDD, ICDM, PKDD, SDM
- Information Analysis: SIGIR, WWW, ECIR, WSDM

#### Community outliers: CVPR and CIKM

#### Akoglu et al. '12 Cohesive groups in attributed graphs

#### Problem:

#### Given a graph with node attributes (features)

- social networks + user interests
- phone call networks + customer demographics
- gene interaction networks + gene expression info

Find cohesive clusters, bridges, anomalies



#### Note: cohesive cluster: similar connectivity & attributes



## **Problem sketch**



Given adjacency matrix A and feature matrix F Find homogeneous blocks (clusters) in A and F \* parameter-free

\* scalable



## **Problem formulation**

How many node- & attribute-clusters?
 How to assign nodes and attributes to clusters?

Main idea: employ Minimum Description Length



# **Problem formulation**



- L (M) : Model description cost
  - 1.  $\log^* n + \log^* f$  n: #nodes, f: #attributes
    - k: #node-clusters, I: #attribute-clusters
  - **3.** nH(P) + fH(Q)

2.  $\log^* k + \log^* l$ 

- $p_i = \frac{r_i}{n}$  size of node-cluster i size of attribute-cluster j  $q_j = \frac{c_j}{f}$
- L(D|M): Data description cost given Model
  - 1. For each block in A and F, #1s:  $\log^* n_1(B_{ij})$

A similar problem (column re-ordering for minimum total run length) is shown to be NP-hard [Johnson+]. (reduction from Hamiltonian Path)

 $= -n_1(B_{ij}) \log_2(P_{ij}(1)) - n_0(B_{ij}) \log_2(P_{ij}(0))$ 



# **Algorithm sketch**



#### The algorithm is iterative and monotonic –will converge to local optimum

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Anomaly detection in graph data (WSDM'13)

# PICS at work (Political books)

#### Examples of "core" liberal and conservative books



Anomaly detection in graph data (WSDM'13)

# PICS at work (Reality mining)



# PICS at work (YouTube)



# Part I: References (attribute graphs)

- C. C. Noble and D. J. Cook. <u>Graph-based anomaly</u> <u>detection</u>. KDD, pages 631–636, 2003.
- W. Eberle and L. B. Holder. <u>Discovering structural</u> <u>anomalies in graph-based data</u>. ICDM Workshops, pages 393–398, 2007.
- Michael Davis, Weiru Liu, Paul Miller, George Redpath: <u>Detecting anomalies in graphs with numeric labels</u>. 1197-1202, CIKM 2011.
  - Jing Gao, Feng Liang, Wei Fan, Chi Wang, Yizhou Sun, Jiawei Han: <u>On community outliers and their efficient</u> <u>detection in information networks</u>. KDD 2010: 813-822.
- Leman Akoglu, Hanghang Tong, Brendan Meeder, Christos Faloutsos. <u>PICS: Parameter-free Identification of Cohesive</u> <u>Subgroups in large attributed graphs</u>. SDM, 2012.

**Substructures** 



## **Tutorial Outline**

- Motivation, applications, challenges
- Part I: Anomaly detection in static data
  - Overview: Outliers in clouds of points
  - Anomaly detection in graph data

#### **Part II:** Event detection in **dynamic** data

- Overview: Change detection in time series
- Event detection in graph sequences

#### Part III: Graph-based algorithms and apps

- Algorithms: relational learning
- Applications: fraud and spam detection



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