Deterministic Graph-Walking Program Mining

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Abstract. Owing to their versatility, graph structures admit representations of intricate relationships between the separate entities comprising the data. We formalise the notion of connection between two vertex sets in terms of edge and vertex features by introducing graph-walking programs. We give two algorithms for mining of deterministic graph-walking programs that yield programs in the order of increasing length. These programs characterise linear long-distance relationships between the given two vertex sets in the context of the whole graph.

Keywords: Graph Walks · Complex Networks · Program Mining · Program Induction

1 Introduction

While data has been stored in the form of tables since time immemorial, more complex data is often represented with graphs. This is because graph databases generalise conventional table-driven data storage methods, allowing for modelling of involved relationships among entities represented therein. As such, graph analysis and mining methods will be at the center of attention when it comes to contextual understanding of relationships between individual datapoints within a large database.

Here we investigate the identification of one type of such relationship between two groups of graph’s vertices. For an illustrative example (Figure 1), consider an individual who has just graduated from high school (starting qualifications $S$) and aims to reach a target career (target qualifications $T$) while being permitted only one study focus at the time – e.g. studying either social or biological sciences, but not both. What sequence of decisions with regards to their study foci should they take? Notice that the choice of focus made at every stage of the individual’s education leads to a restriction on what qualifications they can obtain in the future. Thus, at each stage of their education, they will need to focus on qualifications that are pre-requisites for those that lead to $T$. Attempting to solve the problem on our own, we can search for a sequence of instructions that leads us from $S$ to $T$ either by naively tracing out paths from $S$ and reading out instructions one by one, or by enumerating all possible instruction sequences and then verifying if they indeed do lead from $S$ to $T$.

Informally, let $G$ be a graph where every vertex has some features, and let $S, T$ be vertex sets. We ask the following question: “How is $S$ connected to $T$ in
Fig. 1: A depiction of the qualification pathway $p$ for an individual who has just graduated from high school (the starting qualification in $S$) and aims to become a prosecutor in the United States (target qualifications $T$). Vertices, colours, edges represent qualifications, qualification foci, and dependencies, respectively. Going into college, they will need to choose a focus that maximises their chances of being admitted to a law school (most likely social sciences). In law school, they will need to focus on criminal rather than tax or corporate law and prepare diligently for their barrister examinations. Finally, they will need to satisfy the necessary pre-requisites of civil service before becoming a prosecutor.

Revisiting the example above, if $G$ is a map of qualifications, with $G$ being qualifications and directed edge $(v_1, v_2)$ denoting that $v_1$ is a pre-requisite qualification for obtaining $v_2$, one could iteratively ask “what type of qualifications from among the qualifications I am eligible for now should I achieve to eventually reach my target qualifications $T$”? A good answer would give a sequential list of characteristics of qualifications. Of course, getting all possible qualifications at every stage would likely lead to obtaining qualifications in $T$, but ideally one would not be doing more than absolutely necessary. We illustrate a variant of this example in which each qualification is only characterised by its type in Figure 2.

We investigate this problem and aim to give answers in terms of lists of instructions for a single graph-walking agent that can be present at multiple vertices at the same time. We dub such lists of instructions *simple graph-walking programs*. 

Fig. 2: An example of the qualification program problem with multiple starting qualifications. An individual possessing three different qualifications (vertices in $S$) of the same focus/type (colour) seeks to attain any of the qualifications in $T$ such that they always do qualifications of the same type. Each of their qualifications, however, is a pre-requisite (directed edge) for a slightly different set of later qualifications, and it will take at least four steps to reach $T$ from any qualification in $S$. $p$ gives a program in which they first work towards green, then brown, then red, and finally yellow qualifications, and exactly the qualifications in $T$ are achieved. $p'$ gives a program green-purple-red-yellow, in which there is some overlap with $T$ but an additional yellow qualification not in $T$ is achieved.

Let $G = (V, E)$ be a directed multi-graph, $\mathcal{F}_1, \ldots, \mathcal{F}_z$ spaces of the features appearing in $G$, and $\mathcal{F} := \prod_i \mathcal{F}_i \cup \{0\}$ their product, where $0_i$ denotes that a given graph element is not assigned feature $i$. Let $\phi_V : V \to \mathcal{F}, \phi_E : E \to \mathcal{F}$ be the vertex and edge feature mappings. Let $p : c_1 \cdots c_{2n}$ be a simple graph-walking program – a list of vertex movement selection instructions, i.e. functions on $c_i : \mathcal{F} \to \{0, 1\}$. Consider an agent, located at $E_p^0$ for any time $t \geq 0$, that begins at the set of vertices $S = E_p^0$ and at each time $t \geq 1$ decides to proceed only to those vertices $v$ in out-neighbourhood of $E_p^{t-1}$ connected by edges $e$ whose feature vectors $\phi_V(v), \phi_E(e)$ satisfy $c_{2t-1}(\phi_E(e)) = 1 = c_{2t}(\phi_V(v))$. The problem of simple graph-walking program mining is the problem of finding lists of instructions $p$ such that an agent following it reaches $T$ by the end of the program ($\emptyset \neq E_p^n \subseteq T$). See Figure 3. Alternatively and more in line with the program synthesis literature, we can speak of graph-walking program induction or synthesis, with the triple $(G, S, T)$ forming the inputs for the induction of the programs. We call programs that satisfy $\emptyset \neq E_p^n \subseteq T$ feasible, and programs that achieve the equality exact.
Fig. 3: Two illustrative examples with solutions. Recall the objective to find a sequence of conditions on features that leads an imagined agent from the vertices of $S$ to the vertices of $T$. Left. The simple colour program $p$ can be used to instruct the agent starting at vertices of $S$ to proceed towards $T$. On the first step $E^1_p$ is reached. On the second step, the agent proceeds to the red nodes marked by $E^2_p$. On the third step, the agent proceeds to $T$. green-blue-yellow would be another feasible program. Right. Two simple toset (totally-ordered set) programs $p, p'$ are presented, conditioning on two feature dimensions of a general, unlayered graph: colour and integers. Agent starting in $S$ reaches exactly $T$ if following $p$ ($p$ is feasible and exact) but ends up at a strict superset $E_{p'}$ of $T$ if she follows $p'$ (hence $p'$ is infeasible).

The resulting programs are not frequent patterns, nor do they characterise the graphs locally; they characterize long-distance relationships between groups of vertices in $G$ in terms of $F$. Nevertheless, for a given pair of vertex sets $S, T$ there are often many feasible programs, and our algorithms carry some characteristics of a priori graph pattern mining. We talk of “simple” programs because there are more elaborate program structures that could be studied in this setting (such as those that possess memory), and of “deterministic” programs since the instruction/criterion $c_i$ always gives either 1 or 0 as firm directions to the agent walking the graph.

The difficulty of this problem dwells in it being a cunning composition of two necessary sub-tasks – path search and classification – well-understood and studied in graph theory and machine learning, respectively. This is because it is not enough to find a possible program walk from a vertex in $S$ to a vertex in $T$ – one has to choose from all possible walks for all possible choices of the pair $(s, t) \in S \times T$, and then find a subset of these walks for which a single graph-walking program can be used. In other words, it is necessary to both discover possible walks, and discriminate among them.

The mining algorithms we propose are correct (they return only valid programs) and complete (proceeding in stages, they always yield all valid programs up to some length $\ell$ before looking for longer programs).
This paper reviews related work (Section 2), describes the problem of simple colour program mining, gives an algorithm for the task (Section 3) – which, to the best of our knowledge, has never been addressed in the literature before – and extends simple colour program mining to simple totally-ordered-set programs (Section 4).

2 Related Work

Our effort lies at the intersection of two areas, namely graph program synthesis and analysis of complex networks.

Algorithmic program synthesis [4], traditionally considered a problem in deductive theorem proving, has recently been looked at as a search problem with constraints such as a logical specification of the program behaviour [11], syntactic template [1, 9], and, most recently, previously discovered program fragments and utility functions [10, 16]. Several new methods combine enumerative search with deduction, aiming to rule out infeasible sub-programs as soon as possible [12, 13]. While relevant to us in their intent, the methods are domain-specific and do not extend to programs on graphs.

Under the paradigm of program search within a restricted graph context, Yaghmazadeh et al. [24] study the synthesis of transformations on tree-structured data and employ a combination of SMT solving and decision tree learning. Their synthesis system, HADES, outputs programs in a custom domain-specific language for tree-transformation. Their approach considers entire graphs at the same time and while it does provide insights into construction of programs for graphs, it does not extend to the graph walk scenarios.

Wang et al. [21] give a synthesis algorithm for queries $q$ on a set of tables $T_1, T_2, \ldots, T_k$ that output records of a target table $T_{\text{out}}$. Their approach to query-walk search is syntactic (in contrast to treating the database schema as a graph) and relies on simple enumeration of possible table visits, something our algorithms avoid with further constraints on the search space.

Mendelzon and Wood [18] consider the problem of finding pairs of vertices in a graph connected by simple paths such that the trace of the labels of the vertices traversed satisfies a given regular expression. While being perhaps closest to our work, their goal is to find paths that satisfy a constraint, rather than finding constraints for which connecting paths exist, thus having one degree of freedom fewer.

A sub-branch of graph pattern mining considers the special case of mining frequent paths [14, 15]. We note that while the knowledge of frequent paths in a graph might potentially accelerate the search for solutions for the graph-walking program mining problems, methods for frequent path mining are of little direct use since we seek programs that go between particular sets $S, T$.

Finally, the literature on analysis of complex networks frequently focuses on characterisation of elements of networks in terms of their interactions with their neighbourhoods. Among the examined characterisations are the notions of structural equivalence [5, 7, 17], regular equivalence [22], or other partitioning
strategies [23]. Further, random walks of graphs are frequently employed to help
with analysis of graphs as whole [8,19] or as sum of its communities [2,3], but to
our knowledge, no work so far has investigated the identification of relationships
between nodes related from beyond close neighbourhoods.

3 Simple Colour Programs

Without any loss of generality we restrict ourselves to program mining on simple
directed graphs with featureless edges, to whom directed multi-graphs with edge
features can be converted by replacing every edge with a vertex inheriting edge’s
features and retaining its endpoints as the only neighbours.

We focus on simple colour programs – programs $p : c_1 \cdots c_n$ such that $c_i$ is
the colour of the out-neighbours of the vertices reached by the prefix program
$c_1 \cdots c_{i-1}$ whom the agent executing $p$ should proceed to at step $i$. The program
instructions (criteria) are thus colours.

3.1 Preliminaries

Let $G$ be a simple directed $k$-coloured graph. The colouring does not have to
be proper. Let $\emptyset \neq S, T \subseteq V$. Denote by $c(v)$ the colour of vertex $v$, by $c(A)$
the set of colours of the vertices in $A \subseteq V$, and by $C_c(A)$ the set of vertices
of $A$ with colour $c$. Call set of vertices $A$ monochromatic if $c(A)$ is a singleton
set. Denote the out- and in-neighbours of $A$ by $N_o(A)$ and $N_i(A)$ respectively.

Shorten $n$ applications of $N$, i.e. $N_o(N \cdots N(A))$, to $N_n o(A)$, and similarly for
$N_i$. For convenience, define $N_0 o(A) := A =: N_0 i(A)$.

Definition 1 (Simple Colour Program). $p : c_1 c_2 \cdots c_n$ is a simple colour
program (SCP) of length $n$ iff $1 \leq c_i \leq k$ for all $1 \leq i \leq n$.

Use $\epsilon$ for empty program – the unique program of length 0, $p_i$ for $c_i$, $p_{\leq i}$ for
the prefix $c_1 \cdots c_i$ of $p$ for $1 \leq i \leq n$, and $p_{\geq i}$ for the suffix $c_i \cdots c_n$ of $p$.

Definition 2 (Program Endpoints). For $p : c_1 c_2 \cdots c_n$ an SCP, define $E_p^i(S)$
for $0 \leq i \leq n$ recursively as follows:

1. $E_p^0(S) = S$,
2. For $i > 0$, $E_p^i(S) = C_{c_i}(N_o(E_p^{i-1}(S)))$,

and denote $E_p^n(S)$ by $E_p(S)$.

Definition 3 (Feasible and Exact SCP). $p$ is feasible iff $\emptyset \neq E_p(S) \subseteq T$,
and exact iff $E_p(S) = T$.

Definition 4 (Partial Halting). $p$ partially halts (on $G$) if there exists an
$0 \leq i < n$ and $v$ such that $v \in E_p^i(S)$ but $c_{i+1} \notin c(N_o(v))$.

In other words, $p$ partially halts if it ever reaches a vertex from which it is
impossible to proceed while still following $p$. 
Lemma 1. If $p$ is a feasible program that does not partially halt, then for all $0 \leq i < n$ there exists a colour $c_{i_0}$ such that $\emptyset \neq C_{c_{i_0}}(N_o(E^i_p(S))) \subseteq N^{-i+1}_i(T)$.

Proof. For each $i$, take $c_{i_0} = p_i$.

Definition 5 (Complete Halting). $p$ halts (completely) on $G$ if there exists an $1 \leq i < n$ such that $c_{i+1} \notin c(N_o(E^i_p(S)))$. Equivalently, there is an $1 \leq i < n$ such that $E^{-i+1}_i(S) = \emptyset$.

Lemma 2. Assume that a feasible SCP exists for $S, T$. Then
1. There exists a walk $w$ from $s \in S$ to $t \in T$ such that the colours of the vertices from $s$ to $t$ give a feasible program for $S, T$.
2. If a program that does not partially halt exists, for every $s \in S$ there are $t \in T, w$ as in item 1.
3. If an exact program exists, for every $t \in T$ there are $s \in S, w$ as in item 1.

Proof. Let $p : c_1 \cdots c_n$ be a feasible program.
1. Take any $w_n \in E_p(S)$. If $n = 1$ we are done. If not, prepend it by any $w_{n-1} \in N_i(w_n) \cap E^{n-1}_p(S)$ which is non-empty as $p$ is feasible and therefore does not halt, and observe that $c(w_{n-1}) = p_{n-1}$. Repeat this process for a total of $n$ times. Then $w_0 \in N_i(w_1) \cap E^0_p(S) \subseteq S$ and $w_1 \cdots w_n$ is a walk from a vertex in $S$ to a vertex in $T$ such that the colours of the vertices it visits give precisely the program $p$.
2. If $p$ does not partially halt then for every $s \in S$, $E^0_p(s) \neq \emptyset$ and $E_p(s) \subseteq T$.
   So $p$ is a feasible $\{s\}, T$-program, and hence item 1 applies.
3. If $p$ is exact, $E_p(S) = T$ and the proof of item 1 also gives this stronger statement.

Definition 6 (Cover). For $A, B \subseteq V$ we say that the vertices $A$ cover $B$ by $c$ iff $C_c(N_o(A)) \supseteq B$.

Definition 7 (Injection). For $\emptyset \neq A, B \subseteq V$ we say that the vertices $A$ inject $B$ by $c$ iff $\emptyset \neq C_c(N_o(A)) \subseteq B$. If that is the case, we call $A$ a $c$-injection into $B$.

Definition 8 (Spanning). We say that $A$ outspans $B$ by $c$ iff $C_c(N_o(A)) \setminus B \neq \emptyset$, and that $A$ spans $B$ by $c$ iff $A$ covers $B$ by $c$ but does not outspan $B$ by $c$.

Notice that $A$ $c$-injects $B$ iff $A$ does not $c$-outspan $B$ and $A$ is not a $c$-halting point.

Lemma 3 (Cover-Inject Behaviour of Intermediate Endpoints). For any program $p$ decomposed as $\pi \sigma \delta \alpha$, $E_\pi(S)$ spans $E_{\pi \sigma}(S)$ by $c$ but does not outspan $C_c(N_i(E_{\pi \sigma \delta \alpha}(S)))$.

Proof. Let $p : \pi \sigma \delta \alpha$ be a feasible program.

Since $E_{\pi \sigma \delta \alpha}(S) = C_c(N_o(E_\pi(S)))$, $E_\pi$ spans $E_{\pi \sigma}$ by $c$.

Further, since $E_{\pi \sigma \delta \alpha}(S) \subseteq N_o(E_{\pi \sigma}(S))$, $C_c(N_o(E_\pi(S))) \subseteq C_c(N_i(E_{\pi \sigma \delta \alpha}(S)))$, so $E_\pi$ does not outspan $C_c(N_i(E_{\pi \sigma \delta \alpha}(S)))$. 


Proposition 1. The problems of finding a feasible simple colour program and exact simple colour program are $\text{NP}$. 

Proof. Let $G, S, T$ and a candidate simple colour program $p$ be inputs.

To verify the the certificate $p$ one can simulate the actions of a set graph-walking agent. Starting at $S = E^0_p(S)$, the agent visits vertices $N_o(E^0_p(S)) \subseteq V$ and compare their colour to $c_1$. Searching for edges originating at a vertex, searching for vertex colour, and comparing vertex colours to $c_i$ is a polynomial-time operation. There are always at most $|V|$ vertices whose out-neighbours must be visited, and this operation is repeated for $1 \leq i \leq n$. Hence the verification of the certificate is a polynomial-time operation.

3.2 Viable Injection Basis Enumeration

We present a simple colour program mining algorithm constructing candidate programs from space of possibilities reduced by considering only those injections that cover “enough” vertices to have hope of reaching $T$. This is captured by the notion of pseudo-basis.

Definition 9 (Basis). We say that $B$ is a $c$-basis for $B$ iff $B$ spans $B$ by $c$ and $B$ is a minimal such set, i.e. for any $v \in B$, $B - v$ does not span $B$ by $c$.

Lemma 4. A is a $c$-spanning set for $B$ iff it contains a $c$-basis for $B$ and does not $c$-outspan $B$.

Proof. Let $A$ be a $c$-spanning set for $B$. Then it has a basis (remove vertices until none can be removed without making it a non-spanning set) and by definition does not outspan $B$.

Conversely, let $A$ be a set that contains a $c$-basis $B$ but does not outspan $B$. Since $B = C_c(N_o(B) \subseteq C_c(N_o(A))$, $A$ covers $B$. Hence $A$ $c$-spans $B$.

Definition 10 ($c$-Pseudo-Basis). We say that $B$ is a $c$-pseudo-basis for $(B, M)$ iff $B$ $c$-covers $B$, $B$ $c$-injects $M$, and $B$ is a minimal such set, i.e. for any $v \in B$, $B - v$ does not $c$-cover $B$.

Remark 1. Notice $B$ is a $c$-basis for $B$ if it is a $c$-pseudo basis for $(B, B)$.

The utility of pseudo-bases comes from being a type of injection into $M$ that covers all vertices of the out-neighbourhood designated as essential $(B)$. This allows us to remove from our search space those injections that do not cover sufficiently many of its out-neighbours to fully reach $T$. More specifically, our strategy is to

1. consider all bases $B^1$ for $T$,
2. consider all sets $B^2$ covering each $B^1$ but not outspanning the corresponding monochromatic in-neighbourhoods $M^1$ of $T$, i.e. the pseudo-bases for each $(B^1, M^1)$,
3. do the same for pairings \((B^i_j, M^i_j), i \geq 2\). If the candidate pseudo-basis \(B^i_j\) lies in \(S\) and \(S\) is in turn fully contained in the in-neighbourhood of the appropriate \(c\)-span of \(B^i_j\), a valid program has been found.

In Algorithm 1, let \(Q\) and \(Q_{\text{next}}\) be queues of triples drawn from \(\text{programs} \times \text{vertex-sets} \times \text{monochromatic vertex-sets}\), \(P\) be a set of \(\text{programs}\). Each triple \((p, B, M)\) in \(Q, Q_{\text{next}}\) represents a candidate program \(p\), from where to begin \(B\) in order to reach \(T\), and a monochromatic in-neighbourhood \(M \subseteq N_i(E_{p \leq i}(B))\).

\begin{algorithm}
\textbf{Algorithm 1: (VIBE) Viable Injection Basis Enumeration}
\begin{enumerate}
\item \(\text{Initialisation: } Q_{\text{next}}\) contains only \((\epsilon, T, T)\), \(Q\) and \(P\) are empty
\item \(\text{foreach } \ell \geq 0 \text{ such that } T \subseteq N_\ell^i(S) \text{ do}\)
\item \(Q \leftarrow Q_{\text{next}}\)
\item \(\text{empty } Q_{\text{next}}\)
\item \(\text{while } Q \text{ is not empty do}\)
\item \(\text{pop } (p, B, M) \text{ from } Q\)
\item \(n \leftarrow \text{length of } p\)
\item \(\text{if } n = \ell \text{ then}\)
\item \(\text{if } B \subseteq S \subseteq N_i(E_{p \leq i}(B)) \text{ then}\)
\item \(\text{add } p \text{ to } P\)
\item \(\text{end}\)
\item \(\text{push } (p, B, M) \text{ into } Q_{\text{next}}\)
\item \(\text{continue}\)
\item \(\text{end}\)
\item \(\text{foreach } c \in c(B) \text{ do}\)
\item \(N \leftarrow N_{\ell-n-1}^i(S) \cap N_i(B)\)
\item \(\text{foreach } d \in c(N) \text{ do}\)
\item \(\text{if } \ell \neq n+1 \text{ then}\)
\item \(N_d \leftarrow C_d(N)\)
\item \(\text{else}\)
\item \(N_d \leftarrow N\)
\item \(\text{end}\)
\item \(\text{push } (c, B, N_d) \text{ for } (B, M) \text{ do}\)
\item \(\text{push } (c, B, N_d) \text{ into } Q\)
\item \(\text{end}\)
\item \(\text{end}\)
\item \(\text{end}\)
\item \(\text{end}\)
\end{enumerate}
\end{algorithm}

**Proposition 2.** The following hold.
1. Algorithm 1 is correct in the sense that all programs in \(P\) are exact programs for \(S, T\).
2. Algorithm 1 is complete in the sense that whenever execution exists the loop closing at line 29, \(P\) contains all exact programs for \(S, T\) of length \(\ell\).

Proof. Observe that for every \((p, B, M)\) in \(Q\), \(B \subseteq M\), \(M\) is a monochromatic set, and the spans of \(B\) and \(M\) are the same.

1. First, we show inductively that every triple \((p, B, M)\) in \(Q\) is such that for any set \(B \subseteq A \subseteq M\), \(E_p(A) = T\).

   The base case (stemming from the initialisation of \(Q_{\text{next}}\)) is straightforward as \(E_c(T) = T\). Suppose \(p \neq \epsilon\). Then there is a colour \(c\) and a shorter program \(q\) such that \(p = cq\), as reaching line 25 is the only way for a non-empty program to enter \(Q\).

   So there is a triple \((q, B', M')\) and such that \(B\) is a pseudo-basis for \((B', M')\) (cf. line 24). Thus \(B' \subseteq E_c(B) \subseteq M'\) by Definition 10. But \(E_p(B) = E_q(E_c(B))\), so by the inductive hypothesis \(E_p(B) = T\).

   Now, every program \(p\) in \(P\) must have been added on line 10, so necessarily there is a triple \((p, B, M)\) that was once in \(Q\) s.t. \(B \subseteq S \subseteq N_i(E_{p \leq 1}(B))\).

   Since \(S \subseteq N_i(E_{p \leq 1}(B))\) we have \(E_{p \leq 1}(S) = E_{p \leq 1}(B)\), so

   \[E_p(S) = E_{p > 1}(E_{p \leq 1}(S)) = E_{p > 1}(E_{p \leq 1}(B)) = E_p(B) = T.\]

2. Let \(p\) be an exact program for \(S, T\).

   Focusing on the combinatorial loop of line 4 and ignoring the caching by \(Q_{\text{next}}\), we shall show inductively that for every prefix-suffix decomposition \(\pi \sigma = p\) of \(p\) there is a triple \((\sigma, B, M)\) s.t. \(B \subseteq E_\pi(S) \subseteq M\) that appears on \(Q\).

   For the base case with suffix \(\sigma = \epsilon\), \(p\) is an exact program, so \(T \subseteq E_p(S) \subseteq T\). This is the triple \((\epsilon, T, T)\) found in initialisation.

   Assume the inductive hypothesis holds for shorter suffixes and decompose \(p\) to \(\pi' \sigma\). Since by the inductive hypothesis there is a triple \((\sigma, B, M)\) s.t. \(B \subseteq E_{\pi'}(S) \subseteq M\), \(c \in E_\sigma(B)\) and \(E_{\pi'}(S) \subseteq N \neq \emptyset\) on line 17. Notice also that \(E_{\pi'}\) is further monochromatic whenever \(\pi' \neq \epsilon\), so by the branching on line 19 \(E_{\pi'} \subseteq N_d\). Further, as a consequence of Lemma 3, \(E_{\pi'}(S)\) covers \(E_{\pi' \sigma}\) but does not outspan \(M\), so \(E_{\pi'}(S)\) is a \(c\)-pseudo-basis for \((B, M)\), proving the inductive hypothesis.

   Now, whenever \(\ell = n\) execution will reach line 9 with various triples \((p, B, M)\).

   Decompose \(p = \epsilon p\). Then by the hereproven induction one of them will be such that \(B \subseteq E_c(S) = S \subseteq M\), and by the aboveproven induction also \(E_p(S) = T\). So \(p\) will be added to \(P\) on line 10. This completes the proof of completeness.

Algorithm 1 can be easily modified to also yield feasible programs. This can be done by altering line 24 to give \(c\)-injections into \(T\) if \(n = 0\), and execute the present behaviour otherwise. Alternatively and equivalently, one can just pre-compute all viable \(c\)-injections, their monochromatic peers, and initialize \(Q_{\text{next}}\) to their set in arbitrary order.

The completeness of Algorithm 1 combined with Lemma 3 highlight the role of existence of appropriate pseudo-basis as a necessary and sufficient condition for local feasible program existence.
4 Simple Tosit Programs

Extending on algorithms of Section 3 we now consider a more general setting where there are multiple features at each vertex, and the feature spaces admit a total order. See Figure 3-Right for an example.

Definition 11 (Criterion). Let \( c \) be a triple \((f, \omega, \nu)\) where \( f \) is a feature, \( \omega \) is one of the operators \(<, \leq, =, \geq, >\), and \( \nu \in F_f \). Then \( c \) is an atomic criterion. Inductively, \( c \) is a criterion if it is either an atomic criterion, a conjunction of criteria, or a disjunction of criteria.

Definition 12 (Simple Tosit Program). We say that \( p : c_1c_2\cdots c_n \) is a Simple Tosit Program (STP) if each \( c_i \) is a criterion.

Definition 13 (Criterion Satisfaction). We say that \( v \in V \) satisfies the atomic criterion \( c = (f, \omega, \nu) \) iff \( \phi_V(v)\omega\nu \). We then re-define \( C_c(A) \) in the context of STPs to mean the set of all vertices in \( A \) that satisfy \( c \). If \( c \) is a criterion, we say that \( v \in V \) satisfies \( c \) iff

- \( c \) is an atomic criterion and \( v \) satisfies \( c \) in the sense for atomic criteria, or
- \( c \) is a disjunction of criteria \( c_1 \lor \cdots \lor c_k \) and \( v \) satisfies at least one of \( c_1, \ldots, c_k \), or
- \( c \) is a conjunction of criteria \( c_1 \land \cdots \land c_k \) and \( v \) satisfies all of \( c_1, \ldots, c_k \).

All of the previous notions such as endpoints \( E_p() \), program feasibility, or program exactness, can be readily carried over from SCPs to STPs.

Proposition 3. The problems of finding a feasible simple toset program and exact simple toset program are \( \text{NP} \).

Proof. See the proof of Proposition 1, with the difference that instead of comparing colours we verify whether a criterion (cf. Definition 11) is satisfied, which too is a polynomial-time operation.

Definition 14 (Out-Neighbour Consistency). We say that \( v \in V \) is a vertex with out-neighbours consistent with respect to \( A, B \) (where \( A \cap B = \emptyset \) and \( A, B \subseteq N_o(v) \)) if there exists no pair of vertices \( x \in A, y \in B \) such that \( \phi_V(x) = \phi_V(y) \).

We say that \( S \subseteq V \) is a vertex set with out-neighbours consistent with respect to \( A, B \) (where \( A \cap B = \emptyset \) and \( A, B \subseteq N_o(S) \)) if there exists no pair of vertices \( x \in A, y \in B \) such that \( \phi_V(x) = \phi_V(y) \).

Definition 15 (Building Criteria). Let \( \text{ComputeCriterion}(B, M, E) \) be any algorithm that takes three vertex sets \( B, M, E \) as input and outputs a criterion such that every vertex in \( B \) is classified as “Yes”, “Included” or 1, every vertex in \( E \) is classified as “No”, “Excluded” or 0, and any vertex in \( M \) but not in \( B \) is classified as either.
Such algorithms exist, with CART [6] and C4.5 [20] being two notable examples. In our case it is further important that when the tree pruning phase of these algorithms is initiated, pruning is done only if it does not break the guarantees of Definition 15 or omitted altogether.

**Lemma 5 (Criterion existence for pseudo-bases with out-neighbours consistent).** Let $B, M, E$ be vertex sets such that $B \subseteq M, E \cap M = \emptyset$. If there exists a pseudo-basis $B$ with out-neighbours consistent for $B, M$ then a criterion for $B, M, E$ as per Definition 15 exists.

Proof. Let $b \in B, e \in E$. Since $B$ is a vertex set with out-neighbours consistent w.r.t $B, E$, $b, e$ cannot have the same features. Hence there exists a feature $f$ such that $\phi_V(b) \neq \phi_V(e)$. Thus, there exists a split $s_{b,e}$ on $f$ that separates $b, e$. A conjunction of these splits for all $b, e$ is a criterion for $B, M, E$ as per Definition 15.

If a criterion exists, then both CART and C4.5, if left unterminated, will eventually build a decision tree that achieves the perfect separation. Thus, either can be used as the `BuildCriterion` routine.

Our strategy to tackle STP mining is to find pseudo-bases with out-neighbours consistent for each step of a potential program, and then to find criteria (out-neighbourhood classifiers) that correspond to those pseudo-bases. Lemma 5 shows that once an appropriate pseudo-basis has been found, the criterion can be found thanks to the consistency.

Multiple approaches can be taken to implement this strategy. If getting a solution is the priority, one can perform a depth-first search of pseudo-bases, and the moment the first valid sequence of pseudo-bases encapsulating $S$ at the beginning and hitting exactly $T$ at the end is found, find the step criteria and terminate. Since by Lemma 5 we know that for pseudo-bases with out-neighbours consistent a criterion always exists, there is no utility in computing criteria on the while pseudo-bases are still being determined, as this process presents no benefit to the determination of pseudo-bases. For the sake of consistency with earlier sections we chose to perform a breadth-first search of our pseudo-bases instead.

In Algorithm 2, let $Q, Q_{\text{next}}$ be queues lists of triples drawn from $\text{vertex-sets} \times \text{vertex-sets} \times \mathbb{Z}$, $P$ be a set of programs. The subject of our study is Algorithm 2. Each list $\ell$ in $Q$ is represents a chain of pseudo-bases that might trace out a program path from $S$ to $T$. Every triple $(B, M, n)$ in $\ell$ and $Q_{\text{next}}$ represents from where to begin $B$ to reach $T$, the in-neighbourhood with out-neighbours consistent $B \subseteq M \subseteq N_i(N_o(B))$, and the saved distance $n$ from $B$ to $T$.

**Proposition 4.** The following hold.

1. Algorithm 2 is correct in the sense that all programs in $P$ are exact programs for $S, T$.
2. Algorithm 2 is complete in the sense that whenever execution exists the loop closing at line 30, $P$ contains all exact programs for $S, T$ of length $\ell$, up to criterion equivalence.
Algorithm 2: (BPF) Basis-Path-Finding

Initialisation: $Q_{\text{next}}$ contains only the singleton list $(T, T, 0)$, $Q$, $L$, $P$ are empty

1. for $\ell \geq 1$ such that $T \subseteq N^\ell_S$ do
   2. $Q \leftarrow Q_{\text{next}}$ and empty $Q_{\text{next}}$
   3. while $Q$ is not empty do
      4. pop the list $l$ from $Q$
      5. let $(B, M, m)$ be the head, $n$ the length of $l$
      6. if $n - 1 = \ell$ then
         7. if $B \subseteq S \subseteq M$ then
            8. add $l$ to $L$
         9. end
        10. push $l$ into $Q_{\text{next}}$
      11. continue
   12. $M' \leftarrow N_i(B) \cap N^{\ell-n}_S$
   13. remove from $M'$ vertices with out-neighbours inconsistent w.r.t. $B, N_o(M') \setminus M$
   14. foreach pseudo-basis $B' \subseteq M'$ for $(B, M)$ do
      15. push $(B', M', n)$ into $l$
   16. endforeach
   17. endforeach
   18. foreach list $l$ in $L$ do
      19. $p \leftarrow \epsilon$
      20. pop the head of $l$ and discard
      21. foreach element $(B, M, n)$ in $L$ do
         22. $c \leftarrow \text{ComputeCriterion}(B, M, N^{\ell-n}_S \setminus M)$
         23. $p \leftarrow cp$
      24. end
      25. add $p$ to $P$
   26. endforeach

Proof. The proposition is analogous with the Proposition 2, and as such analogous proofs can be constructed.

Briefly, for correctness, if a candidate list

$$\ell = (B_0, M_0, \ell + 1)(B_1, M_1, \ell) \cdots (B_\ell, M_\ell, 1)(T, T, 0)$$

has been added $L$, then it must have been the case that $S$ is a vertex set with out neighbours consistent spanning $B_1$ but not outspanning $M_1$. Inductively, it must have been the case that $B_k$ spans $B_{k+1}$ but does not outspan $M_{k+1}$. Now, the loop on line 22 ensures that at each step, the program always proceeds to a set of vertices $S_k$ such that $B_k \subseteq S_k \subseteq M_k$. Hence any program in $P$ is correct.
For completeness, just notice that following any \( p \in P \) from the end there is always a pseudo-basis \( B_k \subseteq E_{p_{\leq k}}(S) \) that spans \( B_{k+1} \) but (trivially) does not outspan \( E_{p_{k+1}}(S) \). So a valid chain of pseudo-bases exists, will be found and added to \( L \), and the corresponding chain of criteria logically equivalent to those of \( p \) (but not necessarily the same) will then be added to \( P \).

As in the discussion of Algorithm 1, Algorithm 2 can easily be modified to search for feasible and not just exact programs.

The runtime of the algorithms we propose depends greatly on the network. In the worst case – on a fully connected graph, our algorithms perform a total enumeration of all possible programs. However, real-world labelled graph datasets tend to contain significant amounts of pattern structure, suggesting performance far better than that of the worst case.

5 Conclusion

We have pointed at the previously unaddressed problem of characterising relationships between groups of records in a database in terms of their long-distance connections within the database graph. We have identified the problem of graph-walking program mining as a simple case of this wider challenge, and investigated simple colour and totally-ordered set program mining. We addressed them by giving the Viable Injection Basis Enumeration and Basis-Path-Finding algorithms, and proved their correctness and completeness.

The main observation allowing us to sharply limit the search space is that the set of vertices through whom agent executing a simple program proceeds is bounded below by an appropriate basis and above by consistency with respect to out-vertices. The construct corresponding to these bounds in the process of mining is the criterion pseudo-basis, appearing as a necessary and sufficient condition on local existence of feasible programs. We have further shown that the problems of simple program mining are \( \text{NP} \).

We have hinted that more complex program structures can be employed in graph-walking programs, and that the programs do not need to be deterministic. While adding to the structure of graph-walking programs would likely hinder their interpretation as relationships between sets of vertices, we believe that our current work can be extended by considering probabilistic graph-walking programs, further expanding the utility of graph-walking programs in the context of network analysis and beyond.

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