

# Frequent Generalized Subgraph Mining via Graph Edit Distances

Richard Palme and Pascal Welke

IoT Streams for Predictive Maintenance | SeDaMi

# A Motivating Use Case

Frequent Generalized Subgraph Mining via Graph Edit Distances



# A Motivating Use Case

Frequent Generalized Subgraph Mining via Graph Edit Distances



# A Predictive Maintenance Scenario

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Farmers track their livestock and have to treat them well

# A Predictive Maintenance Scenario

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Farmers track their livestock and have to treat them well
  - before they get sick

# A Predictive Maintenance Scenario

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Farmers track their livestock and have to treat them well
  - before they get sick
  - certainly before they die

# A Predictive Maintenance Scenario

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Farmers track their livestock and have to treat them well
  - before they get sick
  - certainly before they die
  - so that they perform well for a long time

# A Predictive Maintenance Scenario

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Farmers track their livestock and have to treat them well
  - before they get sick
  - certainly before they die
  - so that they perform well for a long time
- Breeders track whole populations of cows and need to decide

# A Predictive Maintenance Scenario

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Farmers track their livestock and have to treat them well
  - before they get sick
  - certainly before they die
  - so that they perform well for a long time
- Breeders track whole populations of cows and need to decide
  - if a breed is a good fit for a changing market or changing climate

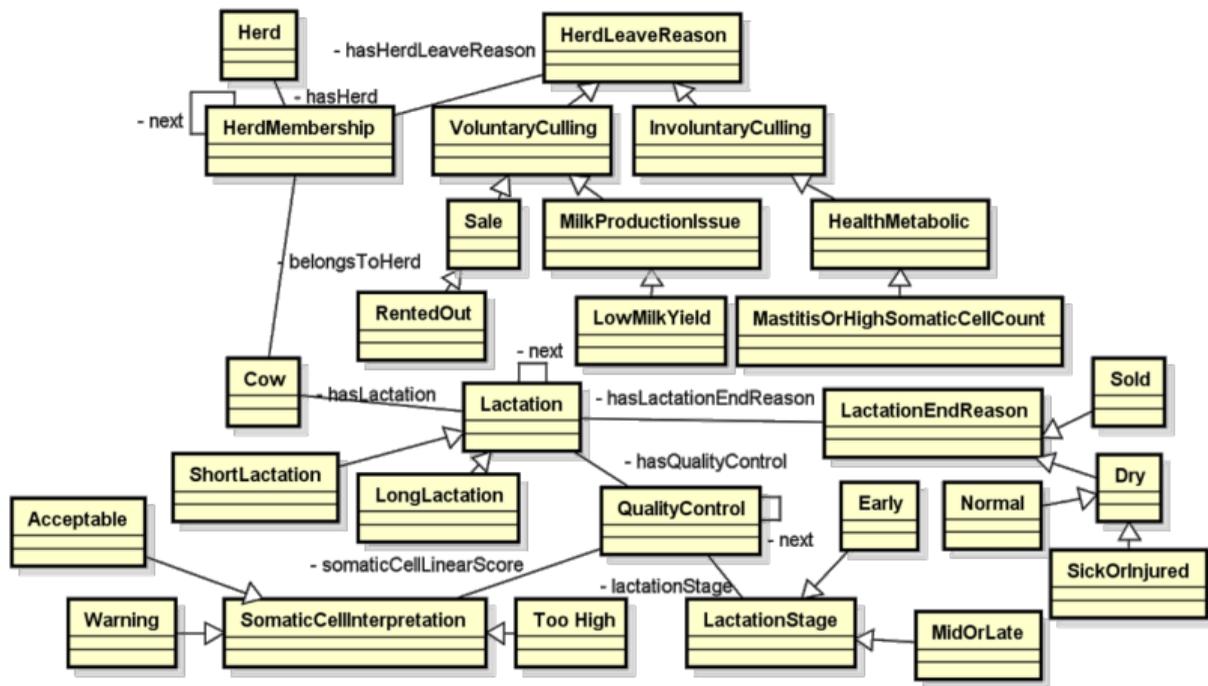
# A Predictive Maintenance Scenario

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Farmers track their livestock and have to treat them well
  - before they get sick
  - certainly before they die
  - so that they perform well for a long time
- Breeders track whole populations of cows and need to decide
  - if a breed is a good fit for a changing market or changing climate
  - which traits to improve by selective breeding

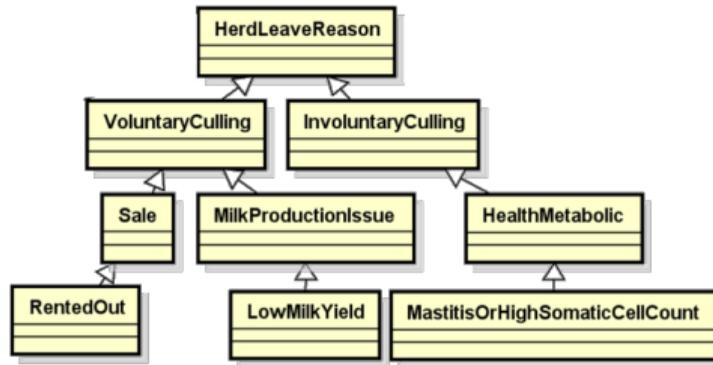
# A Dairy Cattle Performance Ontology

Frequent Generalized Subgraph Mining via Graph Edit Distances



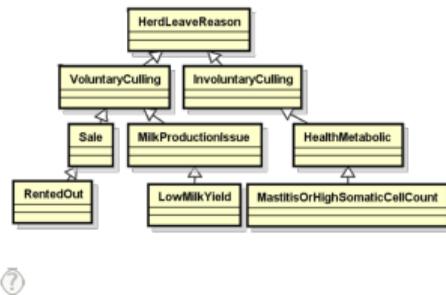
# A Dairy Cattle Performance Ontology

Frequent Generalized Subgraph Mining via Graph Edit Distances



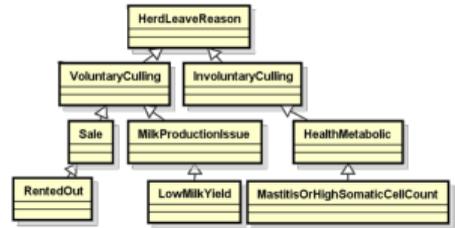
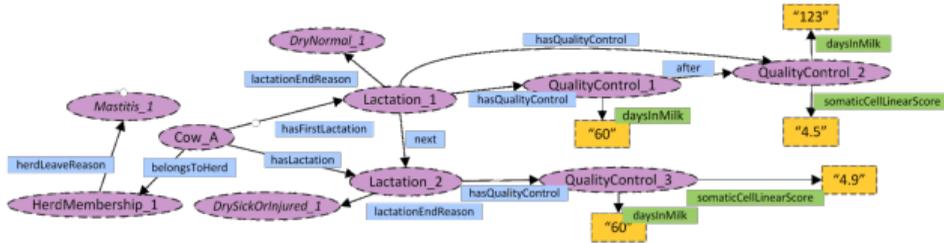
# Dairy Cattle Performance Data

Frequent Generalized Subgraph Mining via Graph Edit Distances



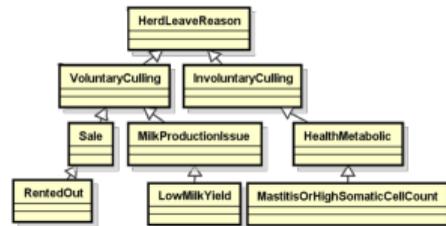
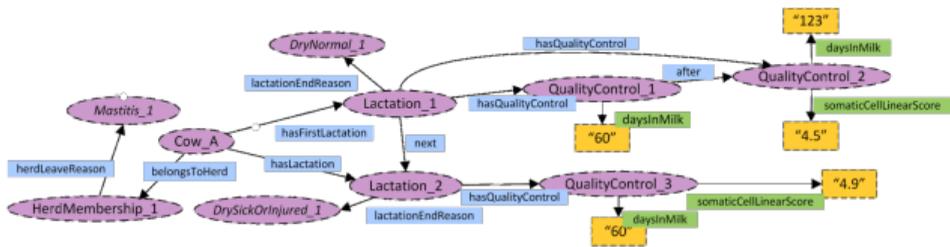
# Dairy Cattle Performance Data

Frequent Generalized Subgraph Mining via Graph Edit Distances



# Dairy Cattle Performance Data

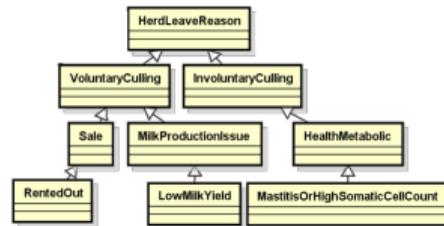
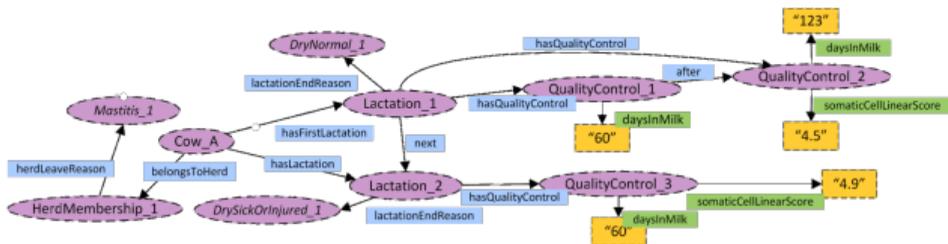
Frequent Generalized Subgraph Mining via Graph Edit Distances



- For each cow, there is a (knowledge) graph recording events

# Dairy Cattle Performance Data

Frequent Generalized Subgraph Mining via Graph Edit Distances



- For each cow, there is a (knowledge) graph recording events
- Are there some reoccurring patterns?

# Generalized Subgraphs

Frequent Generalized Subgraph Mining via Graph Edit Distances

A pattern graph  $H$  is a *generalized sub-graph* (with respect to an ontology  $O$ ) of a graph  $G$  if

# Generalized Subgraphs

Frequent Generalized Subgraph Mining via Graph Edit Distances

A pattern graph  $H$  is a *generalized subgraph* (with respect to an ontology  $O$ ) of a graph  $G$  if

- there is a subgraph isomorphism from  $H'$  to  $G$

# Generalized Subgraphs

Frequent Generalized Subgraph Mining via Graph Edit Distances

A pattern graph  $H$  is a *generalized sub-graph* (with respect to an ontology  $O$ ) of a graph  $G$  if

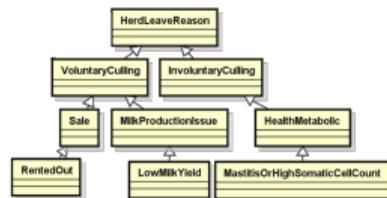
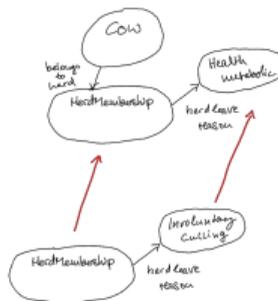
- there is a subgraph isomorphism from  $H'$  to  $G$
- $H'$  can be constructed by replacing vertex labels in  $H$  with *more specific labels* (according to our ontology)

# Generalized Subgraphs

Frequent Generalized Subgraph Mining via Graph Edit Distances

A pattern graph  $H$  is a *generalized subgraph* (with respect to an ontology  $O$ ) of a graph  $G$  if

- there is a subgraph isomorphism from  $H'$  to  $G$
- $H'$  can be constructed by replacing vertex labels in  $H$  with *more specific labels* (according to our ontology)

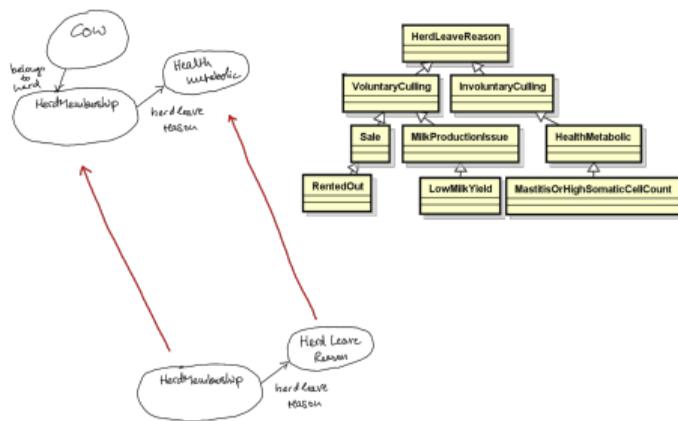


# Generalized Subgraphs

Frequent Generalized Subgraph Mining via Graph Edit Distances

A pattern graph  $H$  is a *generalized subgraph* (with respect to an ontology  $O$ ) of a graph  $G$  if

- there is a subgraph isomorphism from  $H'$  to  $G$
- $H'$  can be constructed by replacing vertex labels in  $H$  with *more specific labels* (according to our ontology)

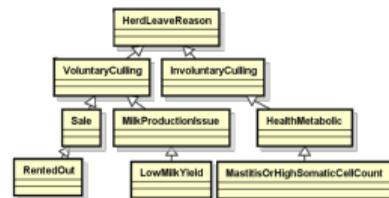
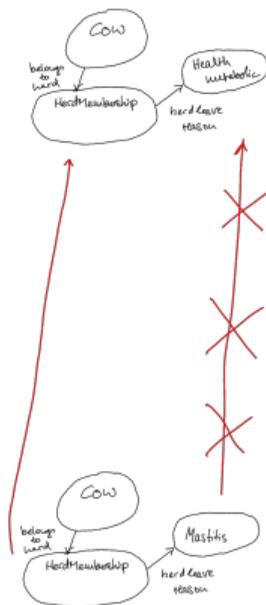


# Generalized Subgraphs

Frequent Generalized Subgraph Mining via Graph Edit Distances

A pattern graph  $H$  is a *generalized subgraph* (with respect to an ontology  $O$ ) of a graph  $G$  if

- there is a subgraph isomorphism from  $H'$  to  $G$
- $H'$  can be constructed by replacing vertex labels in  $H$  with *more specific labels* (according to our ontology)



# Generalized Subgraph Mining

Frequent Generalized Subgraph Mining via Graph Edit Distances

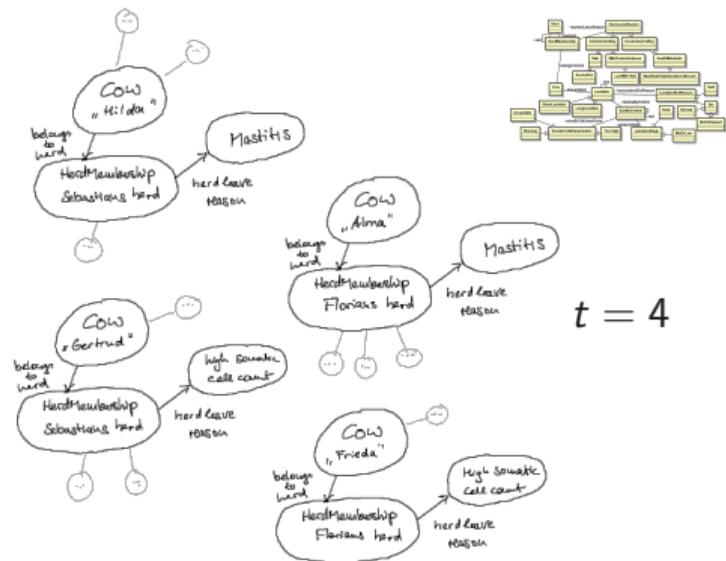
The *Frequent Generalized Subgraph Mining Problem* is then:

# Generalized Subgraph Mining

Frequent Generalized Subgraph Mining via Graph Edit Distances

The *Frequent Generalized Subgraph Mining Problem* is then:

Given: A database  $D$  of graphs, an ontology  $O$  and a frequency threshold  $t$



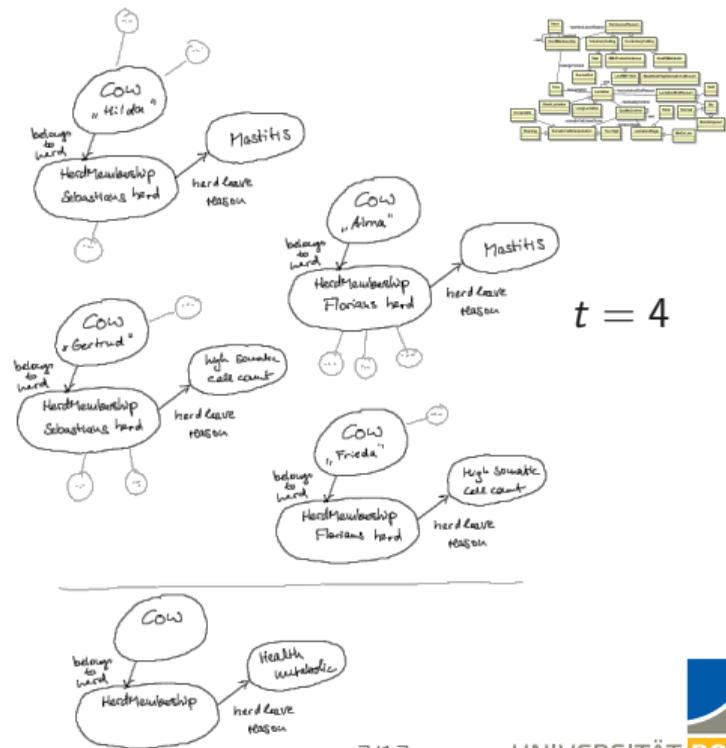
# Generalized Subgraph Mining

Frequent Generalized Subgraph Mining via Graph Edit Distances

The *Frequent Generalized Subgraph Mining Problem* is then:

**Given:** A database  $D$  of graphs, an ontology  $O$  and a frequency threshold  $t$

**Compute:** The set of all graphs that are generalized subgraphs of at least  $t$  graphs in  $D$

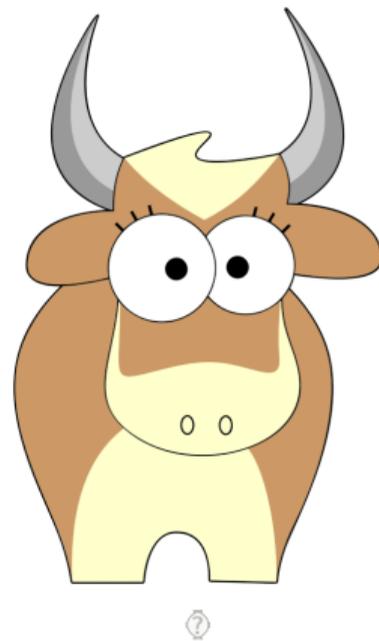


$t = 4$

# How Can This Help with Predictive Maintenance?

Frequent Generalized Subgraph Mining via Graph Edit Distances

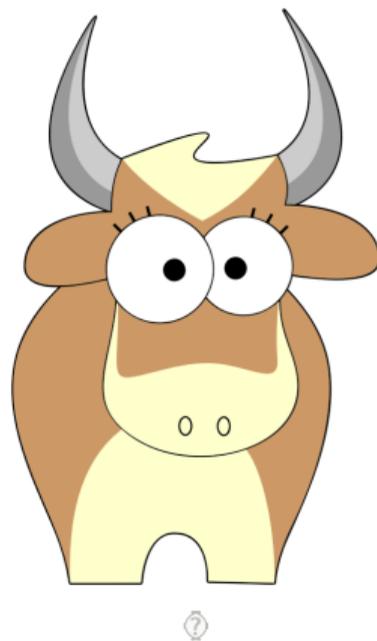
- Not automatically...



# How Can This Help with Predictive Maintenance?

Frequent Generalized Subgraph Mining via Graph Edit Distances

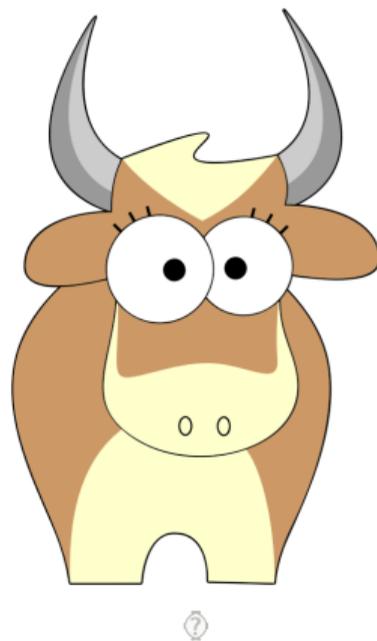
- Not automatically...
- But domain experts can interpret (smaller) frequent patterns



# How Can This Help with Predictive Maintenance?

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Not automatically...
- But domain experts can interpret (smaller) frequent patterns
- And they can interpret changes in frequent patterns



# Existing Approaches

Frequent Generalized Subgraph Mining via Graph Edit Distances

## Frequent Generalized Subgraph Mining has a long history

- ?
- ?

# Existing Approaches

Frequent Generalized Subgraph Mining via Graph Edit Distances

Frequent Generalized Subgraph Mining has a long history

- ?
- ?

And recently gained more traction

- ?
- ?
- ?

# Existing Approaches

Frequent Generalized Subgraph Mining via Graph Edit Distances

Frequent Generalized Subgraph Mining has a long history

- ?
- ?

And recently gained more traction

- ?
- ?
- ?

These papers all modify classical frequent subgraph mining algorithms.

# Existing Approaches

Frequent Generalized Subgraph Mining via Graph Edit Distances

Frequent Generalized Subgraph Mining has a long history

- ?
- ?

And recently gained more traction

- ?
- ?
- ?

These papers all modify classical frequent subgraph mining algorithms.

As a subroutine, they use subgraph isomorphism algorithms.

# Our Approach

# Proposal

Frequent Generalized Subgraph Mining via Graph Edit Distances

We propose to replace subgraph isomorphism computations by *graph edit distance* computations

# Proposal

Frequent Generalized Subgraph Mining via Graph Edit Distances

We propose to replace subgraph isomorphism computations by *graph edit distance* computations

- This makes the problem *harder*

# Proposal

Frequent Generalized Subgraph Mining via Graph Edit Distances

We propose to replace subgraph isomorphism computations by *graph edit distance* computations

- This makes the problem *harder*
- But it allows some nice *freedom and simplicity* in modeling

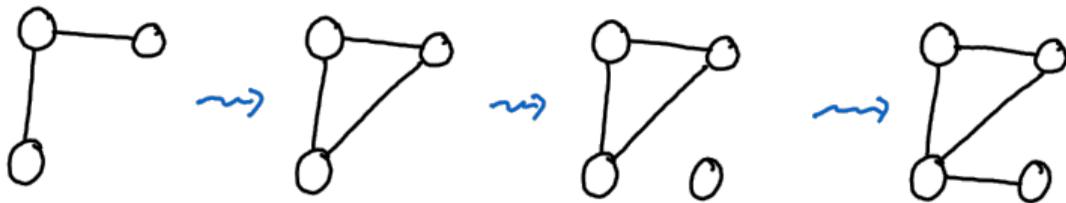
We propose to replace subgraph isomorphism computations by *graph edit distance* computations

- This makes the problem *harder*
- But it allows some nice *freedom and simplicity* in modeling
- And it *simplifies* rather intricate mining algorithms

# Graph Edit Distance

Frequent Generalized Subgraph Mining via Graph Edit Distances

The *graph edit distance* between  $G$  and  $H$  is the smallest cost of a sequence of edits transforming  $G$  into  $H$ .

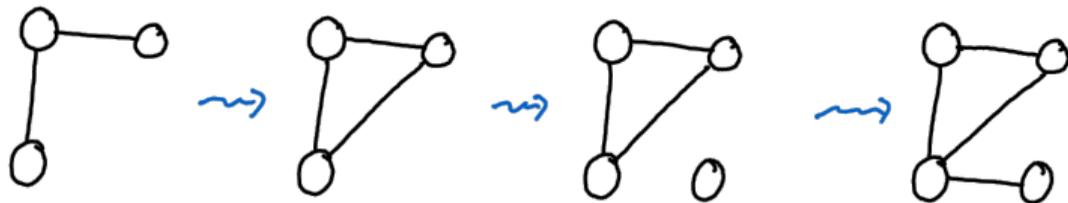


# Graph Edit Distance

Frequent Generalized Subgraph Mining via Graph Edit Distances

Edit operation	Edit cost
Insert an isolated vertex with label $\alpha \in \Sigma$	$c(\varepsilon, \alpha)$
Delete an isolated vertex $u$	$c(\lambda(u), \varepsilon)$
Substitute the label of a vertex $u$ by $\alpha \in \Sigma$	$c(\lambda(u), \alpha)$
Insert an edge with label $\alpha \in \Sigma$	$c(\varepsilon, \alpha)$
Delete an edge $e$	$c(\lambda(e), \varepsilon)$
Substitute the label of an edge $e$ by $\alpha \in \Sigma$	$c(\lambda(e), \alpha)$

The *graph edit distance* between  $G$  and  $H$  is the smallest cost of a sequence of edits transforming  $G$  into  $H$ .



# A Nice Polynomial Time Reduction

Frequent Generalized Subgraph Mining via Graph Edit Distances

The GED can be used to solve the *subgraph isomorphism problem (SGI)* by imposing the following three constraints on the edit cost function:

# A Nice Polynomial Time Reduction

Frequent Generalized Subgraph Mining via Graph Edit Distances

The GED can be used to solve the *subgraph isomorphism problem (SGI)* by imposing the following three constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0 \quad (\text{free insertions})$$

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0 \quad (\text{paid deletions})$$

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \quad (\text{paid substitutions})$$

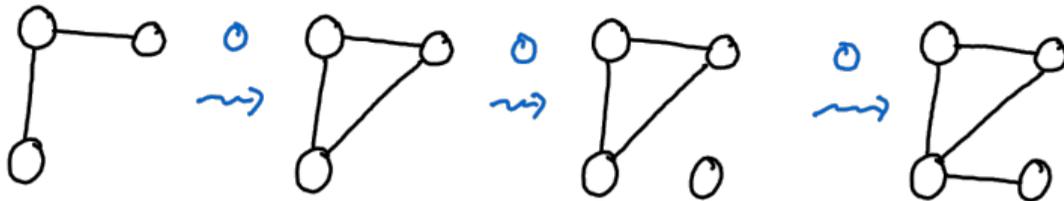
# A Nice Polynomial Time Reduction

The GED can be used to solve the *subgraph isomorphism problem (SGI)* by imposing the following three constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0 \quad (\text{free insertions})$$

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0 \quad (\text{paid deletions})$$

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \quad (\text{paid substitutions})$$



# A Nice Polynomial Time Reduction

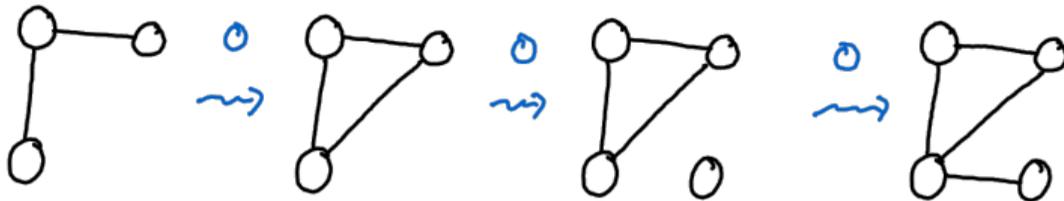
The GED can be used to solve the *subgraph isomorphism problem (SGI)* by imposing the following three constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0 \quad (\text{free insertions})$$

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0 \quad (\text{paid deletions})$$

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \quad (\text{paid substitutions})$$

$$\text{SGI}(H, G) = \text{true} \iff \text{GED}(H, G) = 0.$$



# A Nice Polynomial Time Reduction

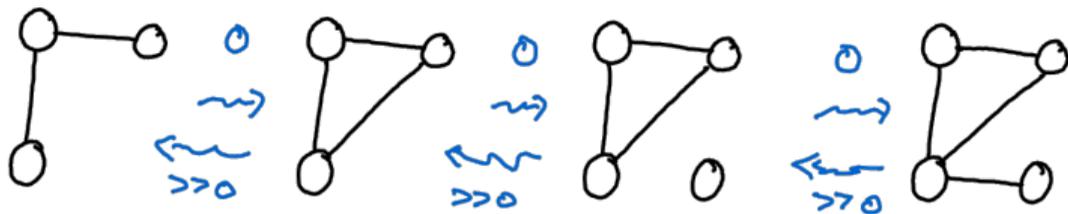
The GED can be used to solve the *subgraph isomorphism problem (SGI)* by imposing the following three constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0 \quad (\text{free insertions})$$

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0 \quad (\text{paid deletions})$$

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \quad (\text{paid substitutions})$$

$$\text{SGI}(H, G) = \text{true} \iff \text{GED}(H, G) = 0.$$



# Another Nice Polynomial Reduction

Frequent Generalized Subgraph Mining via Graph Edit Distances

To solve the *generalized subgraph isomorphism problem (GSGI)*, we impose the following four constraints on the edit cost function:

# Another Nice Polynomial Reduction

Frequent Generalized Subgraph Mining via Graph Edit Distances

To solve the *generalized subgraph isomorphism problem (GSGI)*, we impose the following four constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0$$

(free insertions)

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0$$

(paid deletions)

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \text{ and } \alpha \text{ is not more general than } \beta$$

(paid substitutions)

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) = 0 \iff \alpha = \beta \text{ or } \alpha \text{ is more general than } \beta$$

(free specializations)

# Another Nice Polynomial Reduction

Frequent Generalized Subgraph Mining via Graph Edit Distances

To solve the *generalized subgraph isomorphism problem (GSGI)*, we impose the following four constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0$$

(free insertions)

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0$$

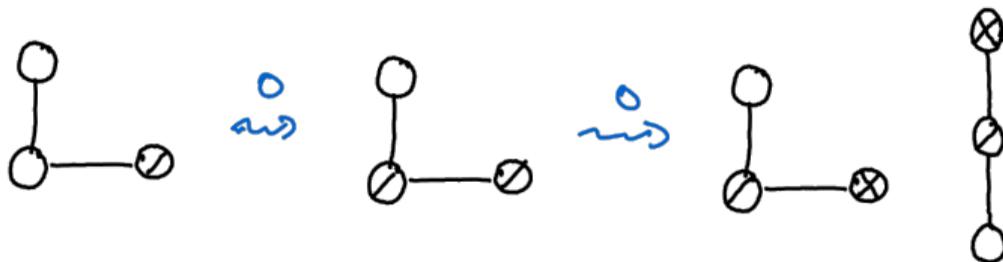
(paid deletions)

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \text{ and } \alpha \text{ is not more general than } \beta$$

(paid substitutions)

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) = 0 \iff \alpha = \beta \text{ or } \alpha \text{ is more general than } \beta$$

(free specializations)



# Another Nice Polynomial Reduction

Frequent Generalized Subgraph Mining via Graph Edit Distances

To solve the *generalized subgraph isomorphism problem (GSGI)*, we impose the following four constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0$$

(free insertions)

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0$$

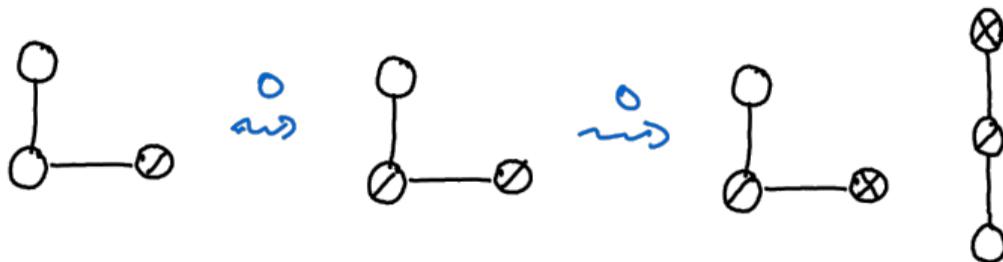
(paid deletions)

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \text{ and } \alpha \text{ is not more general than } \beta$$

(paid substitutions)

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) = 0 \iff \alpha = \beta \text{ or } \alpha \text{ is more general than } \beta$$

(free specializations)



# Another Nice Polynomial Reduction

Frequent Generalized Subgraph Mining via Graph Edit Distances

To solve the *generalized subgraph isomorphism problem (GSGI)*, we impose the following four constraints on the edit cost function:

$$\forall \beta \in \Sigma_\varepsilon: c(\varepsilon, \beta) = 0$$

(free insertions)

$$\forall \alpha \in \Sigma: c(\alpha, \varepsilon) > 0$$

(paid deletions)

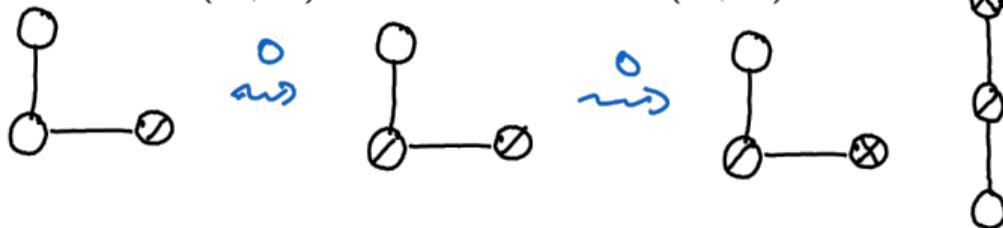
$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) > 0 \iff \alpha \neq \beta \text{ and } \alpha \text{ is not more general than } \beta$$

(paid substitutions)

$$\forall \alpha, \beta \in \Sigma: c(\alpha, \beta) = 0 \iff \alpha = \beta \text{ or } \alpha \text{ is more general than } \beta$$

(free specializations)

$$\text{GSGI}(H, G) = \text{true} \iff \text{GED}(H, G) = 0.$$





# Frequent Generalized Subgraph Mining

Frequent Generalized Subgraph Mining via Graph Edit Distances

- There are fast heuristics 

# Frequent Generalized Subgraph Mining

Frequent Generalized Subgraph Mining via Graph Edit Distances

- There are fast heuristics 
- There was some nice work on lower bounds at ECMLPKDD this year which might be adapted 

# Frequent Generalized Subgraph Mining

Frequent Generalized Subgraph Mining via Graph Edit Distances

- There are fast heuristics 
- There was some nice work on lower bounds at ECMLPKDD this year which might be adapted 
- We say that a graph is a generalized subgraph if it has a small generalized subgraph edit distance

# Implementation

Frequent Generalized Subgraph Mining via Graph Edit Distances

- We implemented a proof of concept graph mining algorithm

# Implementation

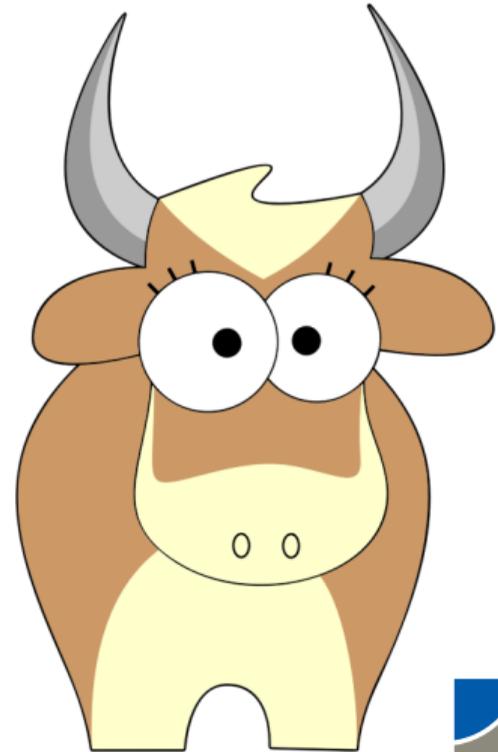
Frequent Generalized Subgraph Mining via Graph Edit Distances

- We implemented a proof of concept graph mining algorithm
- It is available on <https://github.com/RichardPalme/fasm>

# Conclusion

Frequent Generalized Subgraph Mining via Graph Edit Distances

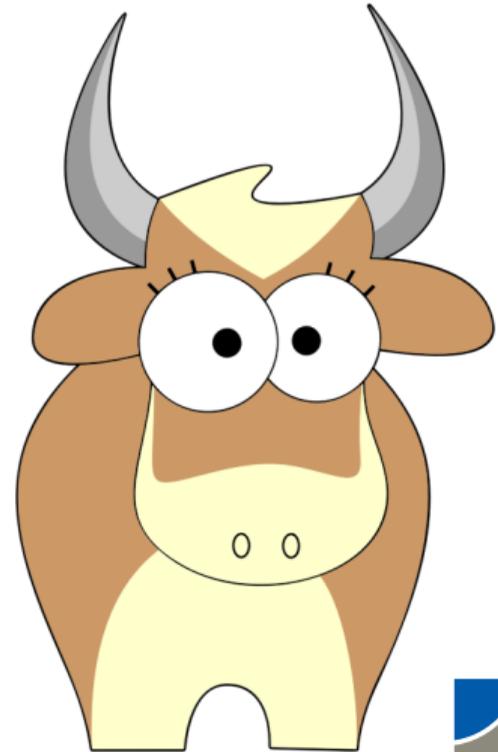
- Generalized Subgraphs can be identified with a specialized variant of the graph edit distance



# Conclusion

Frequent Generalized Subgraph Mining via Graph Edit Distances

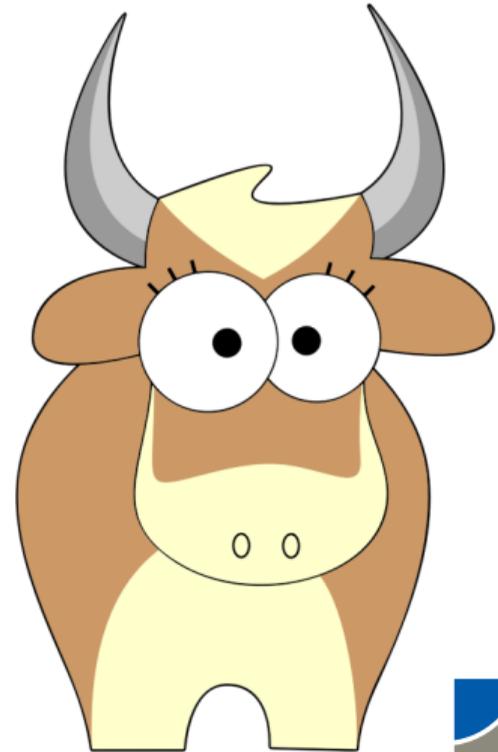
- Generalized Subgraphs can be identified with a specialized variant of the graph edit distance
- This allows to mine generalized patterns in an elegant way



# Conclusion

Frequent Generalized Subgraph Mining via Graph Edit Distances

- Generalized Subgraphs can be identified with a specialized variant of the graph edit distance
- This allows to mine generalized patterns in an elegant way
- We can include interesting costs (checkout the paper) to make the mining practically better



# References I

Frequent Generalized Subgraph Mining via Graph Edit Distances