Frequent Subgraph Discovery
Mining Scientific & Relational Data Sets

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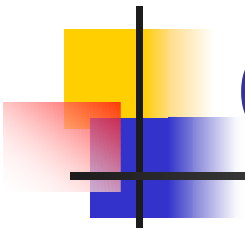
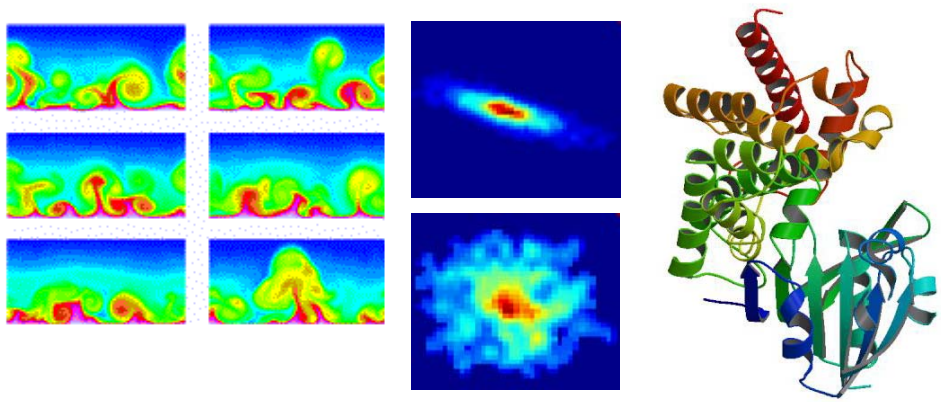


Outline

- Why do we need to use graphs?
- What is frequent subgraph discovery?
- Detail of the algorithm
- Empirical evaluation with synthetic and real datasets
- Conclusions

Data Mining And Scientific Data

- Data mining has emerged as a critical tool for knowledge discovery in large data sets.
  - It has been extensively used to analyze business, financial, and textual data sets.
- The success of these techniques has sparked interest in applying them to various scientific and engineering fields.
  - Astronomy
  - Biology
  - Ecosystem modeling
  - Fluid dynamics
  - Genomics
  - Structural mechanics



Pattern Discovery In Scientific Data

- Most of existing data mining algorithms are based on transaction representation, *i.e.*, **sets of items**.
- Scientific datasets with structures, layers, hierarchy and/or geometry often do not fit well in this transaction setting.
  - e.g., Numerical simulations, 3D protein structures, chemical compounds, etc.

Need algorithms that operate natively on datasets in their native/structured representation

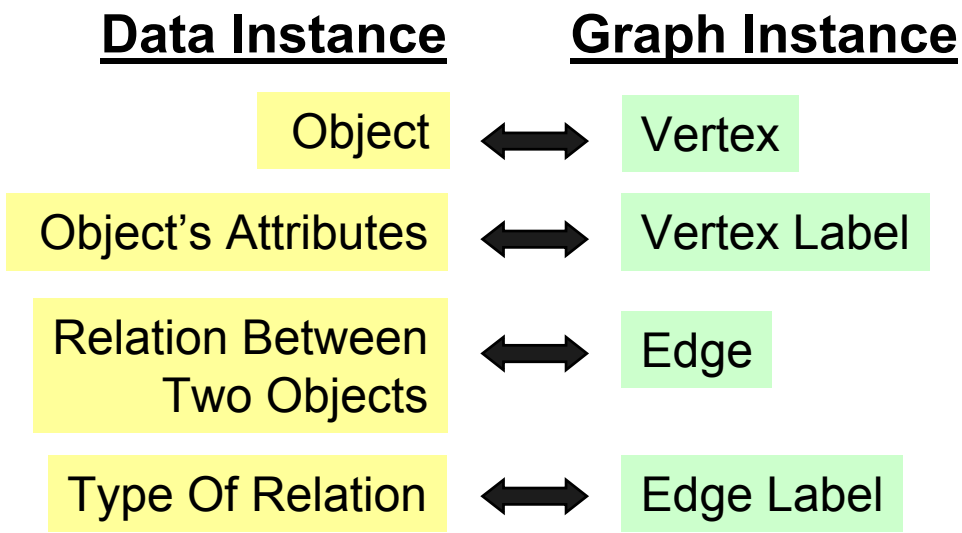
Representation For Scientific Datasets

- Which representation is good?
  - Abstract compared with the original raw (and typically flat) numerical data
  - Yet powerful enough to capture the important characteristics

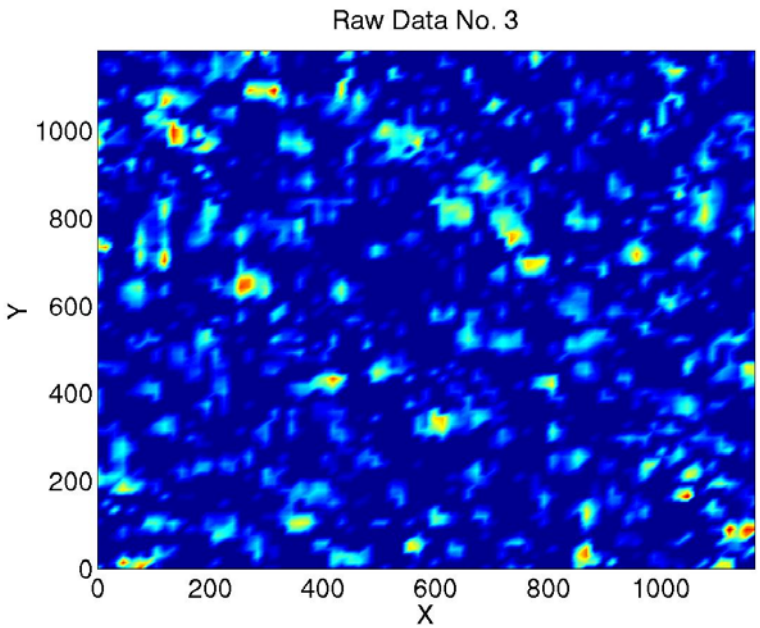
Labeled directed/undirected graphs

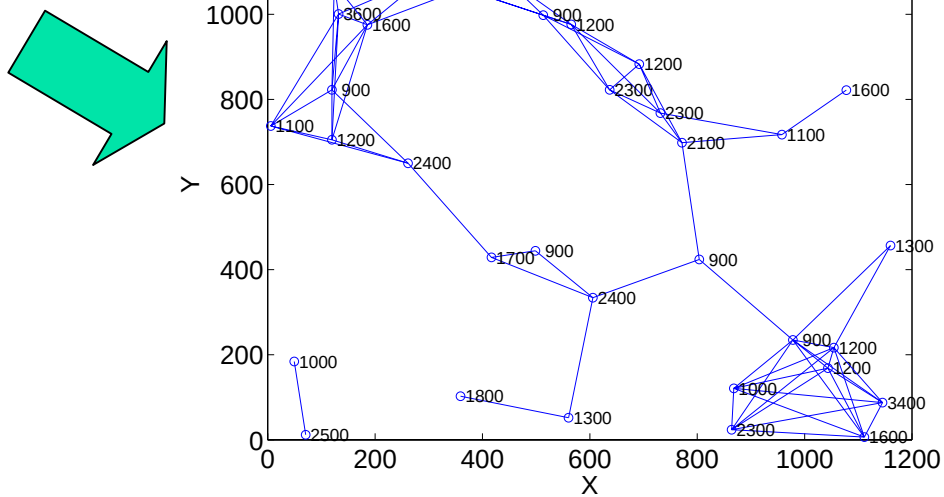
Modeling Data With Graphs…
Going Beyond Transactions

- Graphs can be used to accurately model and represent scientific data sets.
- Graphs are suitable for capturing arbitrary relations between the various objects.



Example


Raw Data No. 3
Y
X
0
200
400
600
800
1000


Corresponding Graph Transaction No. 3
Y
X
0
200
400
600
800
1000
1200
700
1100
2300
1100
3600
1600
900
1200
1200
900
2300
1600
2300
1100
1100
1200
2100
2400
1700
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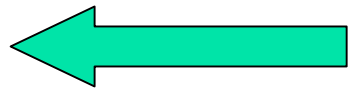
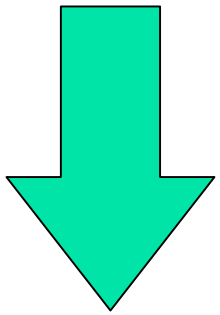
1200
1200
1000
1000
1800
1300
3400
2500
2300
1600

Graph Mining

- Finding patterns in these graph 
- Finding groups of similar graphs
- Building predictive models for the graphs

Interesting Patterns → Frequent Subgraphs

- Discovering interesting patterns



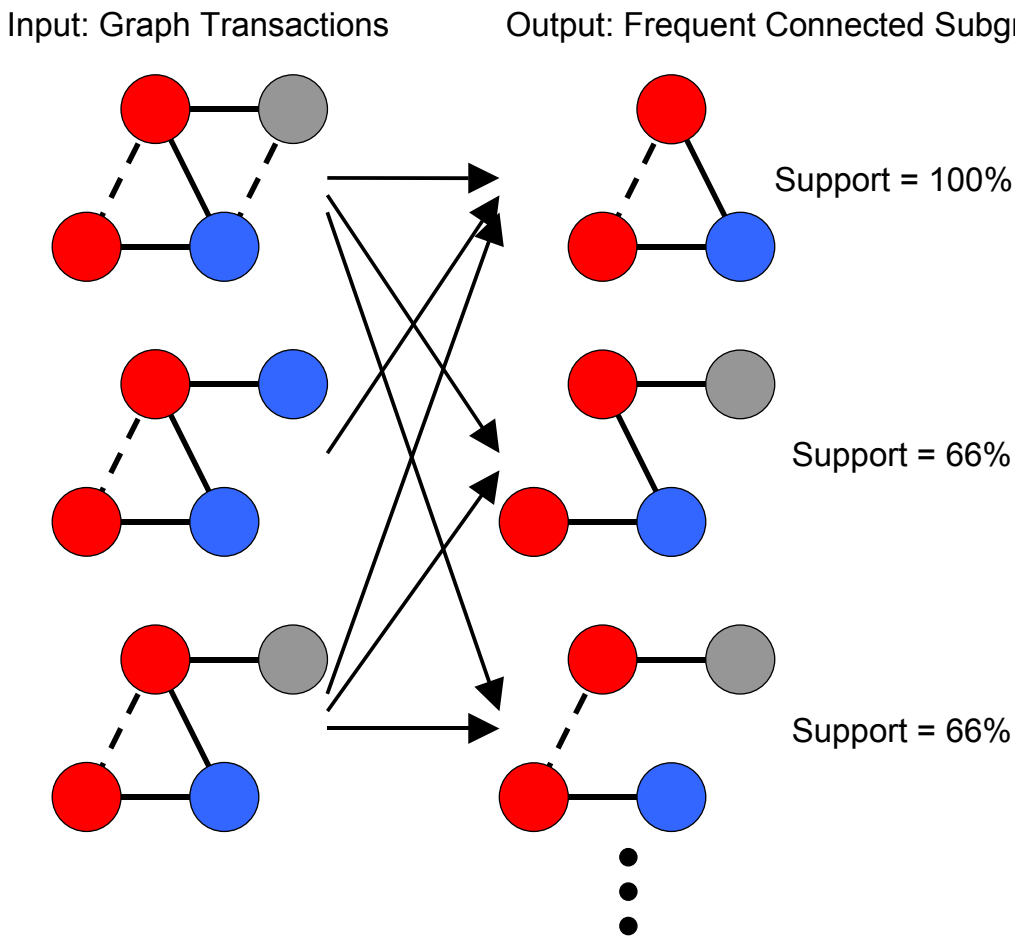
- Finding frequent, recurrent subgraphs

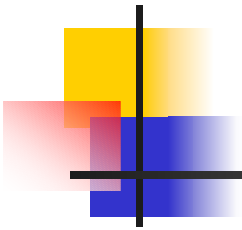
Efficient algorithms need to be developed that operate and take advantage of this representation

Finding Frequent Subgraphs: Input and Output

- Problem setting: similar to finding frequent itemsets for association rule discovery
- Input
  - Database of graph transactions
    - Undirected simple graph (no loops, no multiples edges)
    - Each graph transaction has labeled edges/vertices.
    - Transactions may not be connected
  - Minimum support threshold σ
- Output
  - Frequent subgraphs that satisfy the support threshold
  - Each frequent subgraph is connected.

Finding Frequent Subgraphs: Input and Output





FSG
Frequent Subgraph Discovery Algorithm

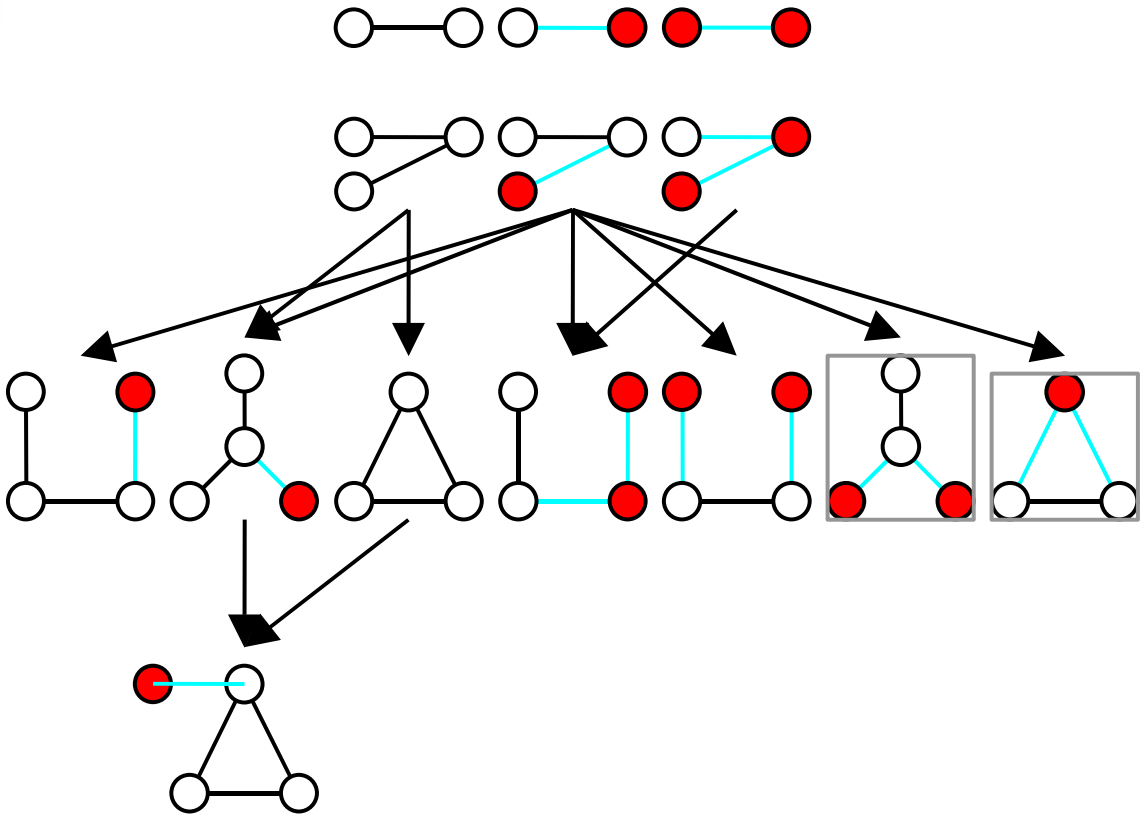
- Incremental and breadth-first fashion on the size of frequent subgraphs (like Apriori for frequent itemsets)
- Counting of frequent single and double edge subgraphs
- For finding frequent size k-subgraphs ($k \geq 3$),
  - Candidate generation

    Joining two size $(k-1)$-subgraphs similar to each other.
  - Candidate pruning by downward closure property
  - Frequency counting

    Check if a subgraph is contained in a transaction.
  - Repeat the steps for $k = k + 1$

    Increase the size of subgraphs by one edge.

FSG: Algorithm



Single edges

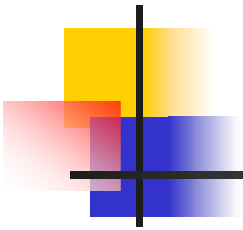
Double edges

3-candidates

3-frequent subgraphs

4-candidates

4-frequent subgraphs



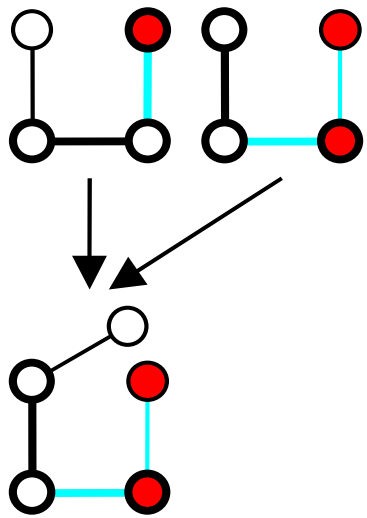
FSG: Methodology

- Edge-based
  - Transaction ↔ Labeled graph
  - Item ↔ Vertex
  - Itemset ↔ Connected subgraph
  - Size of an itemset ↔ Number of edges (size of a subgraph)
- FSG finds frequent connected subgraphs in the bottom-up and breadth-first fashion.

Trivial Operations Become Complicated With Graphs…

- Candidate generation
  - To determine two candidates for joining, we need to perform subgraph isomorphism.
  - Isomorphism for redundancy check
- Candidate pruning
  - To check downward closure property, we need subgraph isomorphism.
- Frequency counting
  - Subgraph isomorphism for checking containment of a frequent subgraph
- How to reduce the number of graph/subgraph isomorphism operations?

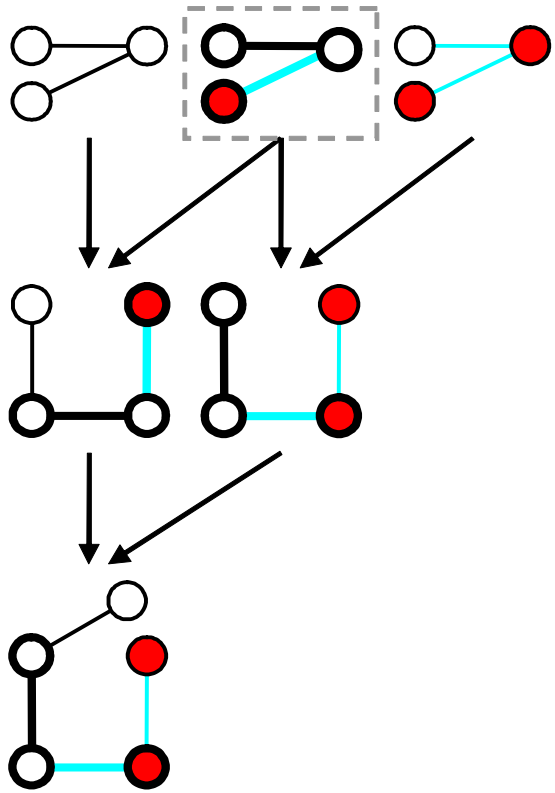
FSG Approach: Candidate Generation



3-frequent

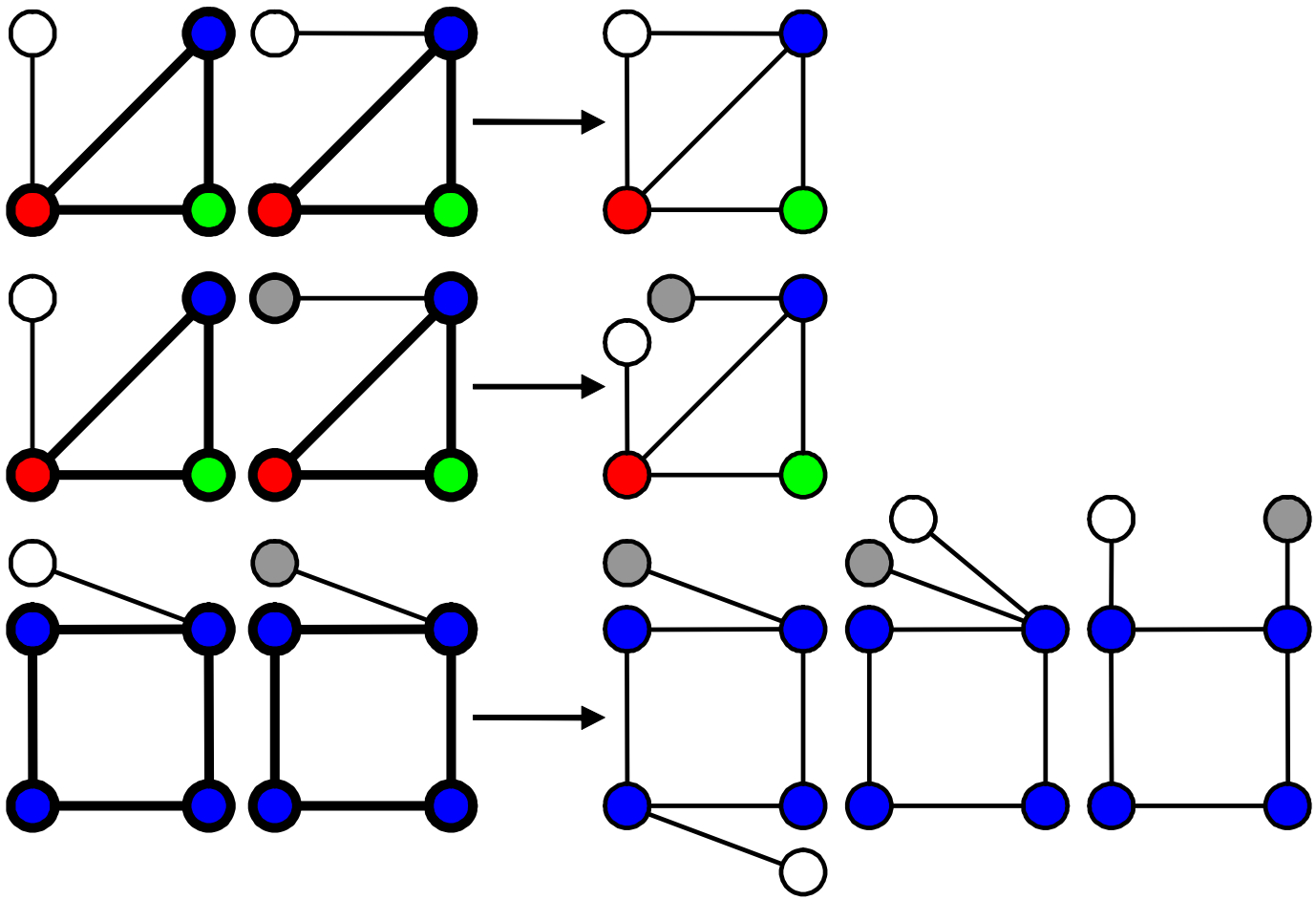
4-candidates

FSG Approach: Candidate Generation

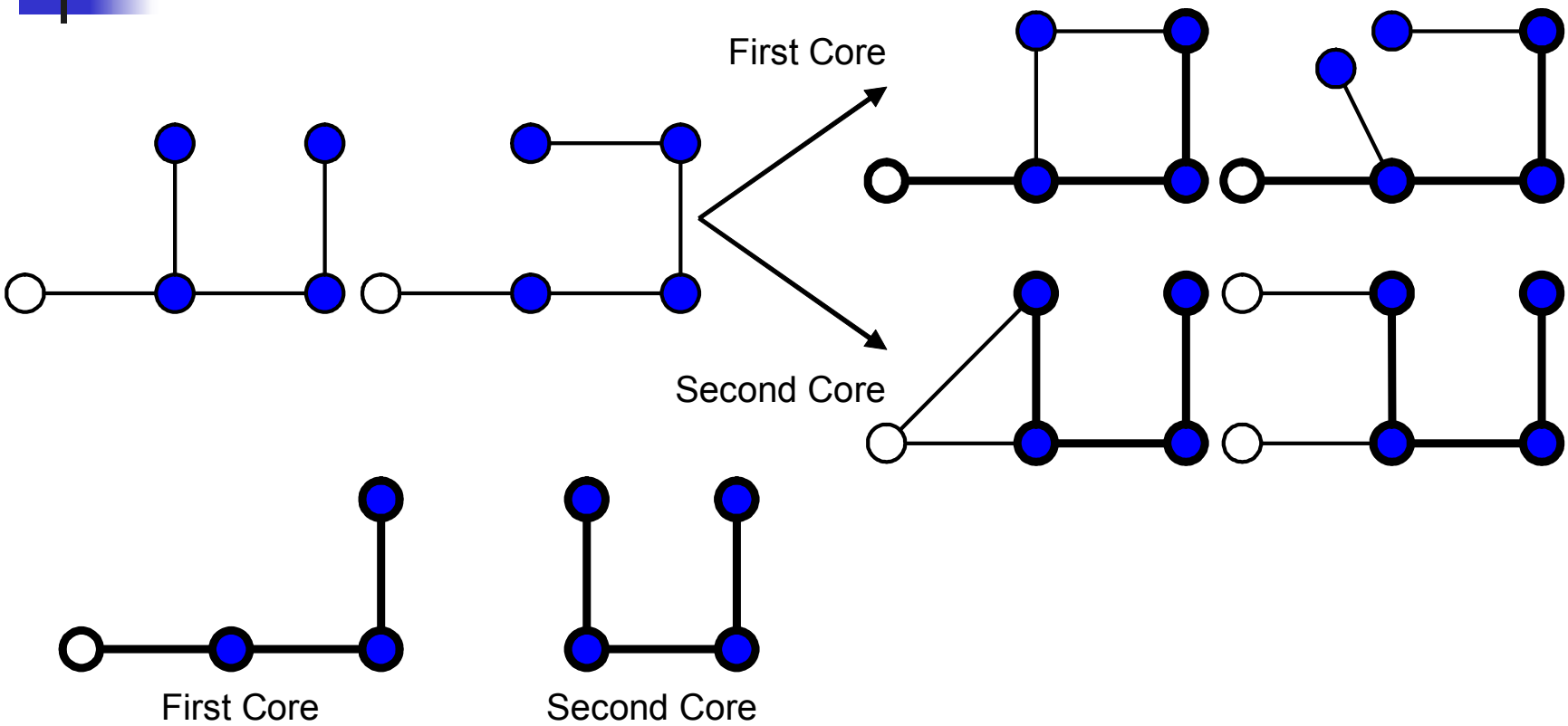


- Intersection of the parent lists of two 3-frequent subgraphs
- Without subgraph isomorphism, we can detect the core of the two 3-frequent subgraphs.
- Redundancy check by canonical labeling

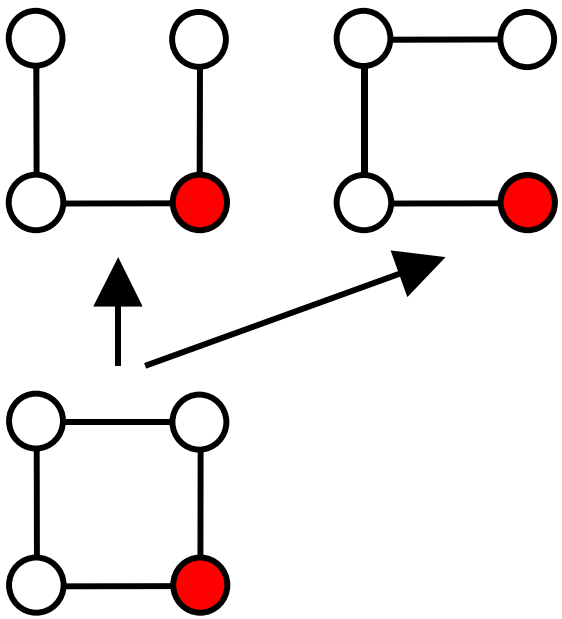
Candidate Generation Based On Core Detection



Candidate Generation Based On Core Detection



FSG Approach: Candidate Pruning



3-subgraphs

4-candidate

- Downward closure property
- Every ($k-1$)-subgraph must be frequent
- Keep the list of those ($k-1$)-subgraphs

FSG Approach: Candidate Pruning

- Pruning of size k-candidates
  - For all the $(k-1)$-subgraphs of a size k-candidate, check if downward closure property holds.
    - Canonical labeling is used to speedup the computation.
  - Build the parent list of $(k-1)$-frequent subgraphs for the k-candidate.
    - Used later in the candidate generation, if this candidate survives the frequency counting check.

FSG Approach: Frequency Counting

Transactions

T1 = {f1, f2, f3}

T2 = {f1}

T3 = {f2}

Frequent Subgraphs

TID(f1) = {T1, T2}

TID(f2) = {T1, T3}

Candidate

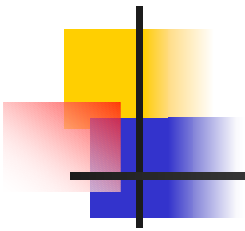
c = join(f1, f2)

TID(c) = subset(TID(f1) AND TID(f2))

- Perform only subg_isomorph(c, T1))
- TID lists require a lot of memory!

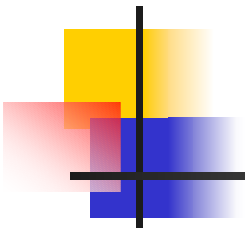
FSG Approach: Frequency Counting

- Frequency counting
  - Keep track of the TID lists.
  - If a size k-candidate is contained in a transaction, all the size $(k-1)$-parents must be contained in the same transaction.
  - Perform subgraph isomorphism only on the intersection of the TID lists of the parent frequent subgraphs of size $k-1$.
    - Significantly reduces the number of subgraph isomorphism checks.
    - Trade-off between running time and memory



Empirical Evaluation

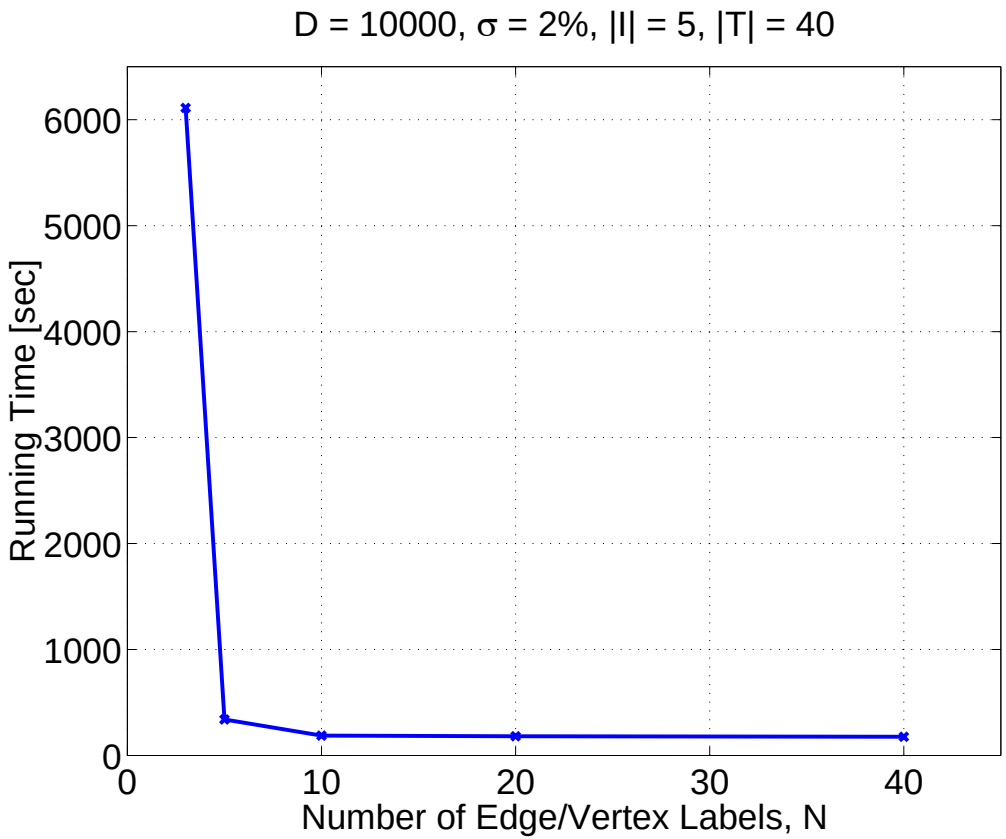
- Synthetic datasets
  - Sensitivity study
    - Number of labels used in input graphs
    - Transaction size
    - Number of transactions
- Real dataset
  - Chemical compounds from PTE challenge
- Pentium III 650 MHz, 2GB RAM



Evaluation: Synthetic Datasets

- Try to mimic the idea of the data generator for frequent itemset discovery, used in the Apriori paper (Agrawal and Srikant, *VLDB*, 1994).
- Generate a pool of potential frequent subgraphs ("seeds").
- Embed randomly selected seeds into each transaction until the transaction reaches the specified size.

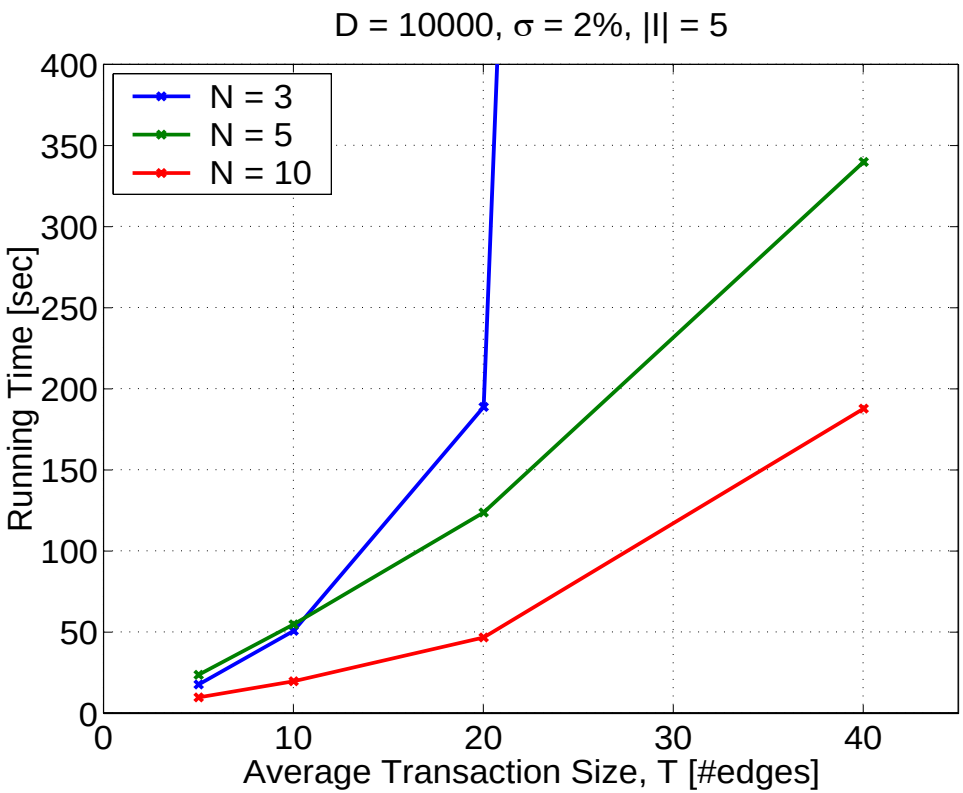
Sensitivity: The Number Of Labels



- 10000 transactions
- 2% support
- Average seed size |I| = 5
- Average transaction size |T| = 40

- More labels → Faster execution

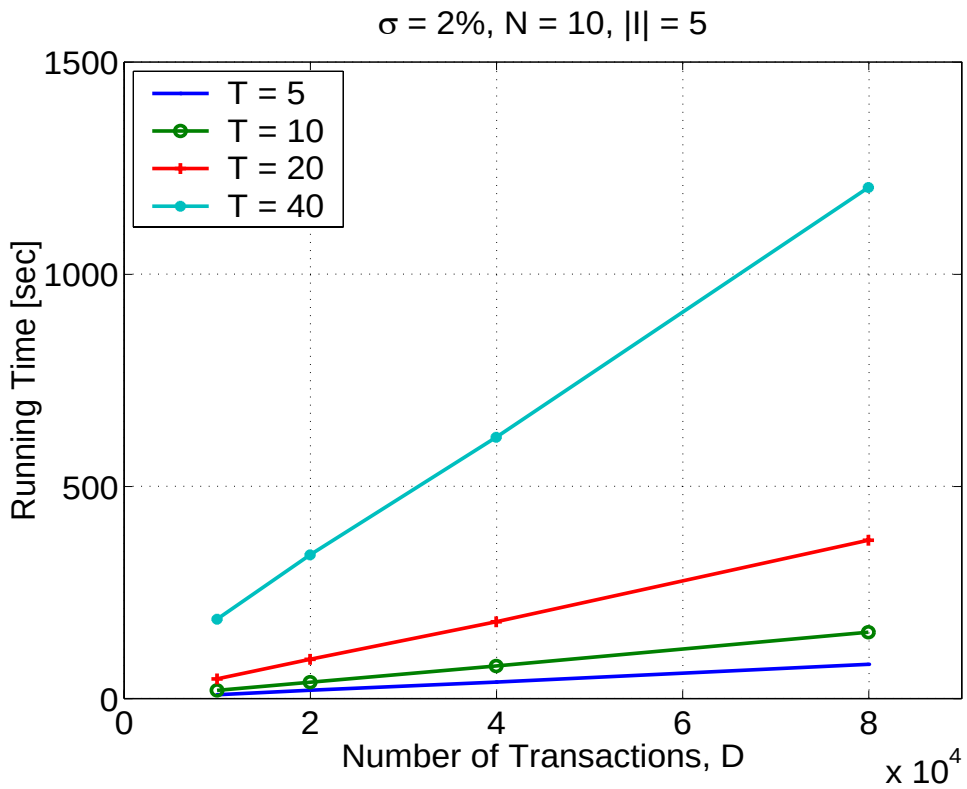
Sensitivity: Transaction Size



- 10000 transactions
- 2% support
- Average seed size
  |I| = 5

- Average transaction size, *T*, significantly affects the execution time, especially with fewer labels.

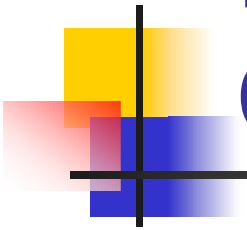
Sensitivity: Number of Transactions



- 2% support
- Transaction size
  T = 5, 10, 20, 40
- Average seed size
  |I| = 5
- 10 edge/vertex labels

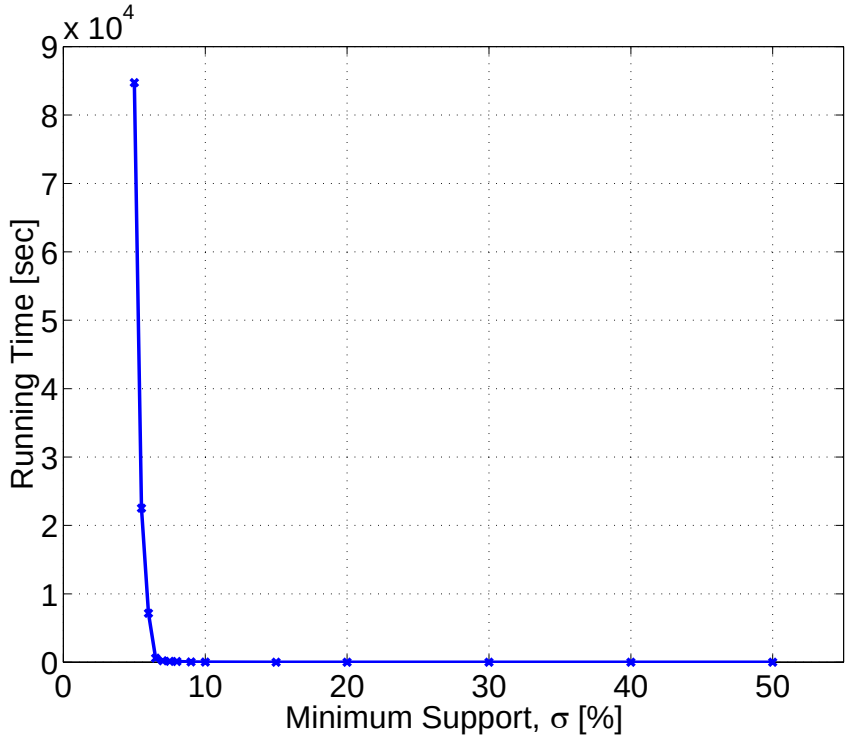
- Linear scalability

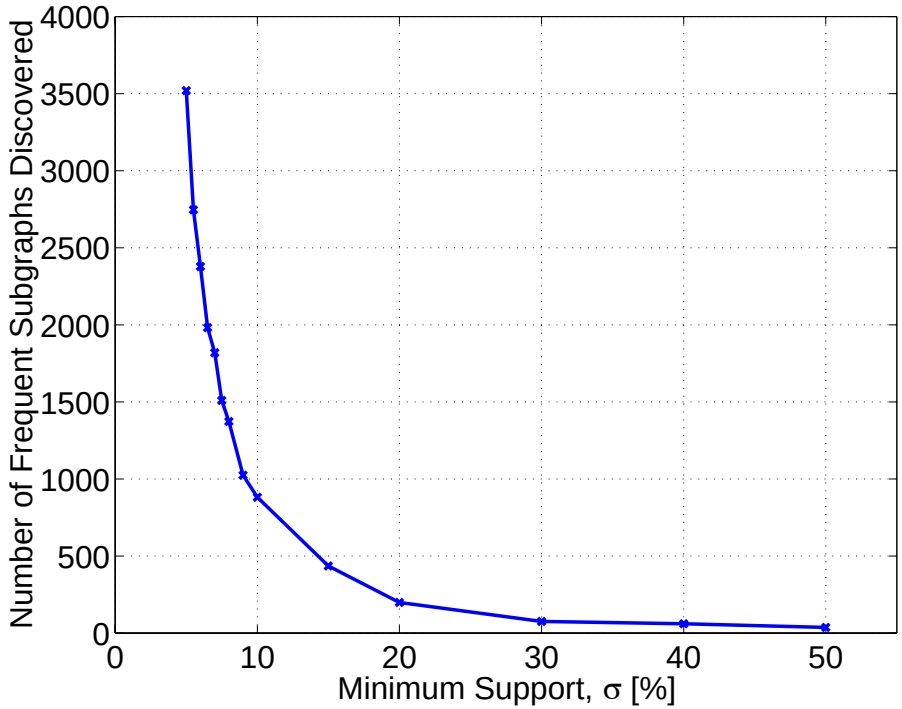
Evaluation: Chemical Compound Dataset



- Predictive Toxicology Evaluation (PTE) Challenge (Srinivasan et al., *IJCAI*, 1997)
- 340 chemical compounds
- Sparse
  - Average transaction size 27.4 edges, 27.0 vertices
  - Maximum transaction has 214 edges.
- 4 edge labels, 66 vertex labels

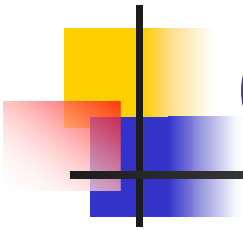
Evaluation: Chemical Compound Dataset





Evaluation: Chemical Compound Dataset

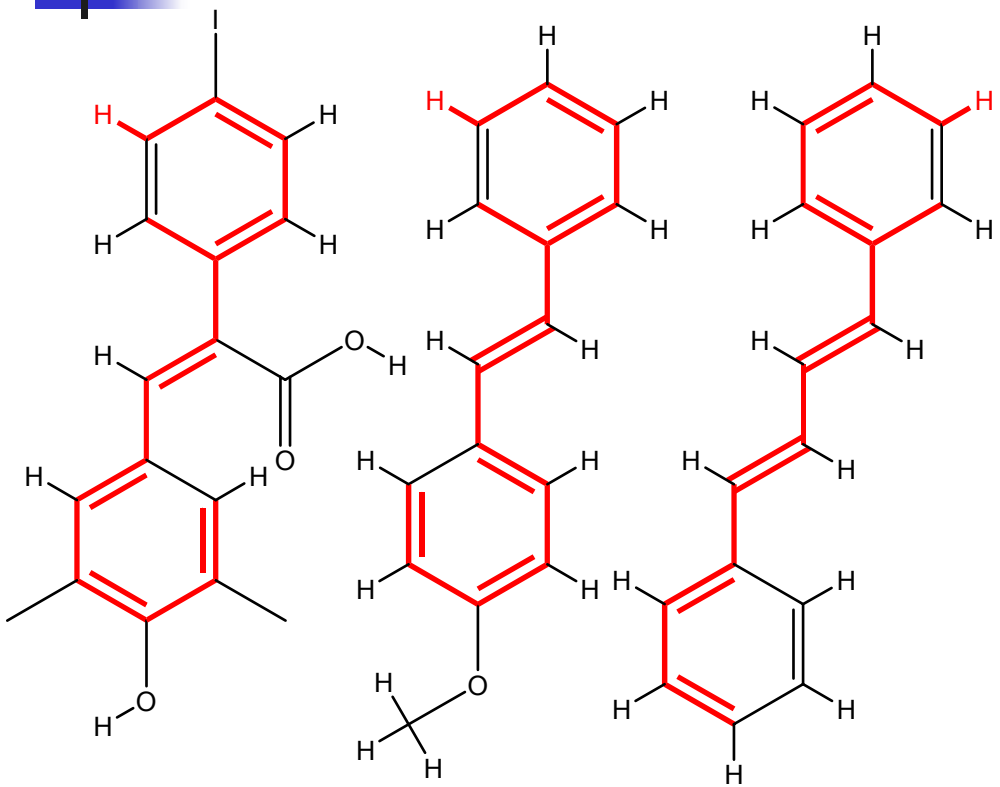
- AGM spent 8 days for support 10% on 400 MHz PC.
  - Inokuchi et al., An apriori-based algorithm for mining frequent substructures from graph data, *PKDD*, 2000
  - Vertex-based
  - AGM finds frequent induced subgraphs that may not be connected
- FSG took 28 seconds for support 10%.



Conclusions

- Linear scalability w. r. t. # of transactions
- FSG runs faster as the number of distinct edge/vertex labels increases.
- Average size of transactions |T|
  - Significant impact on the running time
  - Subgraph isomorphism for frequency counting
  - Edge density
    - Increases the search space of graph/subgraph isomorphism exponentially.
- Suitable for sparse graph transactions

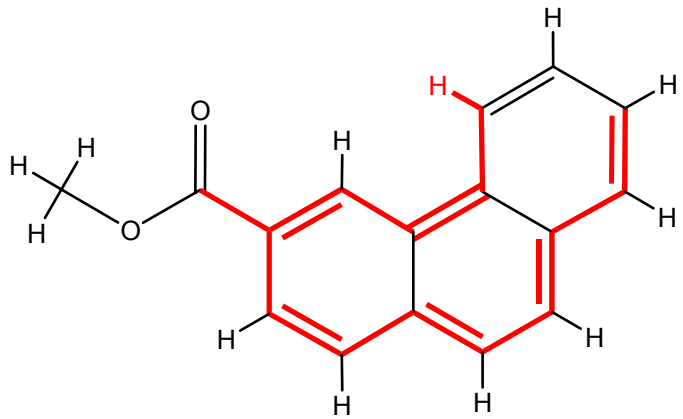
Topology Is Not Enough (Sometimes)



3-(3,5-dibromo-4-hydroxyphenyl)-2-(4-iodophenyl)acrylic acid

1-methoxy-4-(2-phenylvinyl)benzene

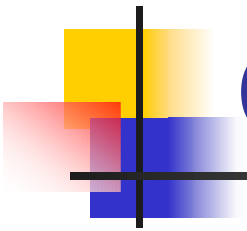
(4-phenyl-1,3-butadienyl)benzene



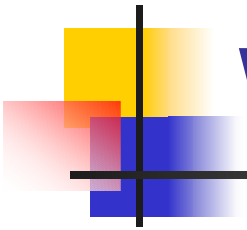
methyl 3-phenanthrenecarboxylate

- 100 chemical compounds with 30 atoms
- Support = 10%
- 3 patterns of 14 edges found

Extension To Discovering Geometric Patterns



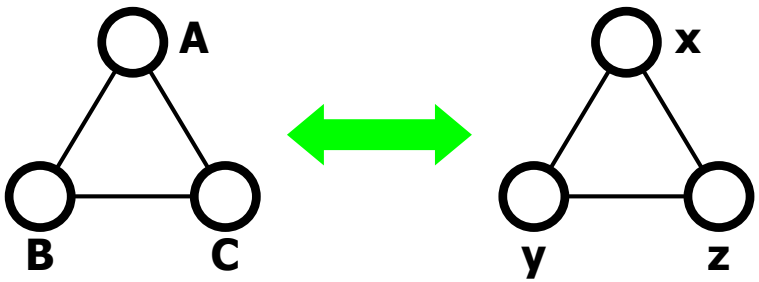
- Ongoing work, no preliminary results. Sorry!
- Geometric graphs
  - Most of scientific datasets naturally contain 2D/3D geometric information.
  - Each vertex has 2D/3D coordinates associated.
  - Geometric graphs are the same as the purely topological graphs except the coordinates (i.e., edges and vertices have labels assigned).



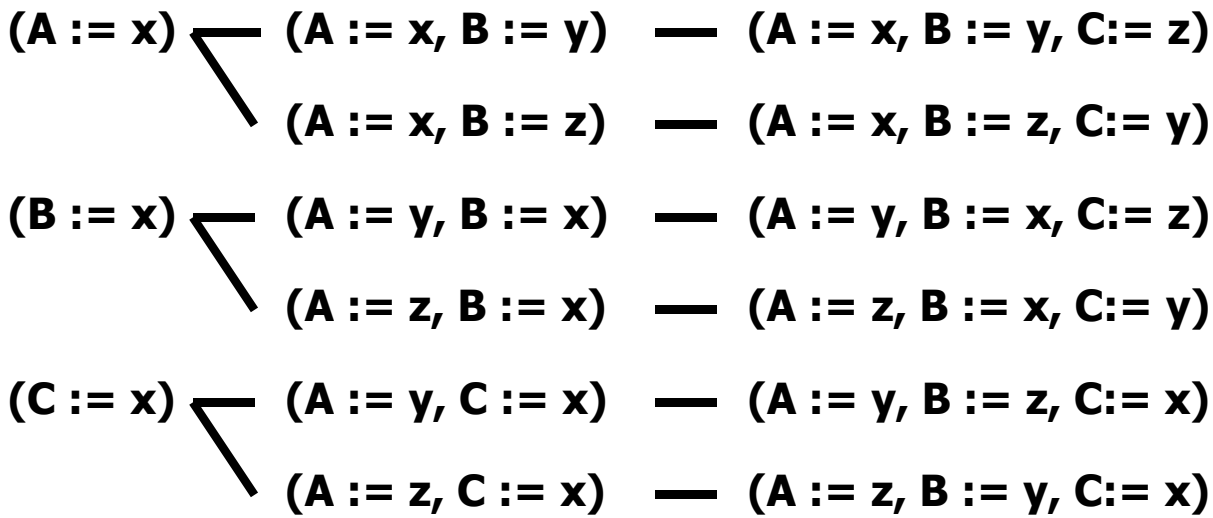
What Is Good With Geometry?

- Coordinates of vertices are helpful
- In topological graph finding, isomorphism which is known to be expensive operation, is inevitable.
  - Candidate generation
  - Frequency counting
- By using coordinates, we can narrow down the search space of (sub)graph isomorphism drastically.
  - Geometric hashing (pre-computing geometric configurations)
    - Rotation
    - Scaling
    - Translation

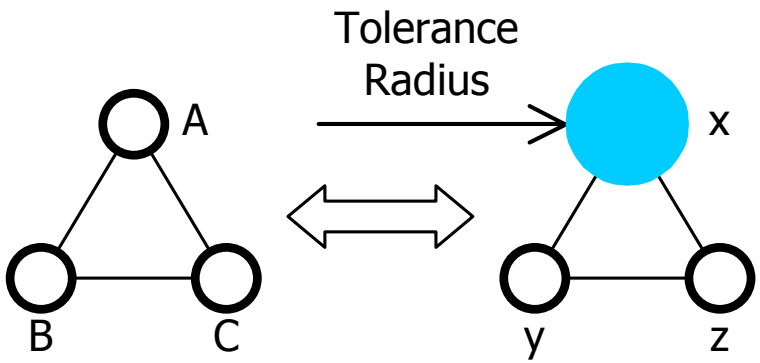
Search Space Of Purely Topological Isomorphism



- Complexity = $O(n!)$
  - n: # of vertices

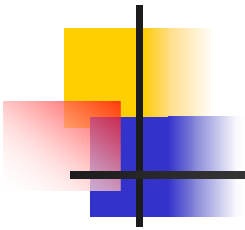


Use Of Coordinates In Geometric Isomorphism



- The radius of the shaded area determines the tolerance of the matching.

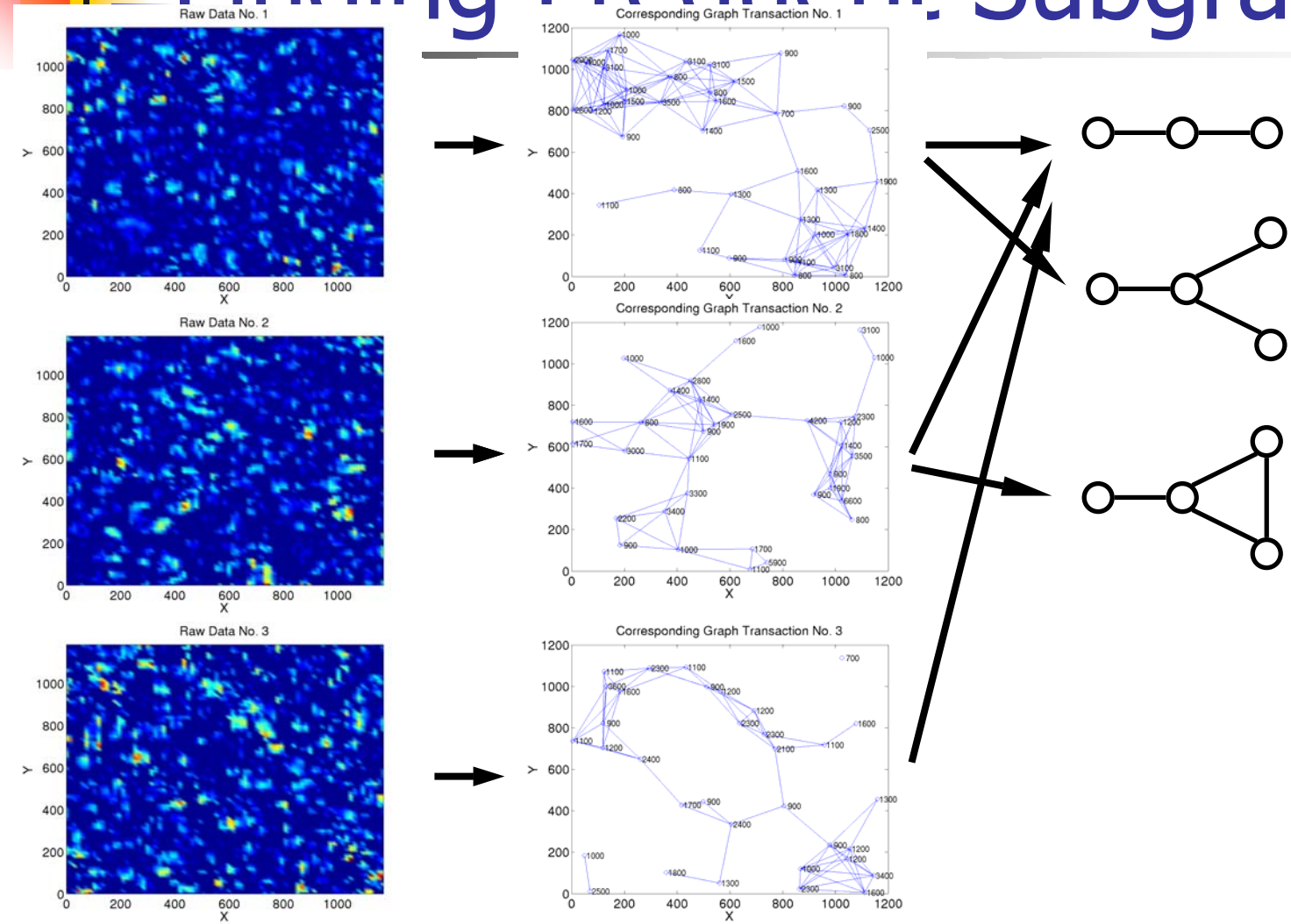
- To seek for a map of "A", we can focus the inside of the shaded area.
  - That eliminates "y" and "z" for a mapping of "A".
- Complexity depends on the # of configurations
  = $O(n^2)$, instead of $O(n!)$ for 2D
  n: # of vertices



Thank you!

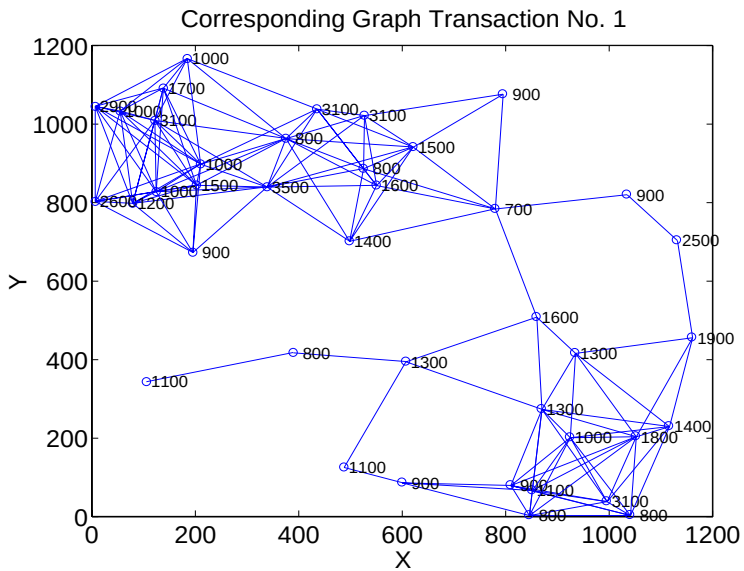
http://www.cs.umn.edu/~karypis

Finding Frequent Subgraphs



FSG: Methodology

- AGM (Inokuchi et al., An apriori-based algorithm for mining frequent substructures from graph data, *PKDD 2000*)
  - Vertex-based
    - Transaction ↔ Labeled graph
    - Item ↔ Vertex
    - Itemset ↔ Induced subgraph
    - Size of itemset ↔ Number of vertices (order of subgraph)
  - Discovered frequent subgraphs may not be connected


Corresponding Graph Transaction No. 1
X
Y
0
200
400
600
800
1000
1200
1000
1700
2900
1000
3100
3100
3100
900
800
1500
1000
800
1600
1500
1500
3500
2600
1200
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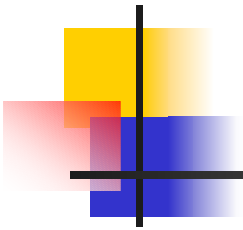
800
800

Graph/Subgraph Isomorphism: Hard Problems



- Graph isomorphism
  - Determine if two graphs are equivalent.
  - Suspected to be neither in P nor in NP-complete.
- Subgraph isomorphism
  - Determine if a graph is a part of another.
  - NP-complete
- Canonical labeling is equivalent to graph isomorphism.
- They are expensive operations, but doable especially when graphs are relatively small.
  - Frequent subgraphs are smaller than the input transactions.
- How to reduce the number of graph/subgraph isomorphism operations?

FSG Approach: Candidate Generation

- To generate a size k-candidate (k edges)
  - Take the intersection of the parent lists of two ($k-1$)-frequent subgraphs
    - To see if two ($k-1$)-frequent subgraphs share the same size ($k-2$)-parent.
    - Parent lists are obtained at the pruning phase.
    - Subgraph isomorphism free!
  - Example
    - parent(c^5) = { g^4, h^4, i^4}, parent(d^5) = { f^4, g^4, h^4}
    - Generate size 6-candidates from the cores g^4 and h^4.
  - Canonical labeling for redundancy check