Efficient Frequent Subtree Mining Beyond Forests

Pascal Welke

Promotionskolloquium

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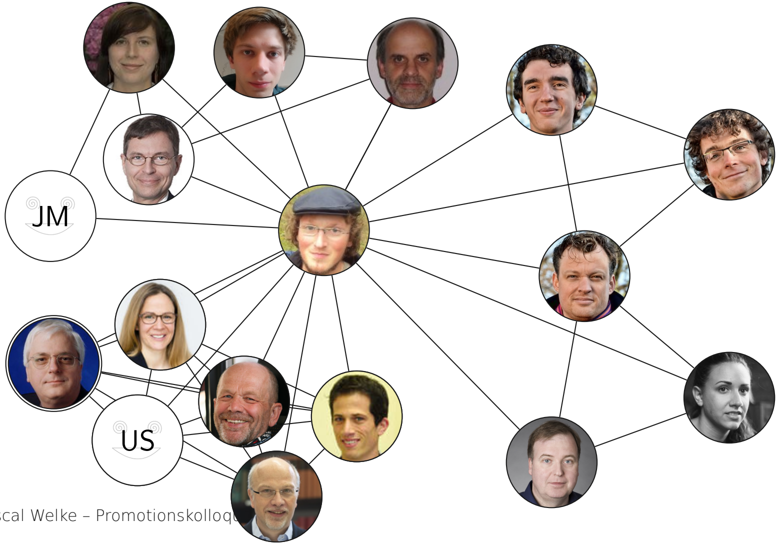
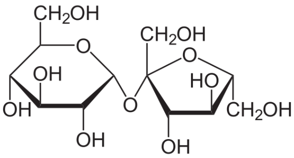
Example: Co-authorship Networks



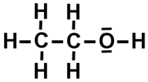
A *graph* $G = (V, E)$ consists of a set of vertices V and a set of edges E connecting pairs of vertices.

(Pictures taken from the home pages of the authors)

Example: Chemical Molecules



Saccharose



Ethanol

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How to Learn From Graphs?

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

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- Similarity based learning methods
  - "close by objects behave similarly"
- Hence: What does "close by" mean if objects are graphs?

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Frequent Subgraph Mining

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Frequent Connected Subgraph Mining (FCSM)

Given a dataset of graphs $\mathcal{D} \subseteq \mathcal{G}$ and an integer threshold $t \leq |\mathcal{D}|$

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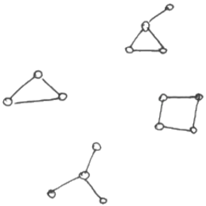

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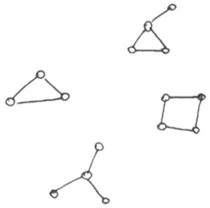


Frequent Connected Subgraph Mining (FCSM)

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 $\mathcal{D}$.

2-frequent subgraphs of $\mathcal{D}$

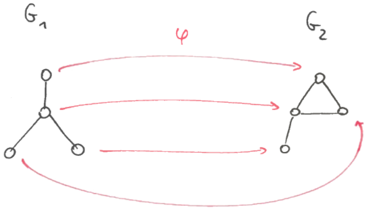
Definition

A *subgraph isomorphism* is an injective mapping

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

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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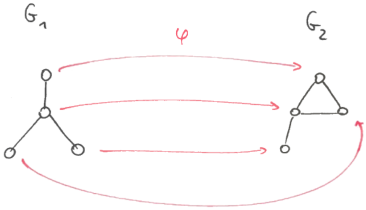

Deciding whether one exists, is *NP-hard*.

FCSM based Similarity Functions

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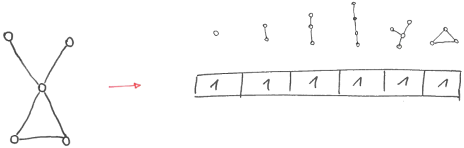
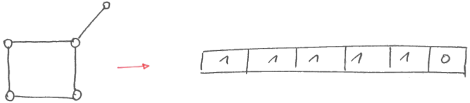
G_1



G_2



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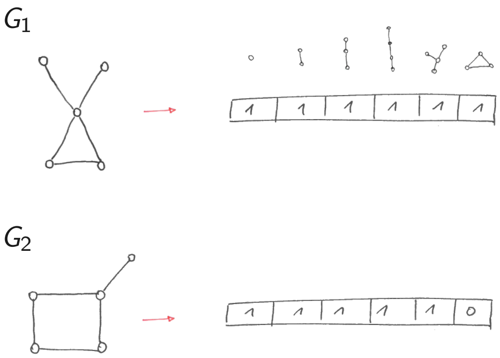

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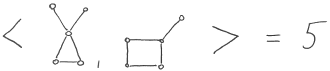

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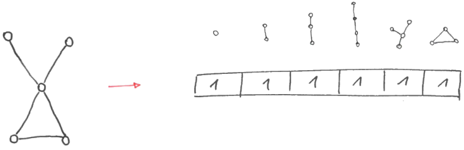

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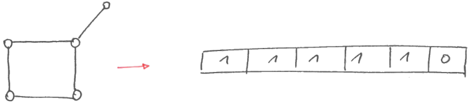

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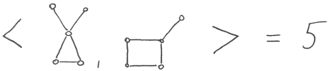

- This allows to apply e.g. all kernel methods to graph databases, like SVMs (Cortes and Vapnik, 1995) etc.

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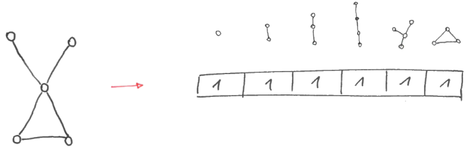

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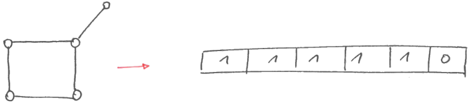

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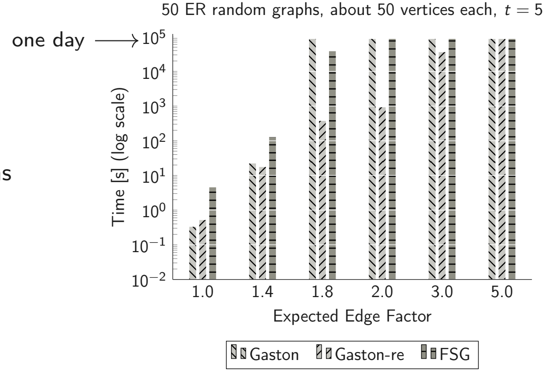

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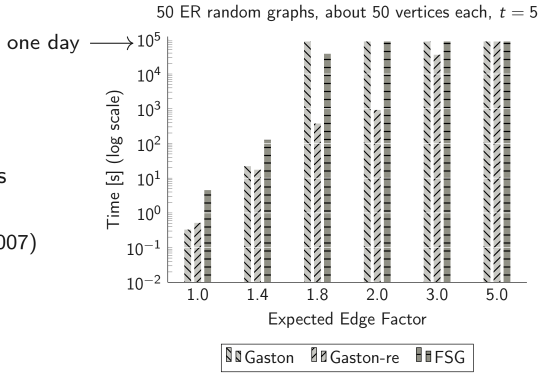

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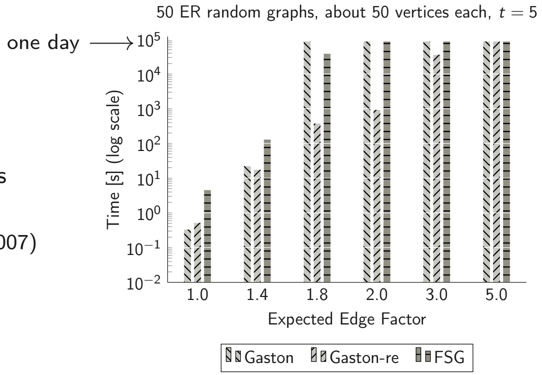

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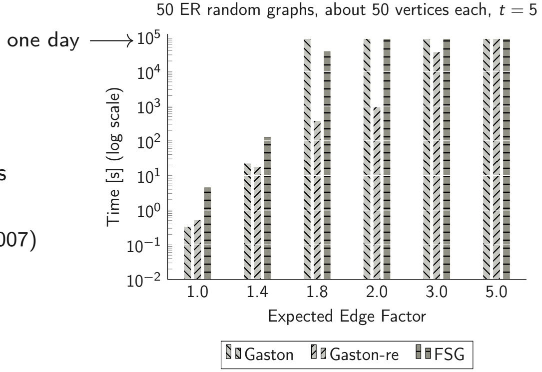

⇒ *There is no system that can reliably mine frequent subgraphs for arbitrary graph databases of small to medium sized graphs*

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3. Fast computation of frequent subgraph based similarity functions
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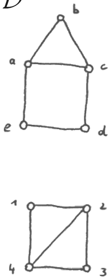
$\Rightarrow$ Resulting in the first *theoretically efficient* and *practically robust* system for frequent subtree mining in arbitrary graph databases

Related Publications

- Pascal Welke, Tamás Horváth, Stefan Wrobel (2019) Probabilistic and exact frequent subtree mining in graphs beyond forests. *Machine Learning Journal*
  - Pascal Welke, Tamás Horváth, Stefan Wrobel (2015) On the complexity of frequent subtree mining in very simple structures. Inductive Logic Programming (ILP), *Springer LNCS*
- Pascal Welke, Tamás Horváth, Stefan Wrobel (2018) Probabilistic frequent subtrees for efficient graph classification and retrieval. *Machine Learning Journal*
  - Pascal Welke, Tamás Horváth, Stefan Wrobel (2016a) Probabilistic frequent subtree kernels. New Frontiers in Mining Complex Patterns (NFMCP), *Springer LNCS*
  - Pascal Welke, Tamás Horváth, Stefan Wrobel (2016b) Min-hashing for probabilistic frequent subtree feature spaces. Discovery Science (DS), *Springer LNCS*
- Pascal Welke (2017) Simple necessary conditions for the existence of a Hamiltonian path with applications to cactus graphs. *CoRR*

Part 1.
Probabilistic Frequent Subtrees

$\mathcal{D}$



Probabilistic Frequent Subtree Mining

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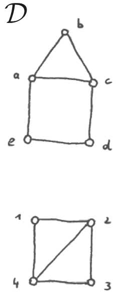

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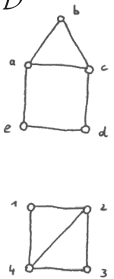

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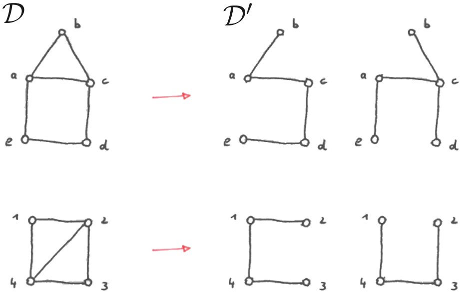

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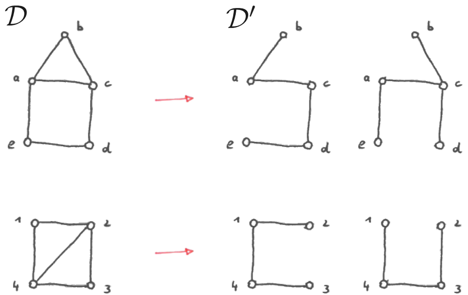
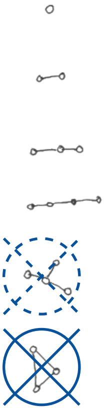
  - $\Rightarrow$ some frequent subtrees might not be found





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Probabilistic Frequent Subtrees can be mined with polynomial delay.

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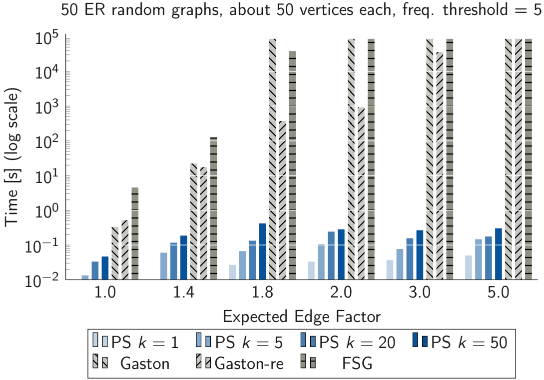
Theorem

Probabilistic Frequent Subtrees can be mined with polynomial delay.

- Does it work in practice?
  - ...in feasible time?
  - ...as basis for similarity based learning?

Runtime of Probabilistic Subtrees (PS)

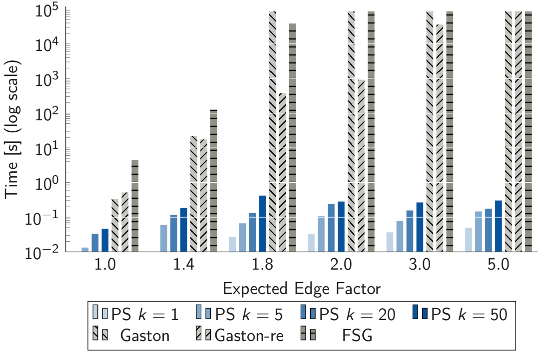


k is the number of sampled spanning trees per graph

Experimental Results

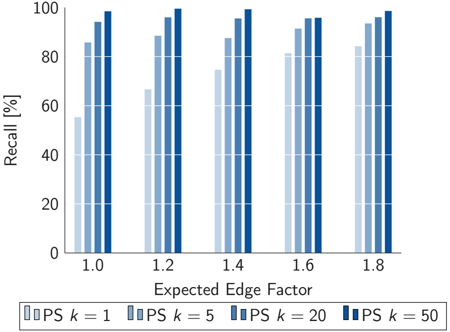
Runtime of Probabilistic Subtrees (PS)

50 ER random graphs, about 50 vertices each, freq. threshold = 5



Recall of PS

same dataset as on left



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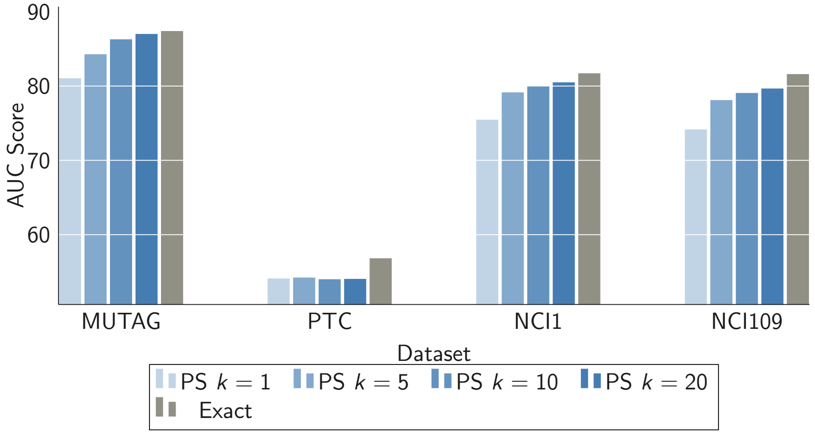
Classification Quality of Probabilistic Subtree (PS) based Learners



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  - our method can efficiently consider only a sample of polynomial size
  - $\Rightarrow$ there is an exponential gap, which might reduce recall

Part 2.
Boosted Probabilistic Frequent Subtrees

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- Improve the probabilistic subgraph isomorphism algorithm

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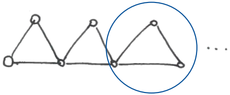

Biconnected Component

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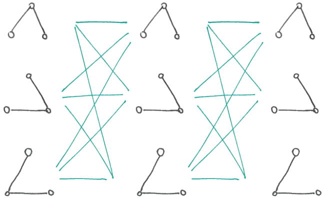

27 spanning trees

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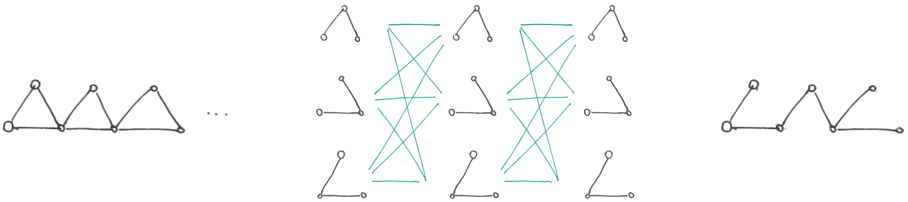

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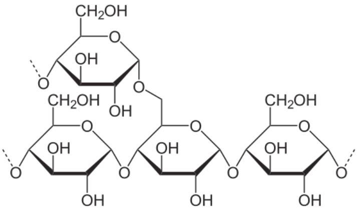

Amylopectin

`commons.wikimedia.org`

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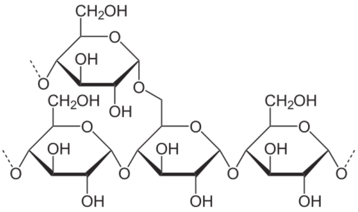

Amylopectin

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...you already see enough graph for $6^4 = 936$ spanning trees

Theorem

Near optimal for trees G

Subtree Isomorphism from a tree H into an arbitrary graph G can be solved in time

$$O\left(f_{\max}^2(G) \cdot |E(G)| \cdot |V(H)|^{1.5}\right)$$

where $f_{\max}(G)$ is the maximum number of spanning trees in any graph induced by the union of biconnected components containing some vertex $v \in V(G)$.

Boosted Subtree Isomorphism

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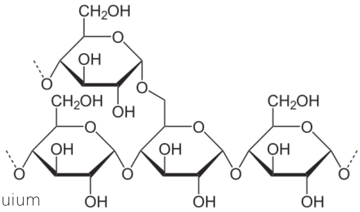

Theorem

Near optimal for trees G

Subtree Isomorphism from a tree H into an arbitrary graph G can be solved in time

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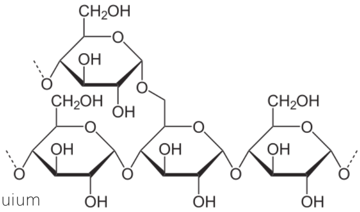

$f_{\max}(G) = 6$

Theorem (Informally)

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This allows to efficiently mine boosted probabilistic frequent subtrees in arbitrary graph databases.

An Algorithm

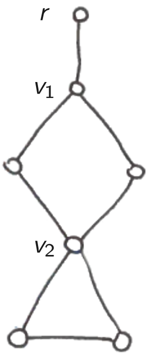
Input : tree H with $|V(H)| > 1$ and an arbitrary connected graph G with $|V(G)| \geq |V(H)|$
Output: True if $H \preccurlyeq G$; o/w False

Main:

set $\mathcal{C} := \emptyset$
pick a vertex $r \in V(G)$ and compute the complete guidance tree $\mathbb{T} = (\mathcal{T}, \mathcal{S})$ of G for the tree skeleton $\mathcal{T}$ rooted at r
for all $v \in V(\mathcal{T})$ in a postorder **do**
  // $\mathcal{S}_v \in \mathcal{S}$ is the bag of v in $\mathbb{T}$
  for all $\tau \in \mathcal{S}_v$ **do**
    for all $w \in V(\tau)$ in a postorder **do**
      $\mathcal{C} := \mathcal{C} \cup$ Characteristics(v, u, τ, w)
      if $(H_u^u, \tau, w) \in \mathcal{C}$ **then return** True
return False

Characteristics(v, u, τ, w):
  $\mathcal{C}_\tau := \emptyset$
  for all $\theta \in \Theta_{vw}(\tau)$ **do**
    for all $u \in V(H)$ **do**
      let τ' be the tree satisfying $\theta = \tau \cup \tau'$
      let C_τ (resp. $C_{\tau'}$) be the set of children of w in τ (resp. τ') and $C_\theta := C_\tau \cup C_{\tau'}$
      let $B = (C_\theta \dot\cup \mathcal{N}(u), E)$ be the bipartite graph with
        $cu' \in E$ if and only if
        $(c \in C_\tau \wedge (H_{u'}^u, \tau, c) \in \mathcal{C}) \vee (c \in C_{\tau'} \wedge (H_{u'}^u, \tau', c) \in \mathcal{C})$
        for all $cu' \in C_\theta \times \mathcal{N}(u)$
      if B has a matching that covers $\mathcal{N}(u)$ **then**
        add (H_u^u, τ, w) to $\mathcal{C}_\tau$
      for all $y \in \mathcal{N}(u)$ **do**
        if B has a matching covering $\mathcal{N}(u) \setminus \{y\}$ **then**
          add (H_u^y, τ, w) to $\mathcal{C}_\tau$
  return $\mathcal{C}_\tau$

Tree H



Graph G

Guidance Trees and Bags of Spanning Trees

Tree H

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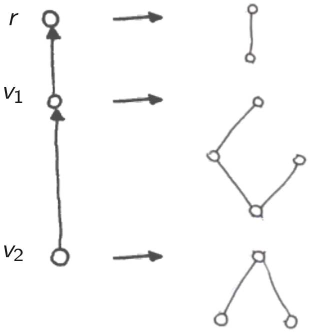

Guidance Tree $\mathbb{T}(G)$

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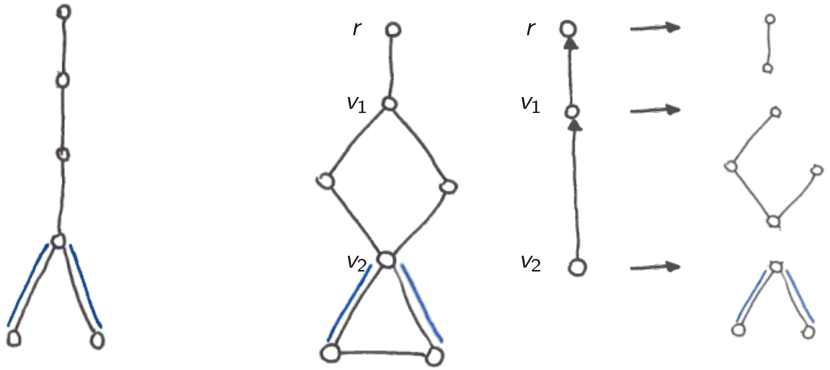

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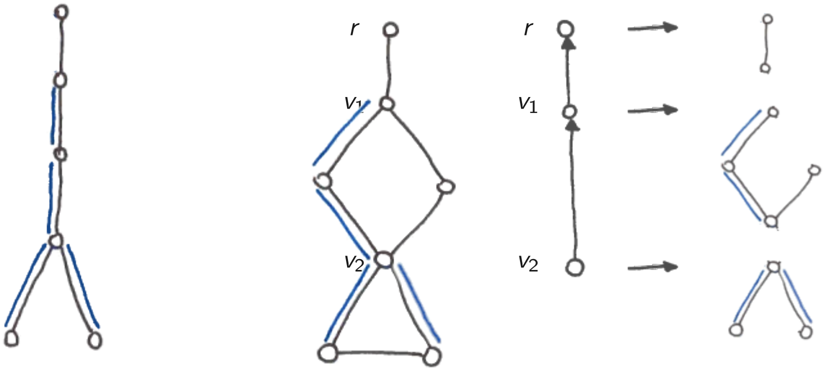

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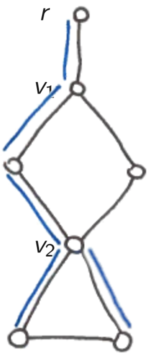

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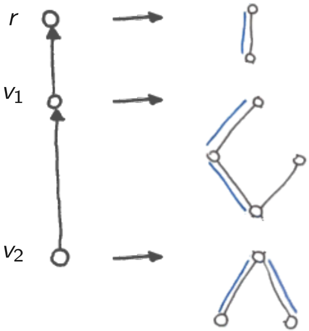

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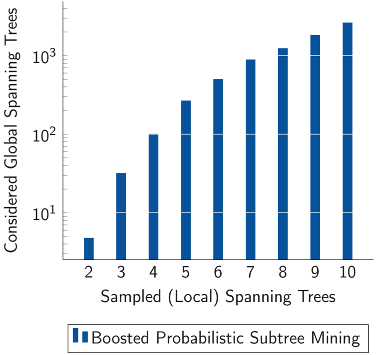
Brownian Motion Dataset (200 graphs à 30 vertices)

Average Number of Considered Spanning Trees per Graph



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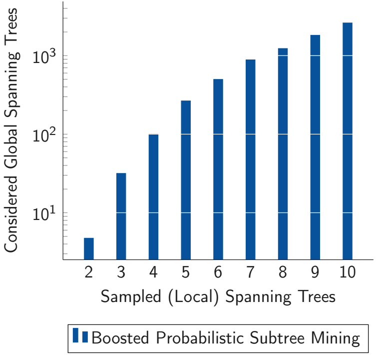
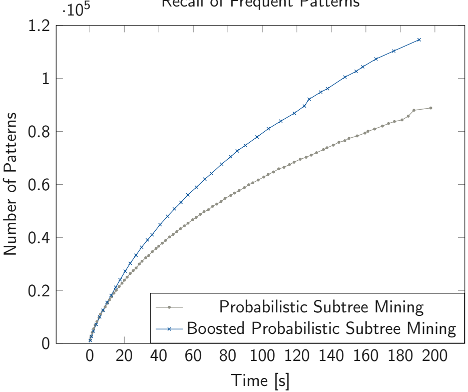


Recall of Frequent Patterns



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  - *conjecture:* we *cannot mine* frequent trees efficiently *beyond locally easy graphs*

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Part 3.

Fast Embedding Vector Computation

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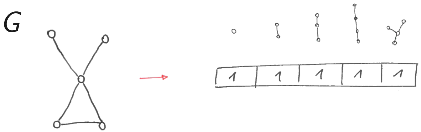
Given a set of tree patterns $\mathcal{F}$ and a (novel) text graph G



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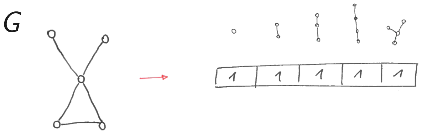

3. Embedding Vector Computation in (B)PS Feature Spaces

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Given a set of tree patterns $\mathcal{F}$ and a (novel) text graph G

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NP-hard problem

(Garey and Johnson, 1979)

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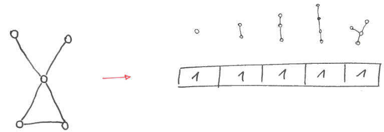

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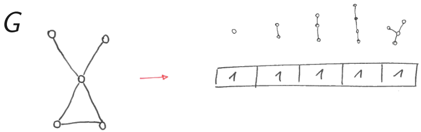

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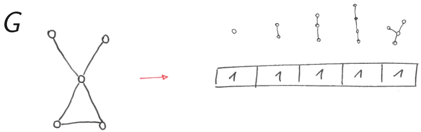
Solution Same as before: *probabilistic embedding operator*

$\Rightarrow$ *efficient* algorithm with *one-sided error*



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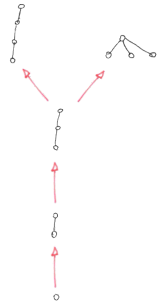

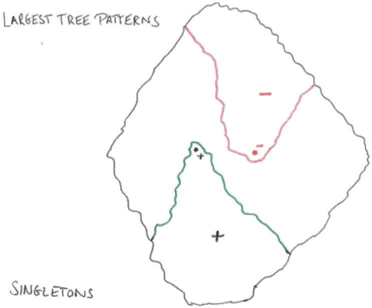

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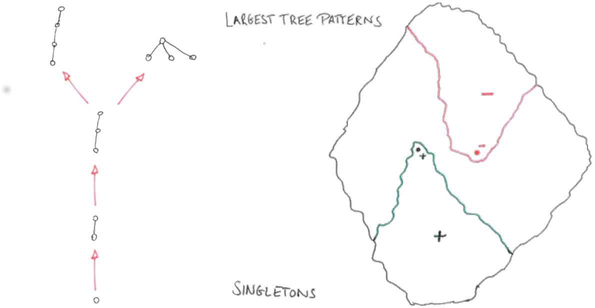

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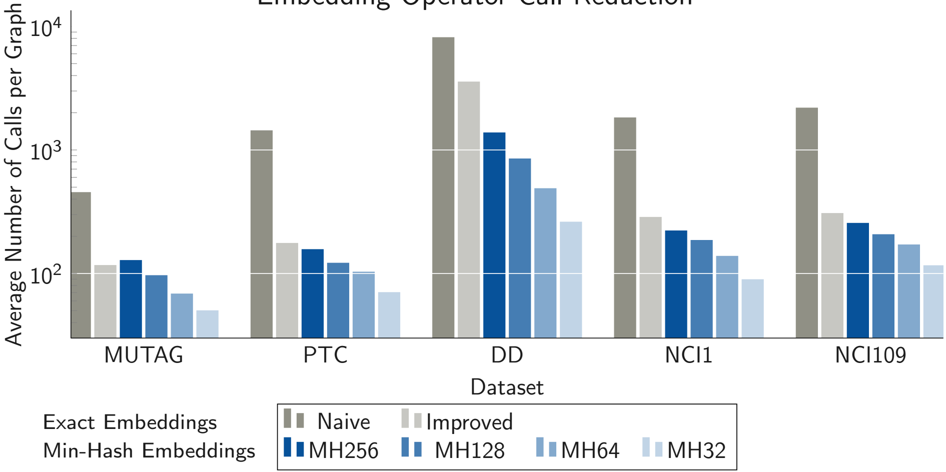
Embedding Operator Call Reduction



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  - for *locally easy graphs*, frequent subtree *mining and embedding* are *computationally tractable*
  - we conjecture: this result is *close to the border between tractable and intractable*

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