On the Complexity of Frequent Subtree Mining in Very Simple Structures

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Problem Setting

Given a database D of graphs and a frequency threshold,

list the set of frequent connected subtrees

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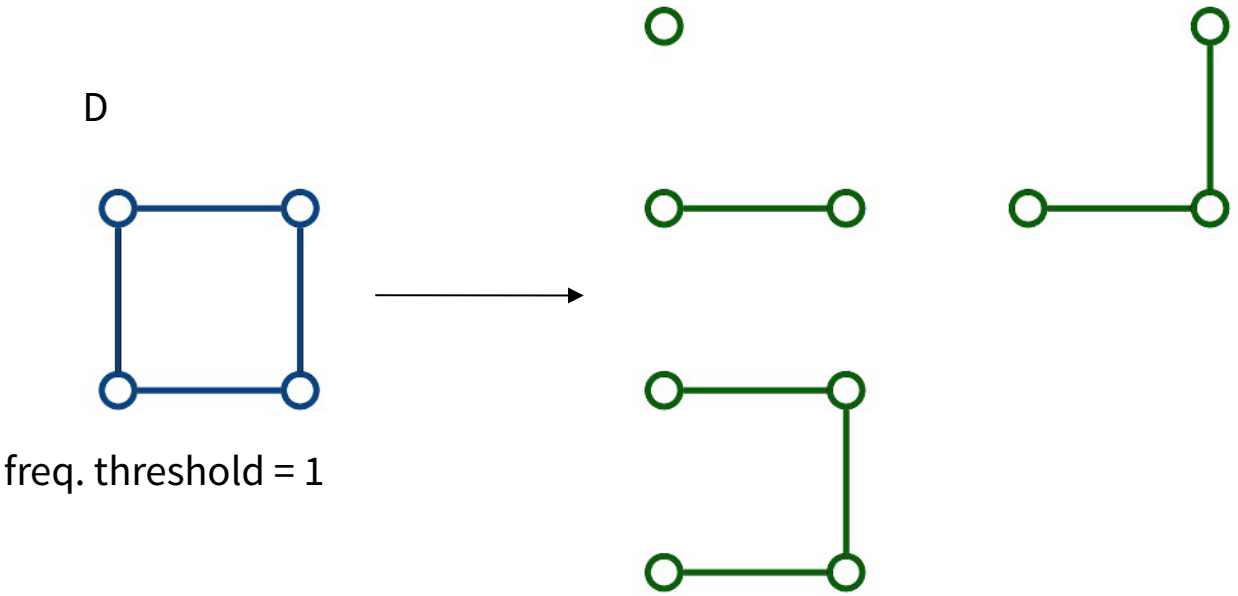
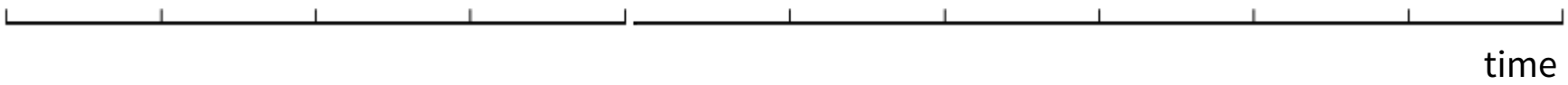
Example:



Efficiency Measures

Polynomial delay: Time between printing consecutive patterns is polynomial in the size of the database D



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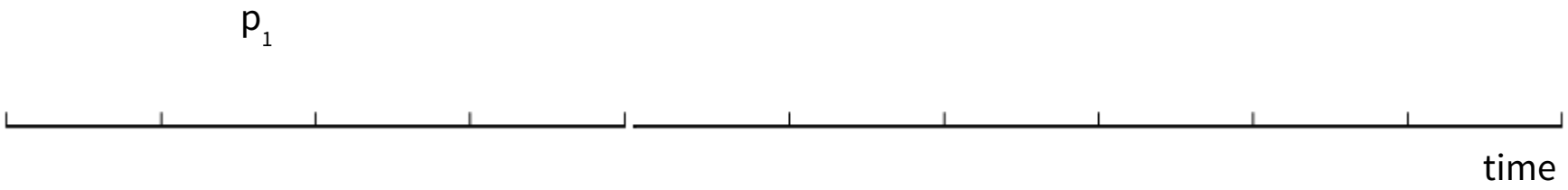

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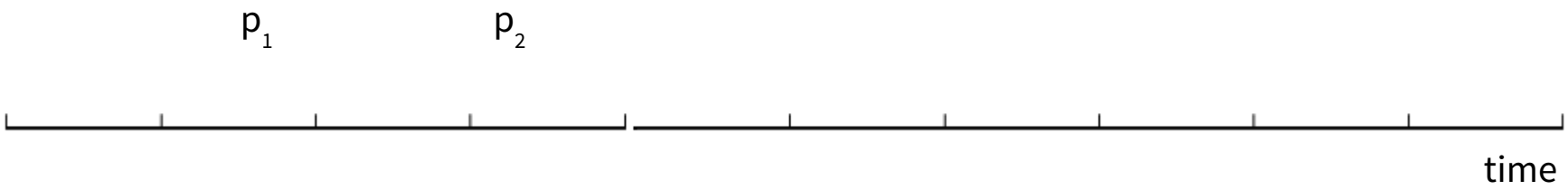

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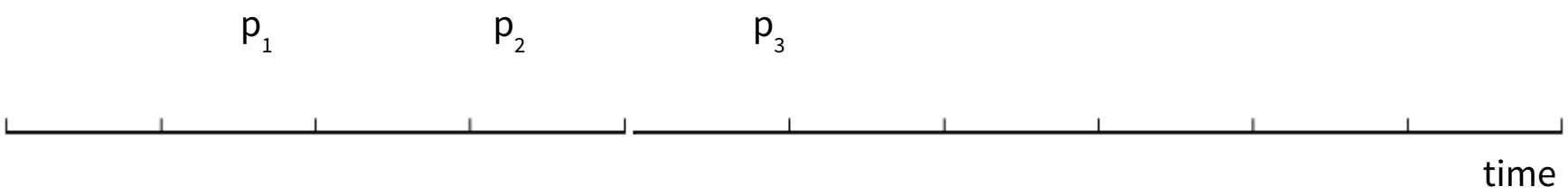

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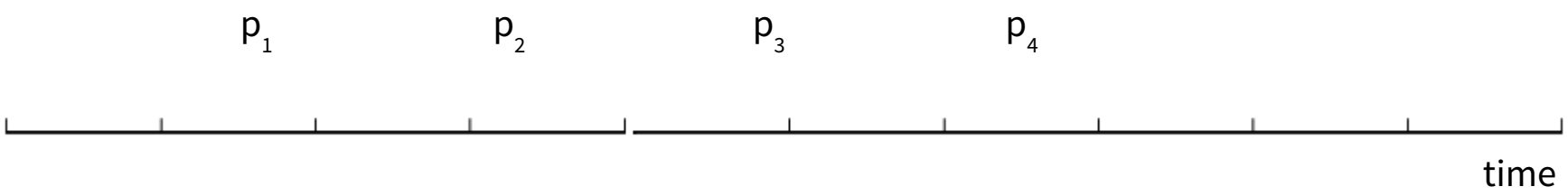

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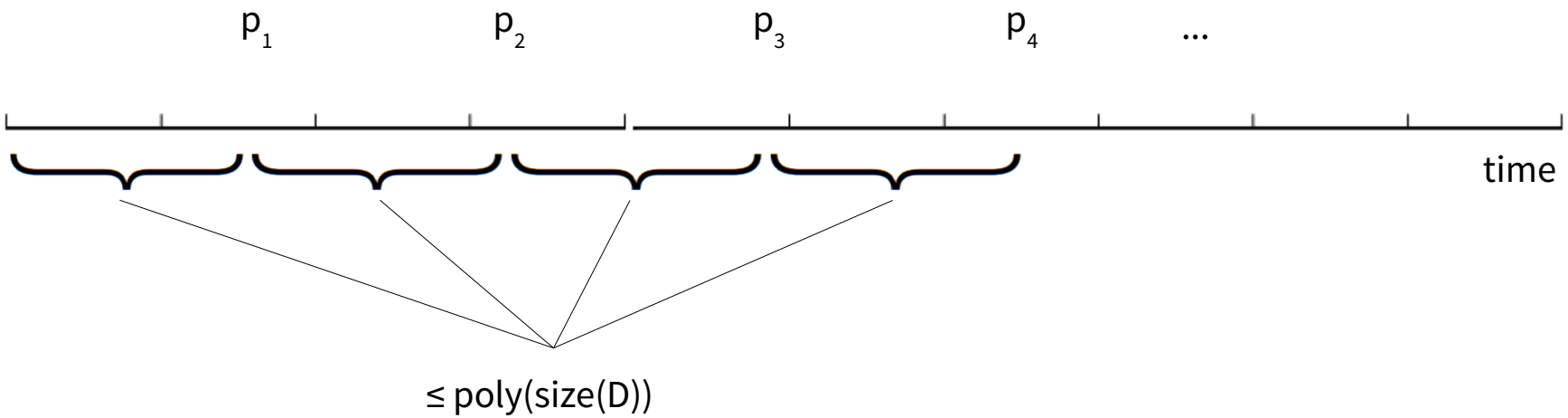

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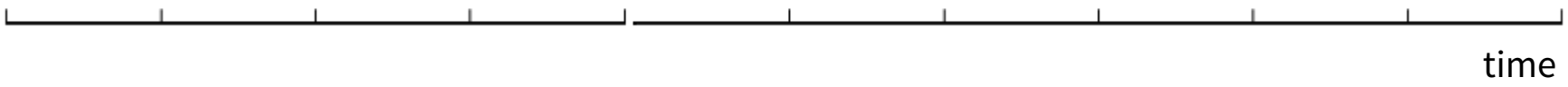
Incremental polynomial time: Time between printing consecutive patterns is polynomial in the size of the database D and the output so far



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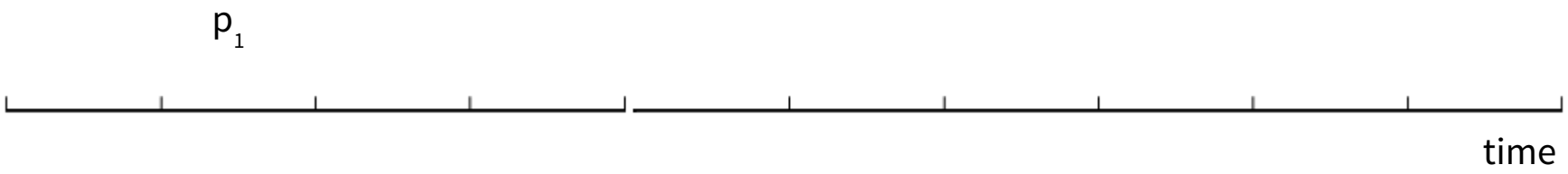

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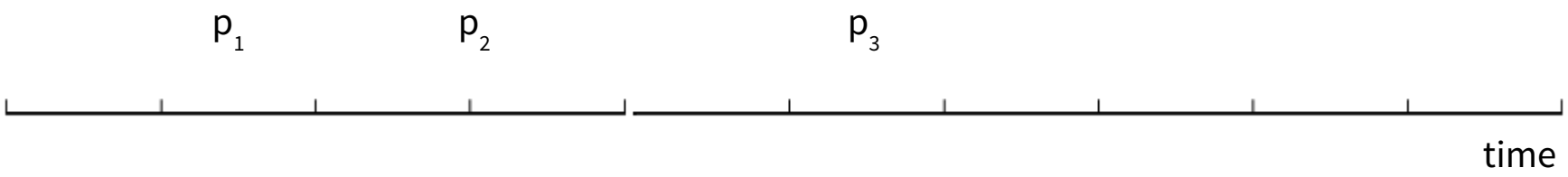

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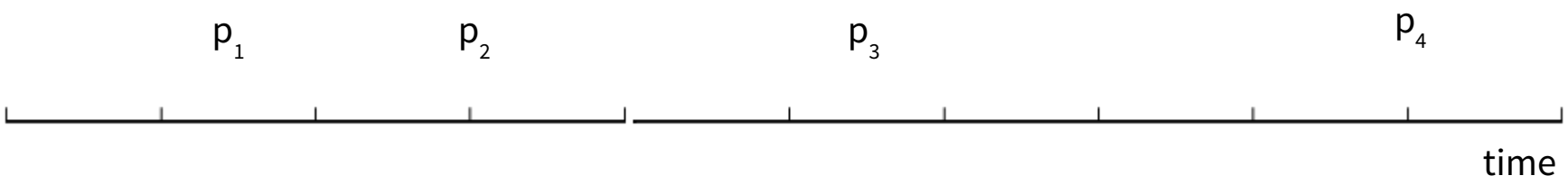

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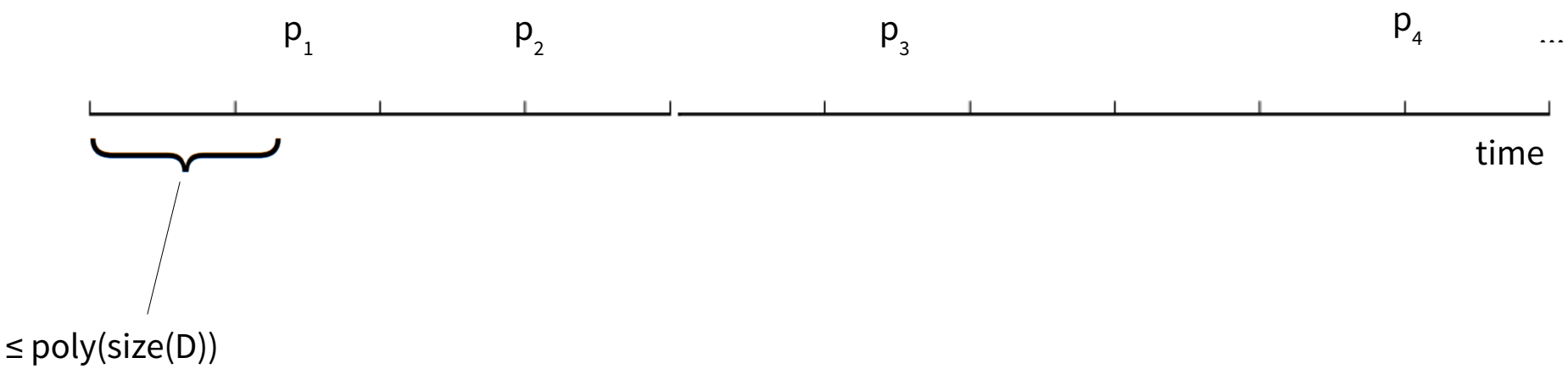

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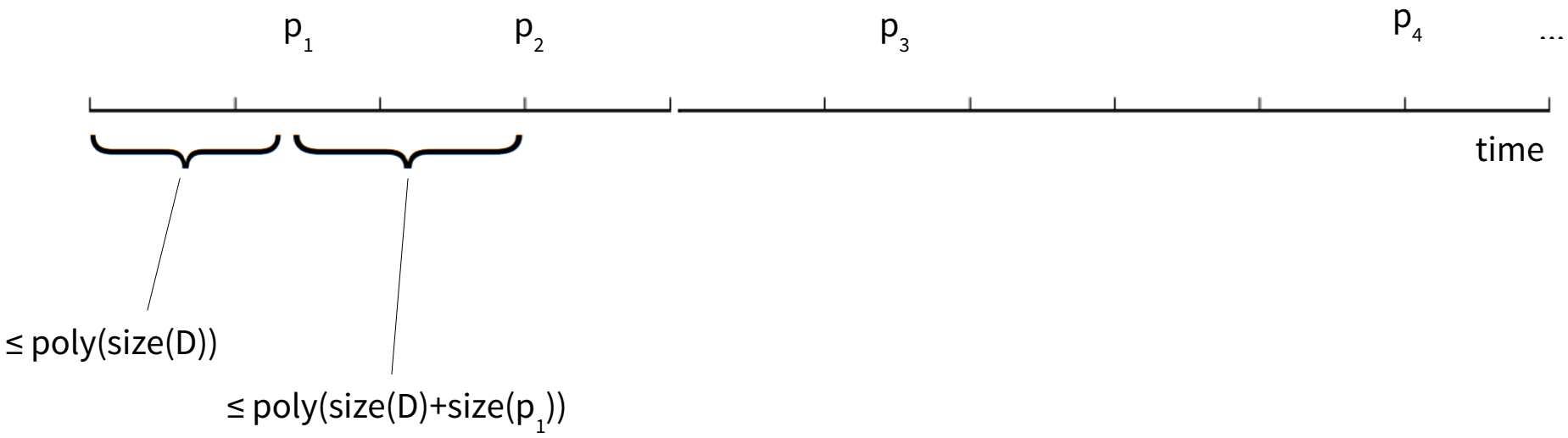

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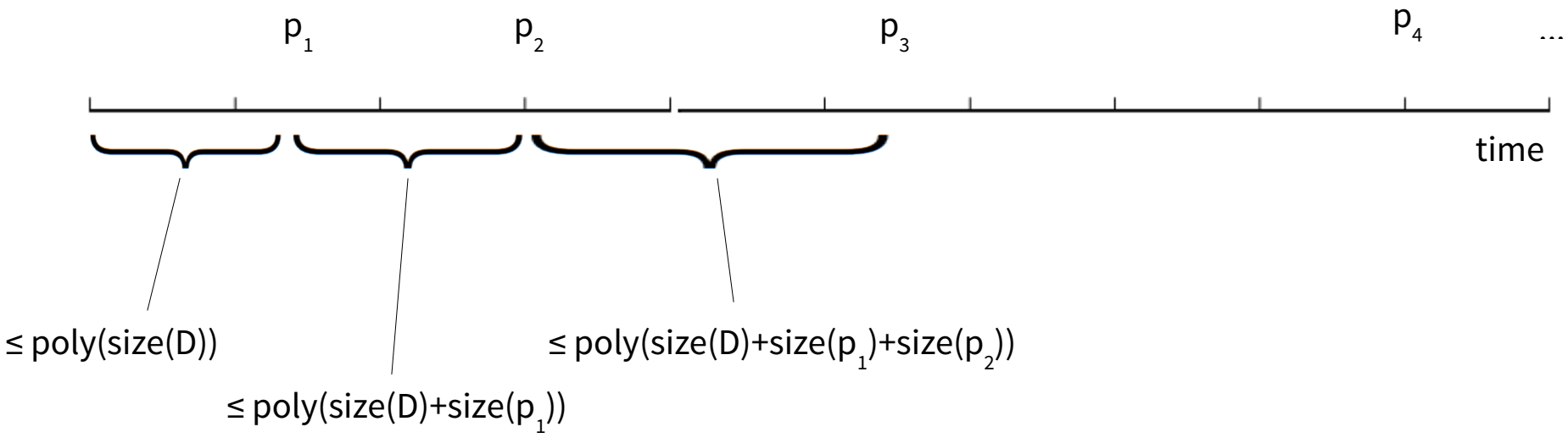

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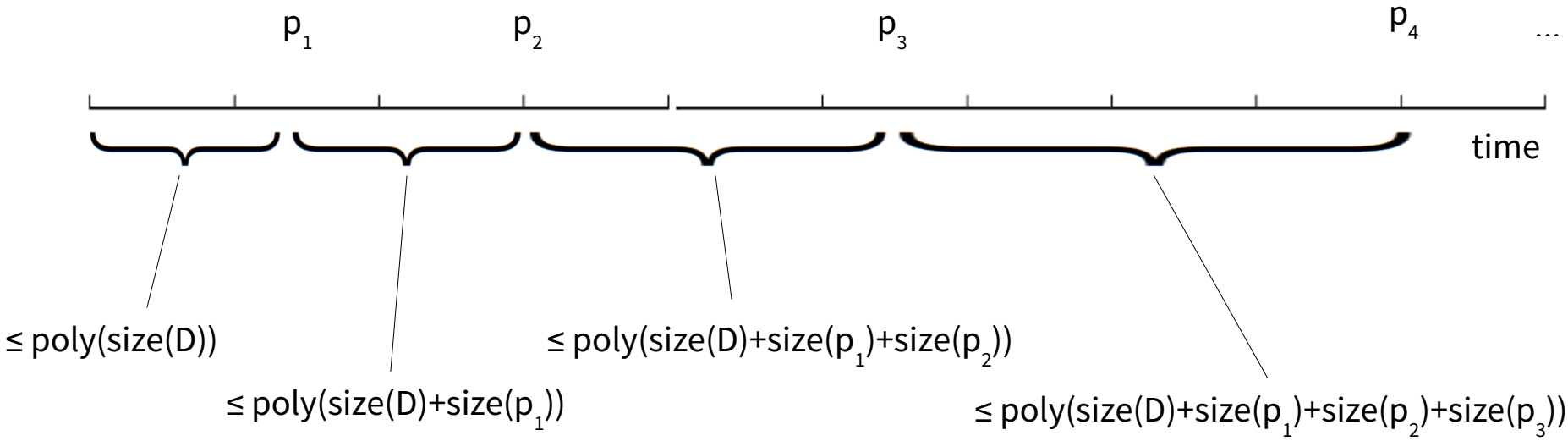

Research Question

- Research so far:

  Identification of graph classes allowing incremental polynomial time enumeration

Bounded Treewidth

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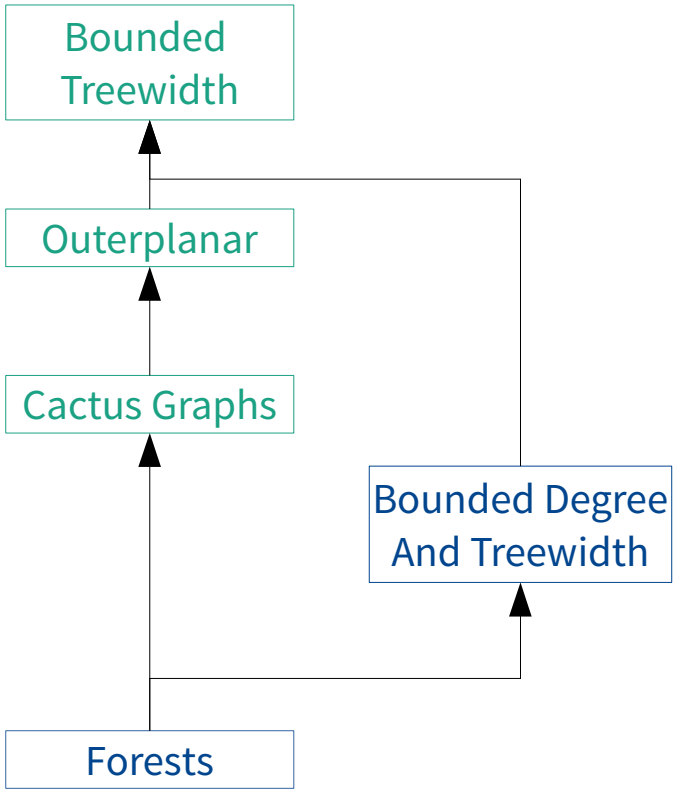
- Question for this work:

  Identification of graph classes allowing polynomial delay enumeration



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Theorem: Frequent subtree mining is possible in cactus graph databases with bounded cycle degree with polynomial delay.

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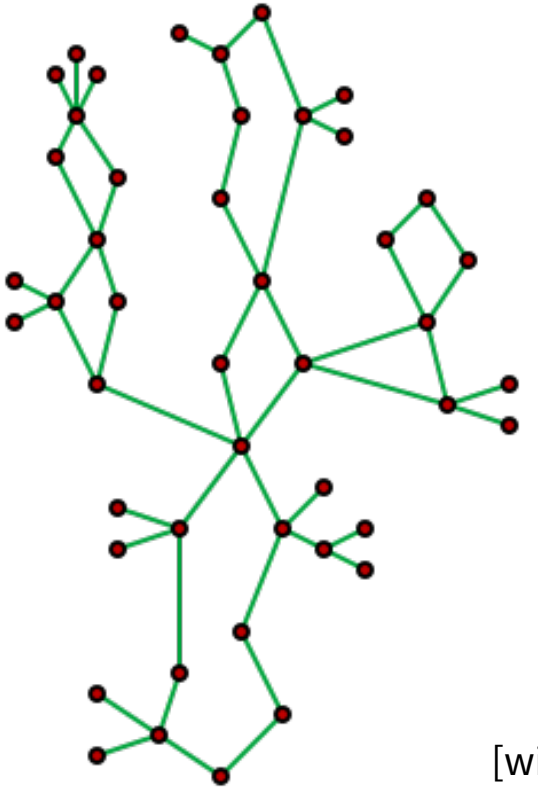

[wikipedia]

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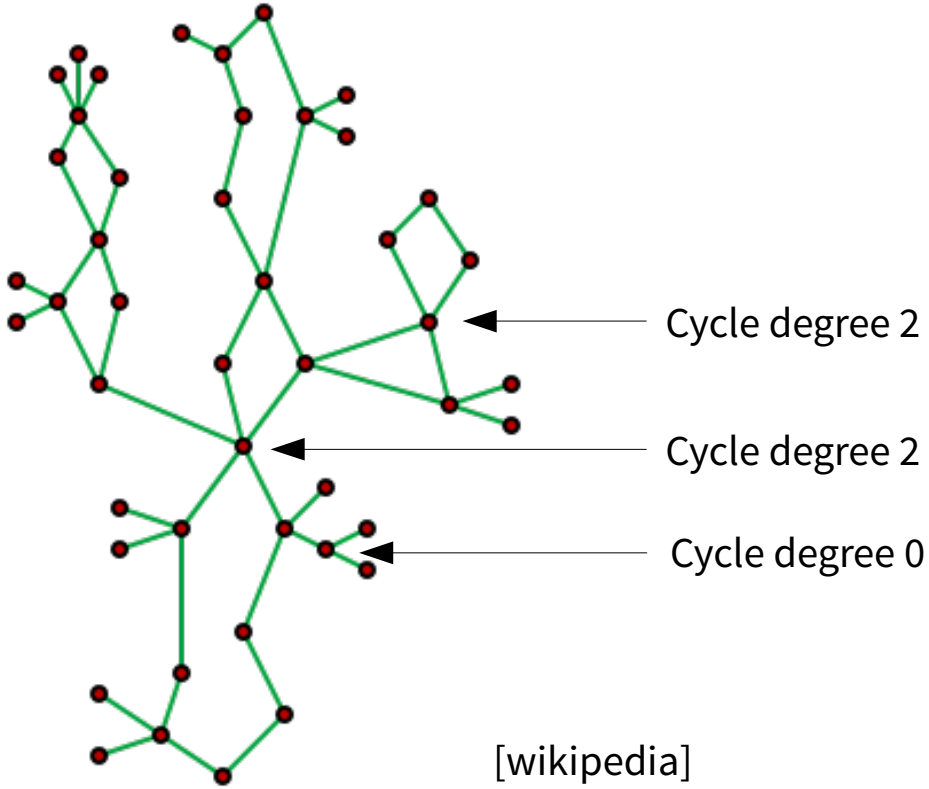

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Proof Sketch: Based on a generalization of [Shamir, Tsur] for pattern matching and a generic subgraph mining framework.

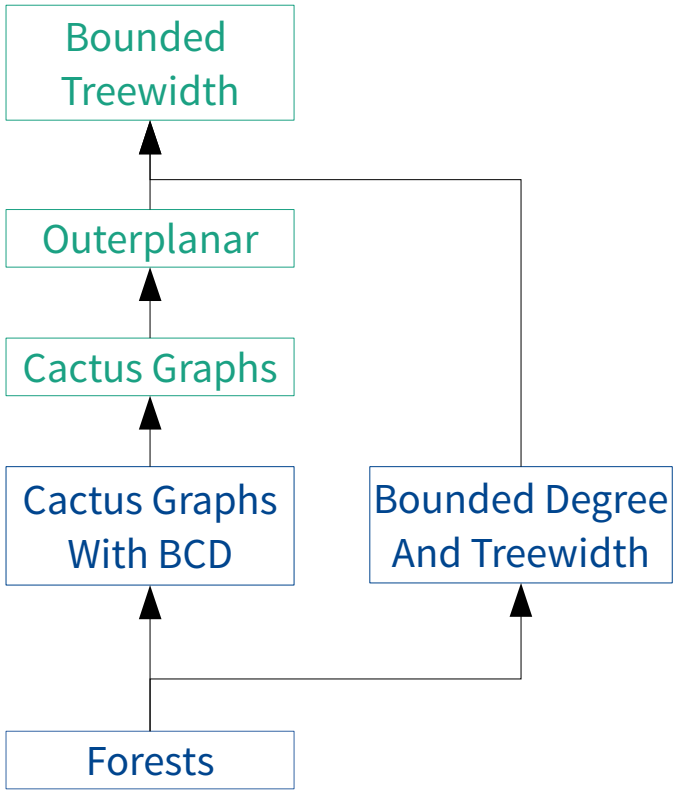
Why is this interesting?

- Many molecular graphs are cactus graphs
- Molecular graphs have very small cycle degrees

Data Set	Size	Max.CycD	Med.CycD	Cactus
NCI-HIV	42,687	4	1	50.08%
NCI-2012	249,533	3	1	63.81%
ZINC-leadlike	8,946,757	2	1	72.84%

Discussion of the Result

- Cycle degree seems a crucial parameter for polynomial delay enumeration
- If removed, there are two options:
  - a) Polynomial delay mining is not possible → P ≠ NP
  - b) Polynomial delay mining is possible → polynomial delay mining for NP-complete matching operators is possible



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