Pascal Welke

DSAA 2020



Example: Co-authorship Networks



Example: Chemical Molecules

Efficient Frequent Subgraph Mining in Transactional Databases



Saccharose



(commons.wikimedia.org)



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- Similarity based learning methods
 - "close by objects behave similarly"





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 - "close by objects behave similarly"
 - $\,\rightarrow$ What does "close by" mean if objects are graphs?





Efficient Frequent Subgraph Mining in Transactional Databases

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 - \rightarrow What does "close by" mean if objects are graphs?



Identification of relevant patterns





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 - "close by objects behave similarly"
 - $\,\rightarrow\,$ What does "close by" mean if objects are graphs?



- Identification of relevant patterns
 - What is a pattern?
 - What is relevant?





Efficient Frequent Subgraph Mining in Transactional Databases

 Let's say we have a few graphs (in a graph database D)





Efficient Frequent Subgraph Mining in Transactional Databases

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- *Frequent subgraphs* are a reasonable choice to define similarities in a domain of graphs

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Frequent Connected Subgraph Mining (FCSM) Given a dataset of graphs $\mathcal{D} \subset \mathcal{G}$ and an

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Frequent Connected Subgraph Mining (FCSM)

Given a dataset of graphs $\mathcal{D} \subseteq \mathcal{G}$ and an integer threshold $t \leq |\mathcal{D}|$ List all connected graphs $P \in \mathcal{P}$ that are subgraph isomorphic to at least t graphs in \mathcal{D} .





Subgraph Isomorphism

Efficient Frequent Subgraph Mining in Transactional Databases

Definition

A subgraph isomorphism is an injective mapping

 $\varphi:V(G_1) \rightarrow V(G_2)$

such that

 $(v_1, v_2) \in E(G_1) \Rightarrow (\varphi(v_1), \varphi(v_2)) \in E(G_2)$





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Deciding whether one exists, is *NP-hard*.





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Efficient Frequent Subgraph Mining in Transactional Databases

Frequent Subtree Mining

		FreeTreeMiner (Rückert and Kramer, 2004)		
FreeTre	eeMiner	HybridTreeMiner	F3TM	
(Chi et al.	, 2003)	(Chi et al, 2004)	(Zhao and Yu, 2008)	





Efficient Frequent Subgraph Mining in Transactional Databases

Frequent Subtree Mining

	FreeTreeMiner (Nicken and Krame, 2000)	
FreeTreeMiner	HybridTreeMiner (Di = 4, 200)	F3TM (ibse and Vo. 1000)



Efficient Frequent Subgraph Mining in Transactional Databases

Frequent Subtree Mining											
		FreeTreeMiner (Nicken and Youme, 2008)									
	FreeTreeMiner (On a st. 2000)	HybridTreeMiner (Di # 4), 2014) (Dist	M and Ye, 2000								2
Frequent Subgraph Mining											!
gSpan (Vas and Has, 2007)											
FSG (Visramushi and Kanjoli, 2001) (Bargels and Berchald, 20	FFSM (Haan et al, 2008)	Ganton (Nijaan and Kab, 2006)		- (Harvá	h and Flamon, 2010)]					
2001 2002	2003	2004	2008		2010	2011	2012	2013	2014	2018	2020

• All these methods enumerate the full set of frequent subtrees/subgraphs



Frequent Subtree Mining												
		FreeTreeMiner (Nielan and Krame, 2010)]									
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Frequent Subgraph Mining												!
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FSG (Fiscamuchi and Karypis, 2001) [Bargelt and Berchuld, 2007]	FFSM (Heas et al. 2008)	Gaston (Nijaan and Kak, 2004)]	(Pherei	th and Ramon, 2018)							
2001 2002	2003	2004	2008		2010	2011	2012	2013	:	2014	2018	2020

- All these methods enumerate the full set of frequent subtrees/subgraphs
- ...so why are we here, ten years later and discussing about this?



Efficient Frequent Subgraph Mining in Transactional Databases

• An acquaintance of yours has 200 graphs



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 - 10-30 vertices each



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Structure of this Talk

Efficient Frequent Subgraph Mining in Transactional Databases

1. Computational complexity of frequent subgraph/subtree mining

- what notions of efficiency are useful?
- is there any hope?



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- 2. Exact algorithms and their problems
 - a quick and general look at counting subgraph support



Structure of this Talk

- 1. Computational complexity of frequent subgraph/subtree mining
 - what notions of efficiency are useful?
 - is there any hope?
- 2. Exact algorithms and their problems
 - a quick and general look at counting subgraph support
- 3. Some more current *inexact* solutions
 - efficient for arbitrary graph databases
 - though *incomplete*, comparable predictive performance to exact frequent subgraphs



Part 1.

Computational Complexity of Frequent Subgraph Mining



Efficient Frequent Subgraph Mining in Transactional Databases

Frequent Connected Subgraph Mining (FCSM) Given a dataset of graphs $\mathcal{D} \subseteq \mathcal{G}$ and an integer threshold $t \leq |\mathcal{D}|$





Efficient Frequent Subgraph Mining in Transactional Databases

 $\begin{array}{l} \textit{Frequent Connected Subgraph Mining (FCSM)} \\ \textit{Given a dataset of graphs } \mathcal{D} \subseteq \mathcal{G} \textit{ and an} \\ \textit{integer threshold } t \leq |\mathcal{D}| \\ \textit{List all connected graphs } P \in \mathcal{P} \textit{ that} \\ \textit{are subgraph isomorphic to at} \\ \textit{least } t \textit{ graphs in } \mathcal{D}. \end{array}$





Efficient Frequent Subgraph Mining in Transactional Databases

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Subgraph Isomorphism is NP-hard.



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 \mathcal{D}

Subgraph Isomorphism is *NP-hard*. (There is a bit more to it (Horváth et al (2007)))

2-frequent subgraphs of \mathcal{D} 0 8 8 4 0 UNIVERSITÄT BONN

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 - we need a bound in the output size



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- Polynomial delay
 - the time between finding two patterns is polynomial in the input size
- Incremental polynomial time
 - something in between



Efficient Frequent Subgraph Mining in Transactional Databases

- Software exists, e.g.
 - FSG (Kuramochi and Karypis (2001))
 - gSpan (Yan and Han (2002))
 - Gaston (Nijssen and Kok (2005)) ...



1

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 - previous work deals with this using some properties of very simple graphs

50 ER random graphs, about 50 vertices each, t = 5



Welke (2019)

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 \Rightarrow There is no system that can reliably mine all frequent subgraphs for arbitrary graph databases of small to medium sized graphs

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Part 2.

Exact Frequent Subgraph Mining Algorithms (& Problems)



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The Timeline, again...

Efficient Frequent Subgraph Mining in Transactional Databases

Frequent Subtree Mining

2

	FreeTreeMiner (Rückert and Kramer, 2004)		
FreeTreeMiner (Chi et al. 2003)	HybridTreeMiner (Chi et al. 2004)	F3TM (Zhao and Yu, 2008)	





The Timeline, again.

Frequent Subtree Mining

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The Timeline, again.

Frequent Subtree Mining

	FreeTreeMiner (Rückert and Kramer, 2004)
only for forest transactions	only for forest transactions
FreeTreeMiner	HybridTreeMiner F3TM
(Chi et al, 2003)	(Chi et al, 2004) (Zhao and Yu, 2008)



Part 3. Efficient Inexact Mining Methods





Possible Ways Out

1. Make the database simpler or smaller (Chen et al (2009))





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- 1. Make the database simpler or smaller (Chen et al (2009)) (Welke et al (20
- 2. Change the embedding operator (Li and Wang (2015)) (Schulz et al (2018))





Possible Ways Out

Efficient Frequent Subgraph Mining in Transactional Databases

- 1. Make the database simpler or smaller (2009) Welke e
- 2. Change the embedding operator (Li and Wang (2015)) (Schulz et al (2018))
- 3. Restrict the pattern language and allow one-sided error (Schulz et al (2018))

Welke et al (2019))

(Welke et al (2020))



<u>A More Recent Timeline</u>

Frequent Subtree Mining

3





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 - not possible in output polynomial time



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- Can we combine exact and approximate tools to achieve "one-size-fits-all" mining?
- Can we devise efficient methods for non-tree patterns?



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Efficient Frequent Subgraph Mining in Transactional Databases

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