Induction of Node Label Controlled Graph Grammar Rules

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Overview

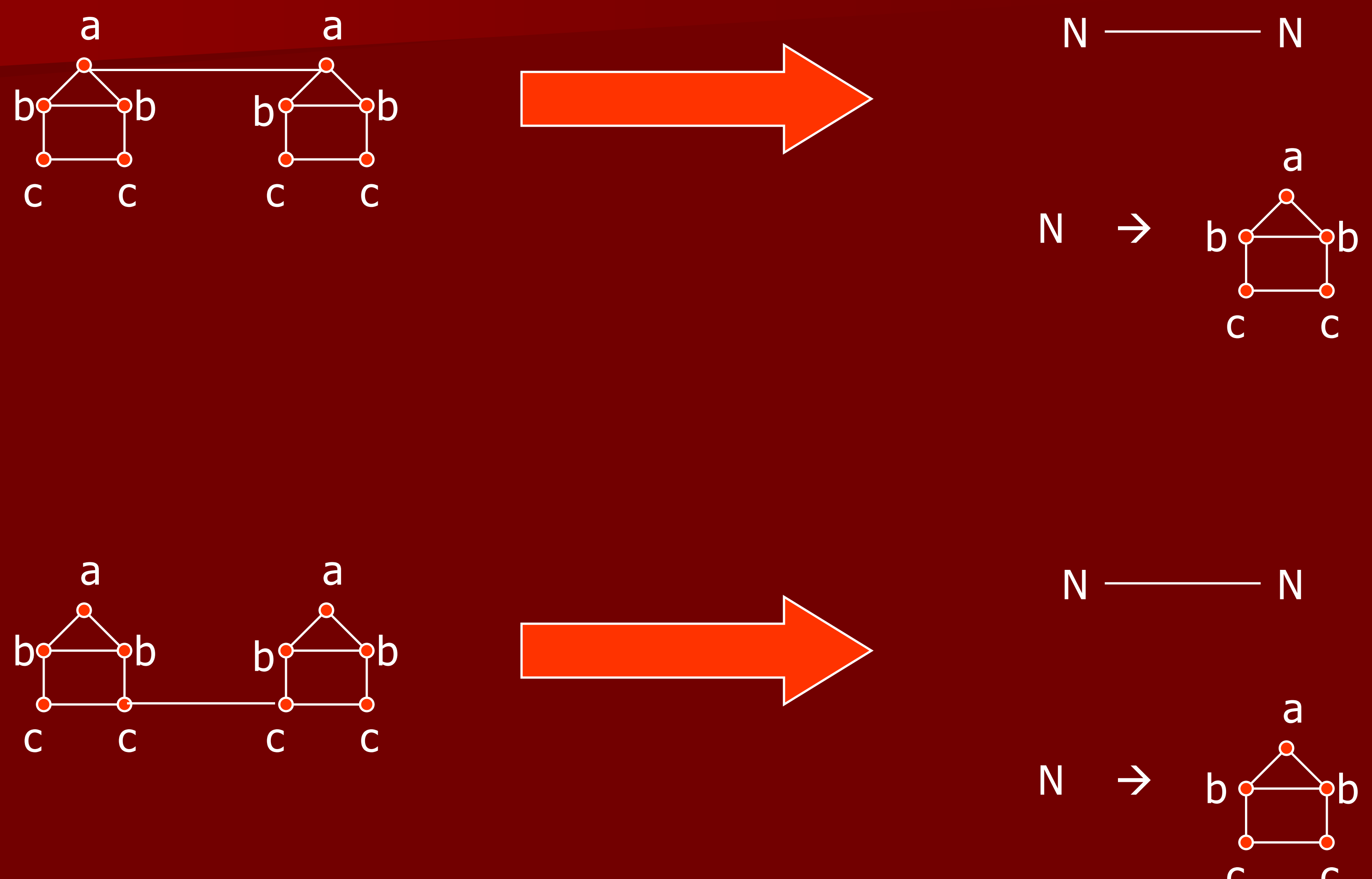
- Motivation
  - Limitations of Subdue-like grammar induction
- Introduction to node label controlled graph grammars (NLC-GGs)
- An algorithm for learning NLC-GG rewrite rules from graphs
- Conclusions & future work

Motivation

- Grammar induction is a popular approach to learning from strings, and a well-studied problem
- Induction of graph grammars might be an interesting approach to learning from graphs
- While graph grammars are well studied (a lot of literature exists on them), there seems to be very little work on *learning* such grammars
- Yet, learning such grammars might be useful
  - Understanding common structure of graphs
  - Active learning: generate new graphs
  - Studying dynamic behavior of networks
  - …

Existing work on learning graph grammars

- Perhaps best known in the learning/mining community: *Subdue* family of algorithms (Holder, Cook, et al., 1994-)
  - Finds frequently occurring subgraph G
  - Compresses graphs by replacing G with a node N and adding *rewrite rule* N -> G
  - Set of rewrite rules can be seen as a graph grammar
  - Heuristic for finding good grammars: maximal compression of graphs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Disadvantage of Subdue

- Disadvantage 1: *compression is lossy*
  - From the point of view of minimal description length (MDL), this is not very nice
- Disadvantage 2: not well in line with existing, well-studied, graph grammars
- Goal of this work is to remove these disadvantages

Theory on graph grammars

- How to define a "graph grammar"?
- Many different methods have been proposed
- Often, on a high level, two kinds of graph grammars are distinguished:
  - Hyperedge replacement grammars
    - Rewrite rule replaces (hyper)edge by new graph
  - Node replacement grammars
    - Rewrite rule replaces node by new graph
- Here we will consider *node replacement grammars*

NLC graph grammars

- *Node Label Controlled* graph grammars (see, e.g., Engelfriet & Rozenberg, 1991)
- = node replacement grammars with rules of the form:

N → G / E

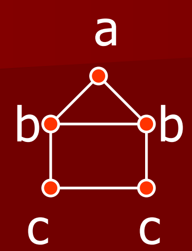
Node label

Labeled graph

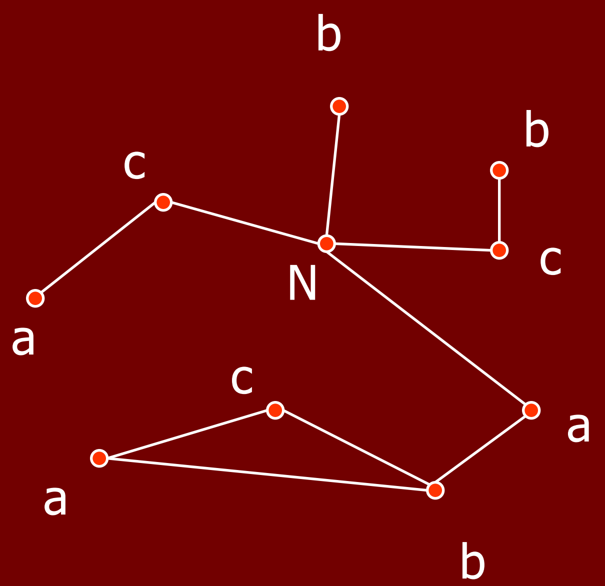
Embedding rules

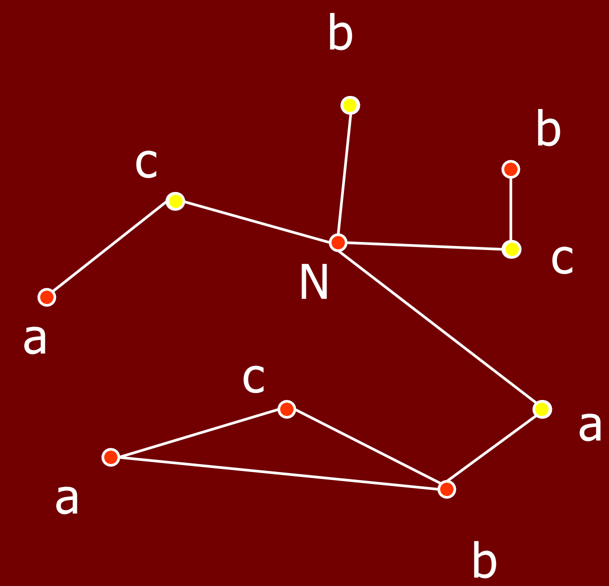
Replace any node with label N by G, connecting G to N's neighborhood according to the embedding rules listed in E. *Embedding rules are based on node labels.*

Example NLC-GG rule

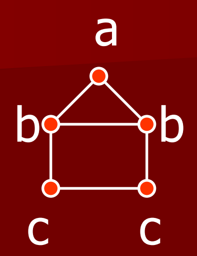
N → 

/ {(a,b), (b,c)}





Example NLC-GG rule

N → 

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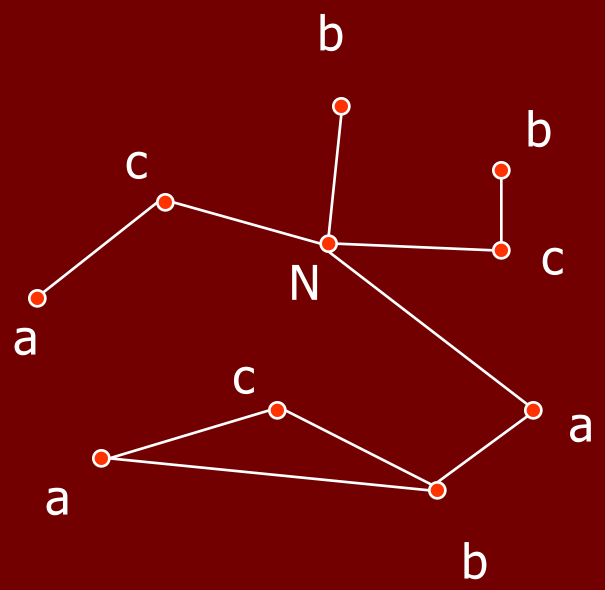
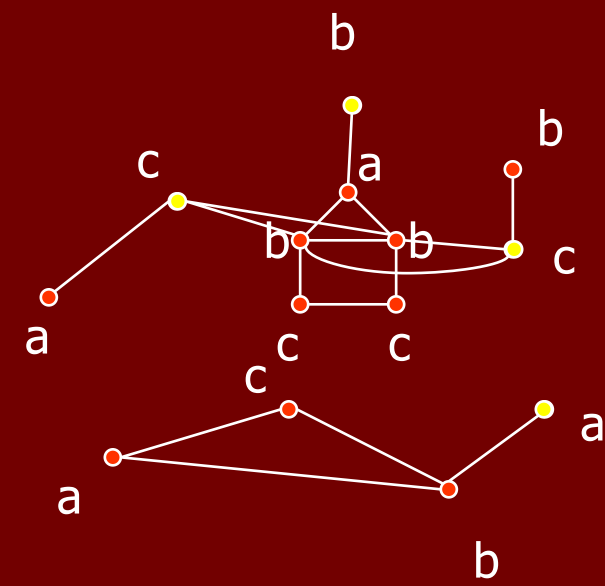
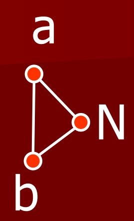


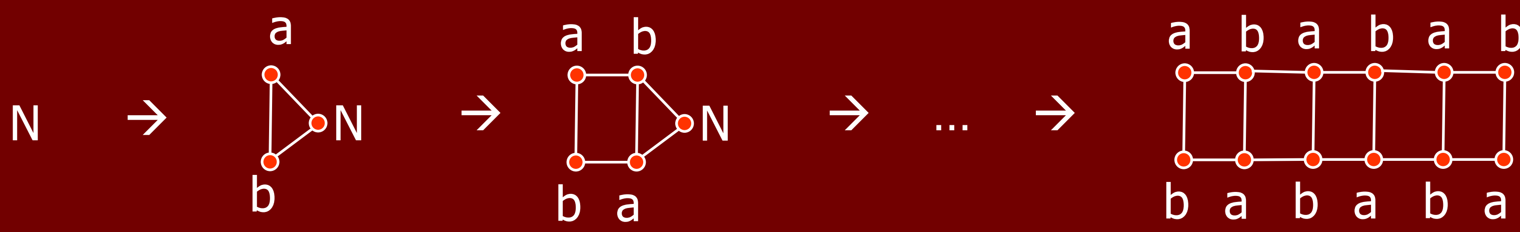


Another example

N → 

/ {(a,b), (b,a)}

N → ε / {}



Research Question

- Question: can we adapt the Subdue operator so that it learns rules of the form N → G / E (instead of N → G) ?
  - This would be a first step towards learning “real” graph grammars (i.e., better in line with existing graph grammar theory)

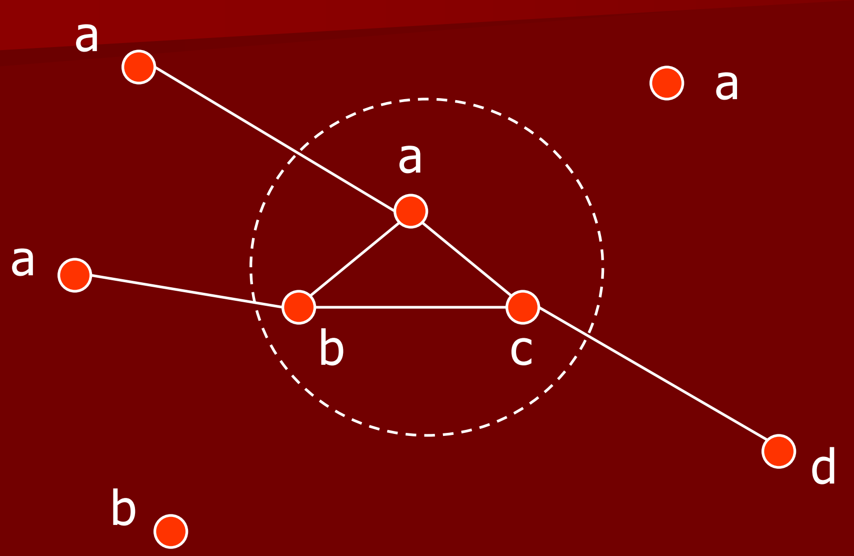
Task: learn rewrite rule

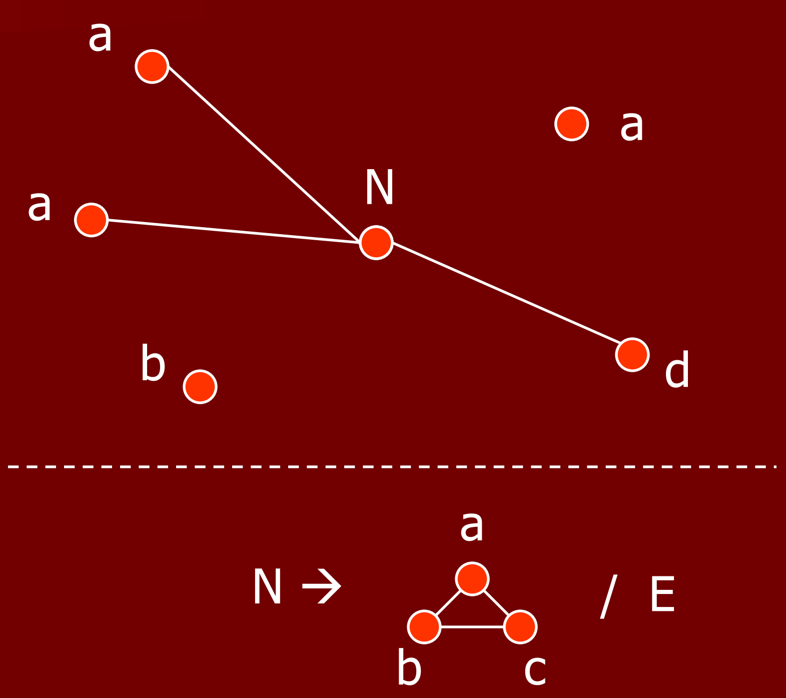
- Subdue learns a rule N → G that leads to maximal compression
- Our goal: Learn a rule N → G / E that leads to maximal compression
  - Find a large G that occurs frequently in the graph, *and* a set E that is compatible with how all these occurrences are embedded in the surrounding graph

Substitutability

- Observation 1: given a single occurrence of some subgraph G, *there may not exist* a set of embedding rules E such that G could be generated and embedded by a rule N → G / E
- We say that a subgraph G is substitutable if such an E does exist
  - In that case, we can substitute some node N for G, and add the rule N → G / E

Substitutability: example





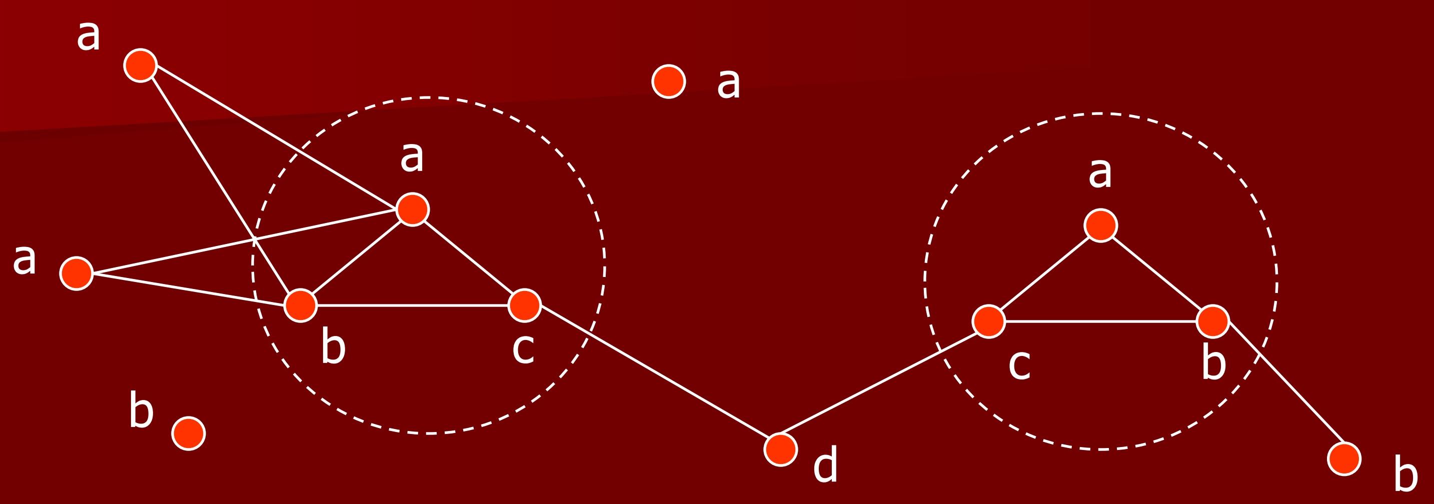
No ruleset E exists such that the encircled graph could have been generated from a node N through N → G / E:

1) 3 nodes (a,a,d) must have been in the environment of N
2) Since we have an edge (b,a), (b,a) must have been in E
3) But then, b should have been connected also to the other a node

Compatibility

- Observation 2: for 2 substitutable occurrences of the same subgraph G, there may or may not exist a single rule N → G / E that could have generated both of them
- We say that the occurrences are compatible if such a rule does exist

Compatibility: example

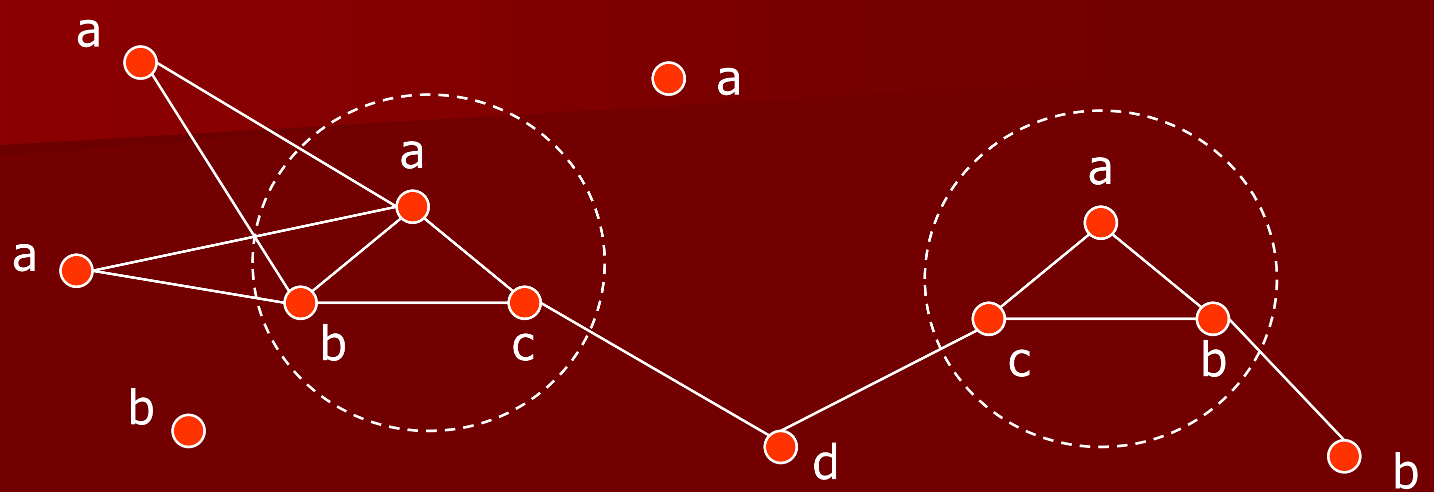


E ⊇ {(a,a), (b,a), (c,d)}

E ⊇ {(b,b), (c,d)}

E ⊇ {(a,a), (b,a), (b,b), (c,d)}

Compatibility: example



$E \supseteq \{(a,a), (b,a), (c,d)\}$

$E \not\supseteq \{(c,a), (a,d), (b,d)\}$

$E \supseteq \{(b,b), (c,d)\}$

$E \not\supseteq \{(a,d), (b,d), (a,b), (c,b)\}$

$E \supseteq \{(a,a),(b,a),(b,b),(c,d)\}$; $E \not\supseteq \{(a,b),(a,d),(b,d),(c,a),(c,b)\}$

Rule-Inset (must be in E)

Rule-outset (must not be in E)

Determining E

- Auxiliary concepts:
  - Given $G \subseteq G'$, and assuming G was generated by some rule N → G / E :
    - The *Node-InSet* of G, NIS(G), contains all nodes in G' – G that must have been in the neighborhood of N
    - The *Rule-InSet* RIS(G), also denoted I, contains all couples (l_1, l_2) that must have been in E
    - The *Rule-OutSet* ROS(G), also denoted O, contains all couples (l_1, l_2) that cannot have been in E
  - We have $I \subseteq E \subseteq L^2 - O$ (with L set of all labels)

1: Determining NIS

- The NIS of a graph G equals the set of all nodes outside G connected to it
  - Each node connected to G must have been in the environment of N (otherwise G couldn’t have been connected to it)
  - For each node not connected to G, either:
    - 1) We know it was not in N’s environment
    - Or 2) we don’t know whether it was or wasn’t
    - (Proof: if node x is not connected to G, any E that yields this embedding from N connected to x would yield the same embedding from N not connected to x)

2: Determining I

- I is the set of couples (a,b) such that E must contain (a,b)
- I contains (a,b) if and only if a node with label a in G is connected to a node with label b outside G
  - If: if edge (a,b) exists, (a,b) must have been in E, otherwise this edge couldnt' have been generated
  - Only if: if no edge (a,b) exists, then for any E, E – {(a,b)} would have given the same embedding; hence, (a,b) not in I

3: Determining O

- O is the set of couples (a,b) that cannot possibly be in E
- O contains (a,b) if and only if there is an a-node in G and a b-node in NIS(G) that are not connected
  - If: if (a,b) were in E, then the a-node and the b-node would have been connected, since the b-node is in NIS(G). Since they are not connected, (a,b) must not be in E.
  - Only if: O contains (a,b) implies that E cannot contain (a,b), i.e., there is a contradiction if (a,b) is in E. Such a contradiction only occurs if there is an a-node in G and a b-node in NIS(G) such that a and b are not connected.

Summary

- Thus, given G (subgraph of G′):
  - Can determine NIS(G) (= nbh(G))
  - Can determine I (= $\{(l(x),l(y)) \mid x \in G \wedge y \in nbh(G) \wedge (x,y) \in G'\}$)
  - From NIS(G), can determine O (= $\{(l(x),l(y)) \mid x \in G \wedge y \in nbh(G) \wedge (x,y) \notin G'\}$)
  - E is a possible embedding rule that might have generated this graph from a graph containing N, using the rule N → G / E, if and only if $I \subseteq E \subseteq L^2 - O$
- If I and O overlap, there are no E's fulfilling the above condition, hence G is not substitutable

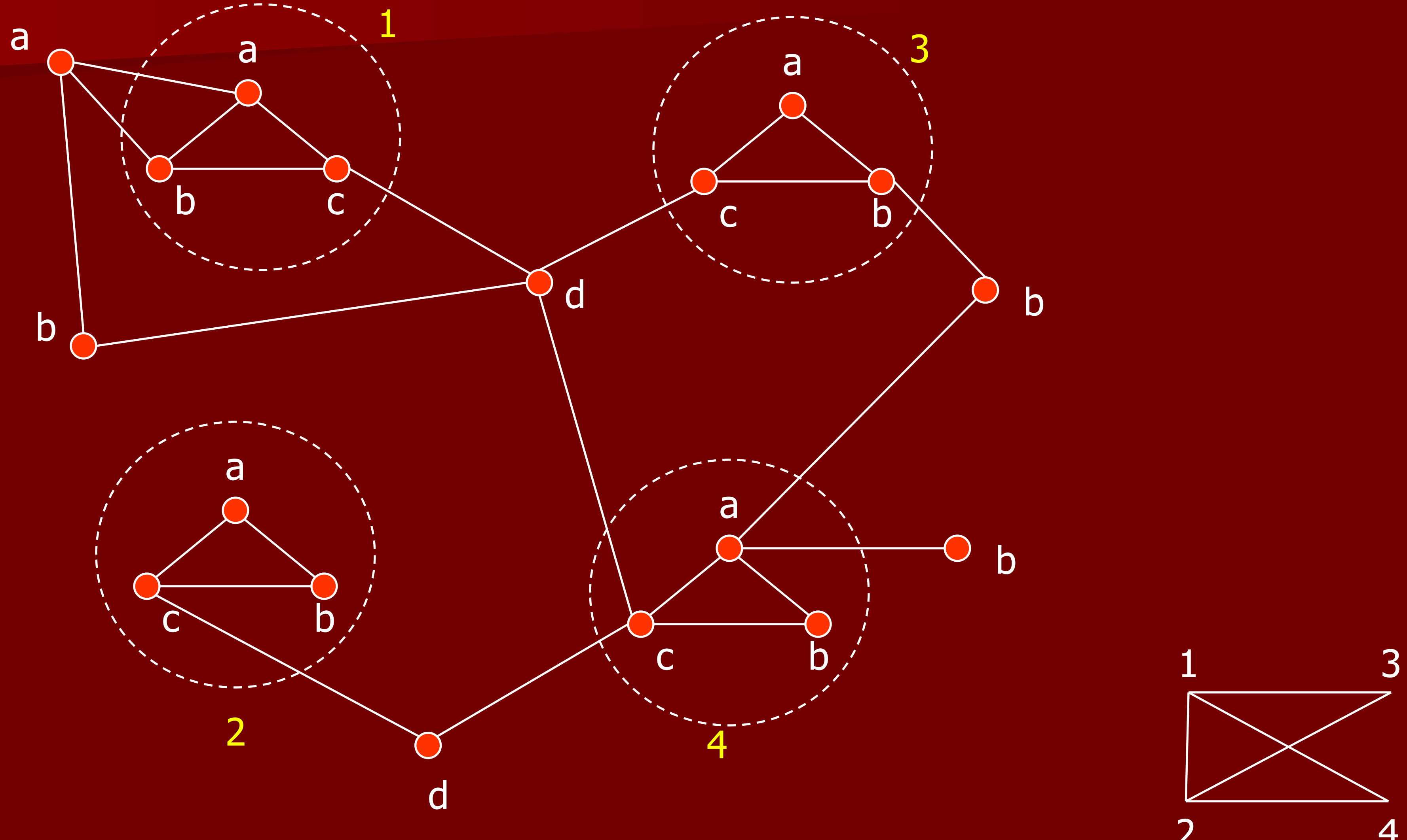
Sets of occurrences

- Take a set of subgraphs G_i (or "occurrences G_i of some subgraph G"), with corresponding I_i and O_i
- E is a possible embedding for all G_i if and only if
  - for all i: $I_i \subseteq E$; in other words, $\cup_i I_i \subseteq E$
  - for all i: $E \subseteq L^2 - O_i$; that is, $E \subseteq L^2 - \cup_i O_i$
- $\Rightarrow$ can define the RIS and ROS of a set of subgraphs (or occurrences of a single subgraph) as follows:
  - $RIS(S) = \cup_{G \in S} RIS(G)$
  - $ROS(S) = \cup_{G \in S} ROS(G)$
- If $RIS(S) \cap ROS(S) \neq \varnothing$, there are incompatible graphs in S

Maximal compatible subset

- Given a set of occurrences $S = \{G_1, \ldots, G_n\}$, find a maximal subset S′ such that S′ is compatible
- Solution:
  - Call two occurrences G_i and G_j *substitution-compatible* iff they *do not overlap nor touch*, and are *compatible*
  - Construct graph with the G_i as nodes and an edge (G_i,G_j) iff G_i and G_j are substitution-compatible
  - Maximal compatible subset = *maximal clique* in this graph
    - Indeed, a set of n occurrences is compatible iff all these occurrences are pairwise compatible
  - Can use existing algorithms for maximal clique finding

Example



Conclusions

- Subdue operator successfully upgraded to learning NLC grammar rules
- Computations seem feasible in practice
  - Computational bottleneck is maximum clique problem, which frequent graph miners already handle with reasonable efficiency

Future work

- Learn recursive rules
  - Currently only non-recursive rules are handled
  - To learn recursive rules, should drop “do not touch” criterion in substitution-compatibility
    - Can it always be dropped safely?
- Extend to ed-NCE grammars
  - Like NLC grammars, but: *directed edges*, *edge labels*, E contains (x,a) where x is *node* in G and a is *label* in neighborhood
  - Shown to be a very powerful (expressive) class of grammars
- Find interesting applications