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Graph-based relational learning with a polynomial time projection algorithm

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Abstract. The paper presents a new projection operator for graphs, named AC- projection, which exhibits good complexity properties as opposed to the graph isomorphism (Θ -subsumption) operator typically used in graph mining. We study the size of the search space and some practical properties of the projection operator. These properties give us a specialization algorithm using simple local operations. Then we prove experimentally that we can achieve an important performance gain (polynomial complexity projection) without or with non-significant loss of discovered patterns quality.

Keywords: Relational learning, Polynomial-complexity projection, Specialization algorithm

1 Introduction

One goal of machine learning is the search of patterns to regroup or separate some elements (examples or counter examples). For this goal, logic-based systems have dominated the area of relational concept learning, especially Inductive Logic Programming (ILP) systems. However, a part of first-order logic can naturally be represented as a graph [6].

In order to learn from a relational description, we need a partial order on expressions of the description language (projection operator which gives a partial order between two expressions). To deal with the complexity of such description, some authors limit the description language [1]. In [2], the author uses a different bias. The examples are described by graphs but the projection operator is not an homomorphism (Θ -subsumption [4]) or a subgraph isomorphism (OI-subsumption [3]). It is a new matching based on arc consistency named AC-projection.

In this paper we present a novel graph mining algorithm, named AC-miner and based on the AC-projection operator, followed by some experimental evaluation of it on classical graph mining data sets.

2 The AC-projection Operator

Definition 1. (*Labeled Graph*) A labeled graph can be represented by a 4-tuple, $G = (V, E, L, l)$, where

- V is a set of vertices,
- $E \subseteq V \times V$ is a set of edges,
- L is a set of labels,
- $l : V \cup E \rightarrow L$, l is a function assigning labels to the vertices and the edges.

Definition 2. (Labeling) Let G_1 and G_2 be two graphs. We named labeling from G_1 into G_2 a mapping $\mathcal{I} : V(G_1) \rightarrow 2^{V(G_2)} | \forall x \in V(G_1), \forall y \in \mathcal{I}(x), l(x) = l(y)$.

Definition 3. (AC-compatible \curvearrowright) Let G be a graph $V_1 \subseteq V(G), V_2 \subseteq V(G)$ V_1 is AC-compatible with V_2 iff

1. $\forall x_k \in V_1 \exists y_p \in V_2 | (x_k, y_p) \in E(G)$
2. $\forall y_q \in V_2 \exists x_m \in V_1 | (x_m, y_q) \in E(G)$.

We note $V_1 \curvearrowright V_2$

Definition 4. (Consistency for one arc) Let G_1 and G_2 be two graphs. We say that a labeling $\mathcal{I} : V(G_1) \rightarrow V(G_2)$ is consistent with an arc $(x, y) \in E(G_1)$, iff $\mathcal{I}(x) \curvearrowright \mathcal{I}(y)$.

Definition 5. (AC-labeling) Let G_1 and G_2 be two graphs. A labeling \mathcal{I} from G_1 into G_2 is an AC-labeling iff \mathcal{I} is consistent with all the arcs $e \in E(G_1)$.

Definition 6. (AC-projection \rightarrow) Let G_1 and G_2 be two graphs. An AC-labeling $\mathcal{I} : V(G_1) \rightarrow V(G_2)$ is an AC-projection iff \forall AC-labeling $\mathcal{I}' : V(G_1) \rightarrow V(G_2)$ and $\forall x \in V(G_1), \mathcal{I}'(x) \subseteq \mathcal{I}(x)$. We note it $G_1 \rightarrow G_2$

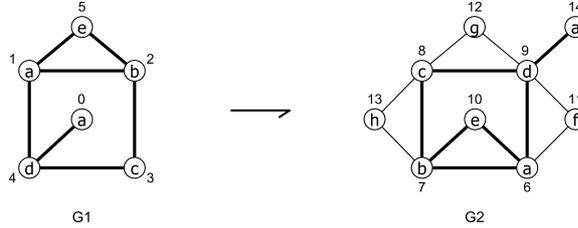


Fig. 1. An AC-projection example ($G_1 \rightarrow G_2$)

Definition 7. (AC-equivalent graphs \Leftrightarrow)

Two graphs G_1 and G_2 are AC-equivalent iff both $G_1 \rightarrow G_2$ and $G_2 \rightarrow G_1$ are fulfilled. We note it $G_1 \Leftrightarrow G_2$.

We have an equivalence relation between graphs using the AC-projection. The smallest element in this equivalence class will be its unique representative, and for which we give then the name of “AC-reduced graph”.

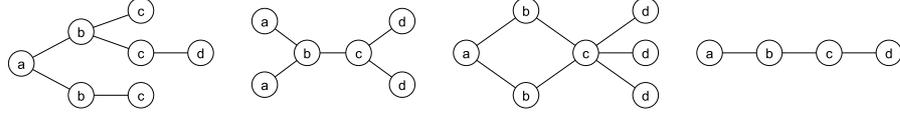


Fig. 2. AC-equivalent graphs and the associated AC-reduced one (extreme right)

3 Search space with AC-projection

In this section, we study the size of the search space using AC-projection. We present some properties of the AC-projection, using this properties we can find an upper bound of the search space. We present this result for one labeled graph G , but these results can be easily extended for n graphs (one for each example). In this case G is the disjoint union of the graphs describing the examples. Notation: For a labeled graph $G:(V,E,L)$ we note $\mathcal{P}_l(V)$, the power set of vertices, in V , with label $l \in L$.

Definition 8. (*AC-graph*) For a labeled graph $G:(V,E,L)$ and a set P of element $\in \bigcup \mathcal{P}_l(V)$ with $l \in L$.

We construct a graph $G':(V',E',L')$ with:

- a vertex v for each element in P . We note $p(v) \in P$ the associated element.
- The label of a vertex v in the label of the element in $p(v)$
- $(V_1, V_2) \in E'$ iff $p(V_1) \sim p(V_2)$

G' is an AC-graph of G .

So an AC-graph is built from a list of set of vertices from a graph G . Now, we study some links between AC-graph and AC-projection.

Proposition 1. For each AC-projection between two graphs G', G there is an associated AC-graph.

Proof. Since an AC-projection \mathcal{I} , gives, for each vertex x of G' , a set of vertex of G . The AC-graph built from an AC-projection is the one build from the set of $I(x)$, $x \in V'$.

Proposition 2. For each AC-graph G' of a graph G we have $G' \rightarrow G$.

Proof. The labeling \mathcal{I} with, for each $V \in G'$, $\mathcal{I}(V) = p(V)$ is an AC-labeling from G' into G by construction.

Now for a graph G we can define a specific AC-graph built from the power set of vertices of G .

Definition 9. (*Max-AC-graph*) For a graph $G:(V,E,L)$ the Max-AC-graph of G is the AC-graph built from the set P of all element $\in \bigcup \mathcal{P}_l(V)$ with label $l \in L$. We note this graph Max-AC-graph(G)

All subgraphs of $\text{Max-AC-graph}(G)$ has an AC-projection into G . Since the Max-AC-graph is the biggest AC-graphe, we have our search space. The complexity of the construction of the Max-AC-graph is $O(2^n)$ where n is the number of vertices in G . This complexity is big but for many structural descriptions (graph with homomorphism projection ..) the size of the search space is bigger by an order of magnitude.

4 AC-miner: A graph mining approach with a polynomial time projection

In this section we will present a basic algorithm for frequent AC-reduced subgraphs mining. The goal of this algorithm is the construction of a part of the $\text{Max-AC-graph}(G)$ where G is the disjoint union of the graphs describing the examples (G is technically materialized by a graph database \mathcal{D} in the following). We are using a support parameter (σ) as a bias which limits the search space.

4.1 AC-compatible extension

Definition 10. (*Vertex group*) Given a graph database \mathcal{D} , a vertex group \mathcal{V} is a set of vertices of the same label l and belonging to graphs in \mathcal{D} . The most general vertex group \mathcal{V}^l is the maximal vertex group of a given label l .

The AC-compatible extension, is the core operation of the AC-miner algorithm. Given a vertex group \mathcal{V} and a vertex label l , the AC-compatible extension consists in finding the maximal subset \mathcal{V} that is AC-compatible with a maximal subset of the most general vertex group (\mathcal{V}^l). The AC-compatible extension is considered to be valid w.r.t. a minimal support parameter (σ) if and only if the vertices in \mathcal{V} appears at least in σ graphs of the graph database \mathcal{D} .

4.2 The AC-miner algorithm

The AC-miner algorithm (see Algorithm 1) starts by adding for each vertex label in the graph database \mathcal{D} its associated most general vertex group \mathcal{V}^l in the *jobs* list (Algorithm 1 line 1). This list contains the remaining vertex group to extend. Then, based on this list (*jobs*) it starts the main computational loop. During each iteration it will try to make an AC-compatible extension for the current vertex group with each one of the graph database labels (Algorithm 1 line 4). If there is an AC-compatible extension, AC-miner will add (if not already done) the two vertex group children as well as an edge between them to the \mathcal{G} AC-graphe and the *jobs* list (lines 6-12). The algorithm will iterates till the *jobs* list becomes empty. At this stage, the algorithm will extract all the connected components from the \mathcal{G} AC-graph. These subgraphs represent the frequent AC-reduced subgraphs.

Algorithm 1: AC-miner

Input : Graph database \mathcal{D} , Minimal Support σ , AC-graphe \mathcal{G} (local)
Output: \mathcal{F} = frequent AC-reduced subgraphs

```

1  $jobs = \{\cup \mathcal{V}^l | l \in \mathcal{D}.getLabels()\};$ 
2 while  $jobs \neq \emptyset$  do
3    $\mathcal{V} = jobs.getFirst();$ 
4   for  $\{\forall l | l \in \mathcal{D}.getLabels(), l \notin \mathcal{V}.getForbidden()\}$  do
5     if AC-compatible-Extension( $\mathcal{V}, \mathcal{V}^l, \mathcal{V}_{child}, \mathcal{V}_{child}^l, \sigma$ ) then
6       if  $\mathcal{V}_{child} \notin \mathcal{G}$  then
7          $\mathcal{G} = \mathcal{G} \cup \mathcal{V}_{child};$ 
8          $jobs = jobs \cup \mathcal{V}_{child};$ 
9       if  $\mathcal{V}_{child}^l \notin \mathcal{G}$  then
10         $\mathcal{G} = \mathcal{G} \cup \mathcal{V}_{child}^l;$ 
11         $jobs = jobs \cup \mathcal{V}_{child}^l;$ 
12         $\mathcal{G}.addEdge(\mathcal{V}_{child}, \mathcal{V}_{child}^l);$ 
13 return  $\mathcal{G}.getConnectedComponents();$ 

```

5 Experiments And Comparative Study

In order to prove the usefulness of the AC-projection for graph mining, we present in the following a qualitative evaluation of the AC-reduced patterns which consists in a calculation of their discriminative power within a supervised graph classification process.

Datasets: We carried out classification experiments on two real-world datasets group widely cited in the literature : The anti-cancer screen datasets (nci) and the AIDS antiviral screen data (aids) as in [7].

Methods: We evaluated the classification accuracy using two different feature sets : Isomorphic and AC-reduced. Each chemical compound is represented by a binary vector with length equal to the number of mined subgraphs. Each subgraph is mapped to a specific vector index, and if a chemical compound contains a subgraph then the bit at the corresponding index is set to one, otherwise it is set to zero.

Results: All classifications have been done using the well-known C4.5 decision tree classifier [5]. We have reported results of the prediction accuracy over 10 cross-validation trials. According to results shown in Figure 3a and 3b, we see that for all datasets we have very few AC-reduced frequent patterns compared to the isomorphic ones. We have on average 35% less patterns. This ratio is bigger for lower supports and can reach up to 58% for the aids dataset with a minimal support of 10%. In the qualitative point of view (Figure 3c) we see that the percentage of correctly classified (PCC) instances is almost the same

for all minimal supports. Taking a more in-depth look to the results, we see that, for some datasets and minimal support values, we even have better PCC for AC-reduced feature set. This is due to the better generalization power of the AC-reduction process, which helped supervised classifiers avoiding over-fitting learning problem.

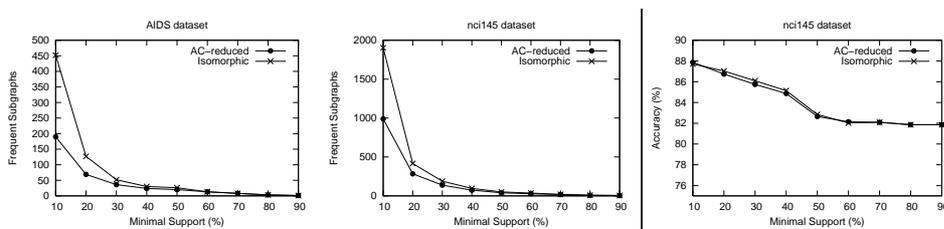


Fig. 3. Comparison of the number of frequent patterns (a,b) and classification accuracy (c) for aids and nci145 datasets

6 Conclusion

In this paper, we have studied the use of a new polynomial projection operator named AC-Projection initially introduced in [2]. We have then presented a novel algorithm named AC-miner which proceeds by specialization of expressions using very simple and fast set and neighborhood operators. This simplicity allows us to obtain a very fast algorithm which can be easily adapted for a depth first or a breadth first search strategy and can be easily parallelized as well. AC-miner is intended to mine frequent AC-reduced subgraphs from a graph database. We have experimentally showed that the number of these subgraphs is clearly smaller than isomorphic subgraphs but having a very comparable quality and discriminative power.

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