Graph Mining Techniques
Subdue

Sharma Chakravarthy
Information Technology Laboratory
Computer Science and Engineering Department
The University of Texas at Arlington, Arlington, TX 76009
Email: sharma@cse.uta.edu
URL: http://itlab.uta.edu/sharma
Course URL: http://wweb.uta.edu/faculty/sharmac

Acknowledgments

- Parts of this presentation are based on the work of many of my students, especially Ramji Beera, Ramanathan Balachandran, Srihari Padmanabhan, Subhesh Pradhan (and others)
- National Science Foundation and other agencies for their support of MavHome, Graph mining and other projects
- Some slides are borrowed from various sources (web and others)

Tutorial Outline

- ***Graph Mining Approaches***
  - Subdue
  - AGM
  - *FSG*
- ***SQL-Based Graph Mining***
  - *HDB-Subdue*
  - *DB-FSG (may be)*
- ***Graph mining applications***
  - Email classification
- Multilayer Network Analysis
- Conclusions
- References

Need for Graph Mining

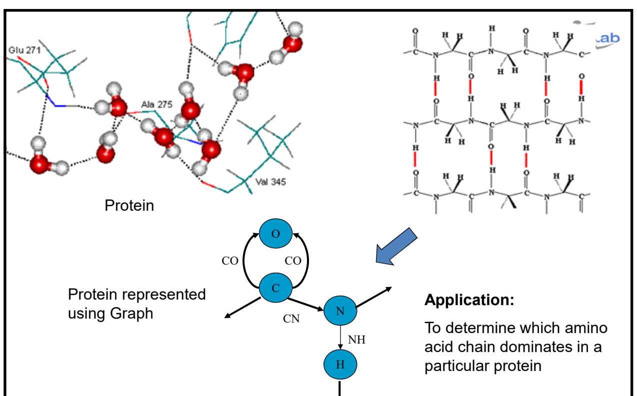
- Association rule mining, decision trees and others mining approaches
  - mine transactional data
  - Do not make use of any structural information
- Graph based mining techniques are used for mining data that are structural in nature
  - chemical compounds, complex proteins, VLSI circuits, social networks, …
  - as mapping them to other representations is not possible or will lead to loss of structural information

Need for Graph Mining

- Significant work in this area includes
  - Subdue substructure discovery algorithm (Cook & Holder),
  - HDB-Subdue (Chakrvarthy, Padmanabhan),
  - Apriori graph mining (AGM) (Inokuchi, Washio, and Motoda),
  - the frequent subgraph (FSG) technique (Karypis & Kuramochi), and
  - gSpan approach (J. Han), also SPIN (Huan, Wang, Prins, and Yang)
- PageRank and HITS are also graph based

Application Domains

- Chemical Reaction *chains*
- CAD Circuit Analysis
- Social Networks
- Credit Domains
- Web analysis
- Games (Chess, Tic Tac toe)
- Program Source Code analysis
- Chinese Character data bases
- Geology
- Web and social network analysis



Graph Based Data Mining

- A Graph representation is an intuitive and an obvious choice for a database that has structural information
- Graphs can be used to accurately model and represent scientific data sets. Graphs are suitable for capturing arbitrary relations between the various objects.
- Graph based data mining aims at discovering interesting and repetitive patterns within these structural representations of data.

Graph Mining: Mapping

Entities/objects	→	*Vertices*
Object's attributes	→	*Vertex label*
Relations between objects	→	*Edges between vertices*
Type of relation	→	*edge label*
Substructure	→	*Connected subgraph*
Substructure Instance	→	*Set of vertices & edges in input graph that match graph representation of data*

Graph Mining Overview

- A substructure is a connected subgraph; need to differentiate between substructures and substructure instances
- A connected subgraph is a subgraph of the original graph where there is a path between any two vertices
- A subgraph $G_s = (V_s, E_s)$ of $G = (V, E)$ is induced if E_s contains all the edges of E that connect vertices in V_s
- Directed and undirected edges are possible; multiple edges between two nodes need to be accommodated; cycles need to be handled

Graph Mining: Complexity

- Enumerating all the substructures of a graph has exponential complexity
- Subgraph isomorphism (or subgraph matching) is NP-complete
- However, graph isomorphism although belongs to NP is neither known to be solvable in polynomial time nor NP-complete
- Generating canonical labels is $O(|V|!)$, where V is the number of vertices
- All approaches have to deal with the above in order to be able to work on large data sets
- Different approaches do it differently; scalability depends on the approach and the use of representation

Subdue

- One of the earliest work in Graph based data mining
  - Uses sparse adjacency matrix for graph representation
- Substructures are evaluated using a metric called Minimum Description Length principle based on adjacency matrices
- Capable of matching two graphs, differing by the number of vertices specified by the threshold parameter, inexactly
- Performs hierarchical clustering by compressing the input graph with best substructure in each iteration

Subdue

- Typically, used for unsupervised discovery of interesting substructures
- Also capable of supervised discovery using positive and negative examples
- Available main memory limits the largest dataset that can be handled
- An SQL-based subdue can address scalability
- A computationally constrained beam-search is used for subgraph generation (pruning the search space)
- A branch and bound algorithm is used for inexact match

FSG

- FSG is used for frequent subgraph discovery
- Given a graph dataset $G = \{G1, G2, G3, \cdots\}$, it discovers all connected subgraphs that are found in at least the support threshold percent of the input graphs
- Uses a (sparse) adjacency matrix for graph representation
- A canonical label is generated by flattening the adjacency matrix of a graph (optimization)
- At each iteration FSG generates candidate subgraphs by adding one edge to the previous iteration's frequent subgraph (optimization)
- Graph isomorphism is checked by comparing canonical labels (optimization)

AGM

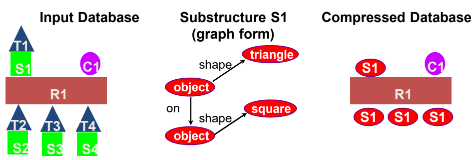
- First to propose apriori-type algorithm for graph mining
- Detects frequent induced subgraphs for a given support
- Follows apriori algorithm
- Not much optimization; hence performance is not that good and is not scalable!

gSpan

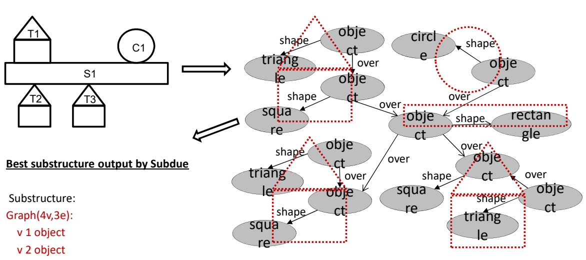
- Avoids candidate generation
- Builds a new lexicographical ordering among graphs and maps each graph to a unique minimum DFS code as its canonical label
- Seems to outperform FSG
- Amenable to parallelization
- Does not handle cycles and multiple edges

Subdue Example

- Came from AI
- Examples are different from what we normally see in mining



SUBDUE : Overview



Best substructure output by Subdue

Substructure:
Graph(4v,3e):
v 1 object
v 2 object
v 3 triangle
v 4 square
u 1 2 over
u 1 3 shape
u 2 4 shape

Subdue Substructure Discovery System

- Subdue Substructure discovery system is a graph-based data mining system that discovers interesting and repetitive patterns within graph representations of data.
- It accepts as input a forest and identifies the substructure that best compresses the input graph using the minimum description length (MDL) principle.
- It is capable of identifying both exact and inexact (isomorphic) substructures within a graph
- It uses a branch and bound algorithm for inexact matches (substructures that vary slightly in their edge and vertex descriptions).

Subdue

- Unsupervised learning
  - Subdue finds the most prevalent substructure from a set of unclassified input graphs
- Supervised learning
  - Subdue finds discriminating patterns from a set of classified (positive – G+ and negative – G- graphs)
- Hierarchical conceptual clustering
  - Compresses G with S and iterate
- Incremental Subdue?

Subdue

- Inferring graph grammars and graph primitives from examples
- Applications
  - Data mining
  - Pattern recognition
  - Machine learning

Graph Representation

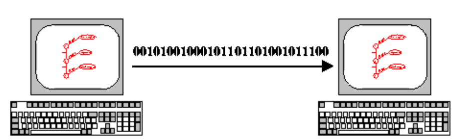
- Subdue represents data as labeled graph.
  - Vertices represent objects or attributes
  - Edges represent relationships between objects
  - Input: Labeled graph
  - Output: Discovered patterns and instances and their compression value.
- A substructure is a connected subgraph
- Graph isomorphism is used to identify similar (not merely exact) substructures

MDL Principle

- Theory to minimize description length (DL) of data (graph)
- information theoretic approach
- Has been shown to be good across domains
- Evaluates substructures based on their ability to compress the DL of a graph
- Description length = DL(S) + DL(G/S)
  - Depends upon the representation
  - Substructure that best compresses the original is chosen

MDL Principle

- Best theory: minimizes description length of data
- Evaluate substructure based ability to compress DL of graph
- Description length = DL(S) + DL(G|S)



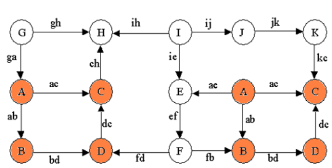
MDL Principle (cont.)

- Minimizes description length (MDL) of data
- Substructures are evaluated based on their ability to compress the DL of the entire graph
- MDL = description length of the original graph / description length of the compressed graph

$$MDL = \frac{DL(G)}{DL(S) + DL(G \mid S)}$$

- High MDL value is desirable !
- DL(G) – Description length of the input graph
- DL(S) – Description length of sub graph
- DL(G|S) – Description length of the input graph where the sub graph has been substituted

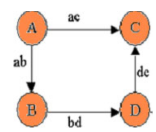
Example: Subdue



Input (partial)

- The input is a file, with all the vertex labels, vertex numbers, edges (using vertex numbers) and the edge directions

v 1 A
v 2 B
v 3 C
v 4 D
d 1 2 ab
d 1 3 ac
d 2 4 bd
d 4 3 dc



- 'd' stands for a directed edge and 'u' stands for undirected. 'e' stands for directed.

Subdue Approach

- Create a substructure for each unique vertex
- Expand each substructure by adding an edge (and may be a vertex)
- Maintain **beam** number of substructures for expansion
- Halting conditions
  - Discovered substructures > **limit**
  - List maintaining the substructures to be expanded becomes **empty**
  - **Max size** of substructure to be discovered is reached

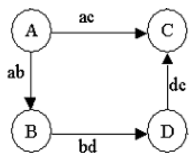
Output

➢ Output

Substructure: MDL value = 1.21789, instances = 2

Graph (4v,4e):

v 1 A
v 2 C
v 3 B
v 4 D
d 1 2 ac
d 1 3 ab
d 4 2 dc
d 3 4 bd



Subdue Parameters

➢ *Threshold* determines the amount of variation permissible in the vertex and edge descriptions during inexact graph match.

➢ *Nsubs* determines the maximum number of substructures that are returned as the set of best substructures

➢ *Beam* determines the maximum number of substructures that are retained for expansion in the next iteration of the discovery algorithm

➢ Minsize constrains the size of substructures returned as best to be equal to or more than the specified parameter value

➢ Limit is a upper bound on the number of substructures detected

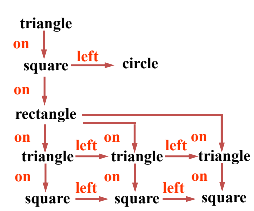
Subdue Algorithm

```
Subdue(Graph, BeamWidth, MaxBest, MaxSubSize, Limit)
   ParentList = {};     ChildList = {};     BestList = {}
   ProcessedSubs = 0
   Create a substructure from each unique vertex label and its single-vertex instances; insert the resulting
         substructures in ParentList
while ProcessedSubs <= Limit and ParentList is not empty do
   while ParentList is not empty do
      Parent = RemoveHead(ParentList)
      Extend each instance of Parent in all possible ways; Group the extended instances into Child
         substructures
      foreach Child do
         if SizeOf(Child) <= MaxSubSize then
            Evaluate the Child     //by using MDL
            Insert Child in ChildList in order by value  //highest to lowest MDL value
            if Length(ChildList) > BeamWidth then Destroy the substructure at the end of ChildList
      ProcessedSubs = ProcessedSubs + 1
      Insert Parent in BestList in order by value
      if Length(BestList) > MaxBest then Destroy the substructure at the end of BestList
      Switch ParentList and ChildList
return BestList
```

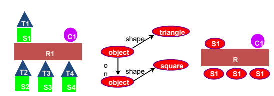

Algorithm (Contd.)

1. Create substructure for each unique vertex label

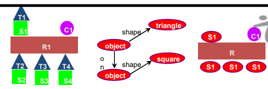
Substructures:



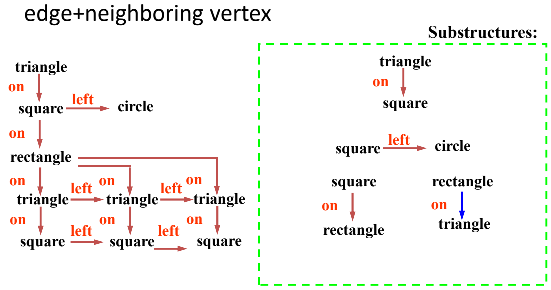
triangle (4), square (4), circle (1), rectangle (1)



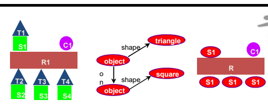
Algorithm (Contd.)



2. Expand best substructure by an edge or edge+neighboring vertex



Algorithm (cont.)



3. Keep only best substructures on queue (specified by beam width)
4. Terminate when queue is empty or #discovered substructures >= limit
5. Compress graph and repeat to generate hierarchical description
6. Constrained to run in polynomial time

Graph Match

- Exact Graph match
- Inexact Graph match

Exact graph match is likely to be restrictive for real life applications.

Inexact Graph Match

- Some variations may occur between instances
- Want to abstract over minor differences
- Difference = cost of transforming one graph to make it isomorphic to another
- Match if cost/size < threshold

Inexact Graph Match

- Minimum graph edit distance

cumulative cost of graph changes required to transform the first graph into a graph isomorphic to the second graph.

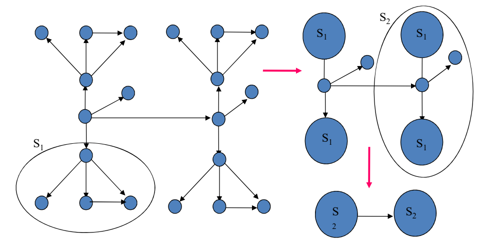
- Uses Branch and bound algorithm

Variants of Subdue

- Hierarchical reduction
- Concept learner using positive and negative examples
- Similarity detection in social networks
- Inductive learning
- Partitioned and parallel approaches
- Database approach to some of the above

Hierarchical Reduction

- Input is a labeled graph
- A substructure is connected subgraph
- A substructure instance is a subgraph isomorphic to substructure definition
- Multiple iterations can create hierarchy



Supervised Concept Learning Using Subdue

- Need for non-logic-based relational concept learner

SubdueCL

- Accept positive and negative graphs as input examples
  - Find hypotheses that describes positive examples and not negative examples

SubdueCL

- Find substructure compressing positive graphs, but not negative graphs
- Find substructure *covering* positive graphs, but not negative graphs
- Learn multiple rules

Concept Learning Subdue

- Positive graph G+, Negative graph G-
- Find substructure that compresses positive instances but not (or more than) negative instances
  - Value (G+, G-, S) = DL(S) + DL(G+|S) + DL(G-) – DL(G-|S)
- One of the limitations of this compression-based concept learner is that it only looks for substructures which compress the entire positive graph more than the entire negative graph.
- Therefore, it is biased to look for a substructure that offers more compression as compared to a substructure that covers a greater number of positive examples.

Concept Learning SUBDUE

- Positive graph G+
- Negative graph G-
- Concept:
- Alternative set covering measure
  - Error (substructure) $= \frac{\#PosExNotCovered + \#NegExCovered}{\#PosEx + \#NegEx}$
  - For a substructure to be good, Error should be minimum
  - Hence, Value (of a substructure) = 1 – Error
- Coverage: A substructure covers an example if the substructure matches a subgraph of the example

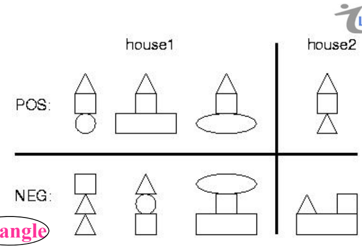
Hypotheses detection using coverage

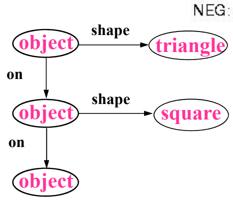
```
Main(Gp, Gn, Beam, Limit)
  H = {};
  repeat
    repeat
      BestSub = SubdueCL(Gp, Gn, Beam, Limit)
       if BestSub = {}
          then Beam m= Beam * 1.1
    until (BestSub <> {})
    Gp = Gp  - {p in Gp | BestSub covers p}
    H = H + BestSub
  until Gp = {}
  return H
end
```

SubdueCL Algorithm

```
SubdueCL(Gp, Gn, Limit, Beam)
  ParentList = (All substructures of one vertex in Gp) mod Beam
  repeat
    BestList = {}
    Exhausted = TRUE
    i = Limit
    while ( (i > 0 ) and (ParentList ≠ {}) )
      ChildList = {}
      foreach substucture in ParentList
        C = Expand(Substructure)
        if CoversOnePos(C,Gp)
          then BestList = BestList ∪ {C}
        ChildList = ( ChildList ∪ C ) mod Beam
        i = i – 1
      endfor
      ParentList = ChildList mod Beam
    endwhile
    if BestList = {} and ParentList ≠ {}
      then Exhausted = FALSE
           Limit = Limit * 1.2
  until ( Exhausted = TRUE )
  return first(BestList)
end
```


Example





Empirical Results

- Comparison with ILP (inductive logic programming) systems
- Non-relational domains from UCI repository

	Golf	Vote	Diabetes	Credit	TicTacToe
FOIL	66.67	93.02	70.66	66.16	100.00
Progol	33.33	76.98	51.97	44.55	100.00
SubdueCL	66.67	94.88	64.21	71.52	100.00

- Subdue has also been extended for multiple classes

Graph-based Anomaly Detection [KDD03]

- Anomalous substructure detection
  - Examine entire graph
  - Report unusual (low MDL compression) substructures
    - low count
    - lower MDL
    - lower compression in subsequent passes

size * count can be used as a heuristic

Graph-based Anomaly Detection [KDD03]

- Anomalous subgraph detection
  - Partition graph into distinct, separate structures (subgraphs)
  - Determine how anomalous each subgraph is compared to others
    - How early compressed?
    - How much compression?

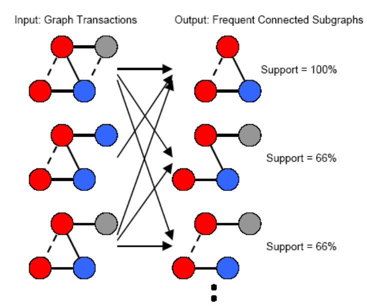
FSG

- Aims at discovering interesting sub-graph(s) that appear frequently over the entire set of graphs in contrast to discovering a interesting sub-graph(s) that appear within a single graph (or a forest) as in Subdue/HDB-Subdue
- It is designed along the lines of Apriori algorithm.

Problem Definition

- discovering all connected subgraphs that occur frequently over the entire set of graphs.
  - Subdue: best n are output (n is user defined)
- vertex : corresponds to an entity
- edge : correspond to a relation between two entities

Example of Frequent sub-graph discovery



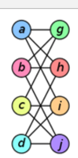
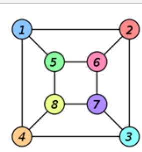
Definitions

- Gs will be an induced subgraph of G if Vs is a subset of V and Es contains all the edges of E that connect vertices in Vs.
- Two graphs *G*1 = (*V*1;*E*1) and *G*2 = (*V*2;*E*2) are *isomorphic* if they are topologically identical to each other, that is, there is a mapping from *V*1 to *V*2 such that each edge in *E*1 is mapped to a single edge in *E*2 and vice versa
- An automorphism : an isomorphism mapping where G1 = G2 (on the same graph).

© Sharma Chakravarthy

Example (from wiki)

- The two graphs shown below are isomorphic, despite their different looking drawings

Graph G	Graph H	An isomorphism between G and H
		*f*(*a*) = 1 *f*(*b*) = 6 *f*(*c*) = 8 *f*(*d*) = 3 *f*(*g*) = 5 *f*(*h*) = 2 *f*(*i*) = 4 *f*(*j*) = 7

- The formal notion of "isomorphism", e.g., of "graph isomorphism", captures the informal notion that some objects have "the same structure" if one ignores individual distinctions of "atomic" components of objects in question

© Sharma Chakravarthy

Conclusions

- Graph mining is a powerful approach needed by many real-world applications
- There is need for both Subdue class of mining algorithms and frequent subgraph class of algorithms
- Scalability is an extremely important issue
- Our approach to using SQL has yielded very promising scalability results (800K vertices and 1600K edges)

© Sharma Chakravarthy

Comparison

	Subdue	FSG	AGM	gSpan	HDBSubdue
Graph Mining	✓	✓	✓	✓	✓
Multiple edges	✓	×	×	×	✓
Hierarchical reduction	✓	×	×	×	✓
Cycles	✓	✓	✓	×	✓
Evaluation metric	MDL	Frequency	Support, Confidence	Frequency	DMDL (frequency)
Inexact graph match With threshold	✓	×	×	×	×
Memory limitation	✓	✓	✓	✓	×

© Sharma Chakravarthy

Scalability Issues

- Subdue is a main memory algorithm.
- Good performance for small data sizes
- Entire graph is constructed before applying the mining algorithm
- Takes a very long time to even to initialize for 1600K edges and 800K vertices graph
- Scalability is an issue

SQL-Based Graph Mining

- We have mapped the Subdue algorithm using SQL (HDB-Subdue)
  - Handles multiple edges between nodes
  - Handles cycles/loops
  - Performs Hierarchical reduction
  - Dveloped DMDL tailored to databases
- Can handle graphs of Millions of edges and vertices
- DB-FSG does frequent subgraph mining
- Working on inexact matching