SET MATRICES AND THE PATH/CYCLE PROBLEM

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ABSTRACT. Presentation of set matrices and demonstration of their efficiency as a tool using the path/cycle problem.

INTRODUCTION

Set matrices are matrices whose elements are sets. The matrices comprise abilities of data storing and processing. That makes them a promising combinatorial structure. To prove the concept, this work applies the matrices to the path/cycle problem, see [1, 2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 15, and many others]. The problem may be generalized as a problem to find all paths and all cycles of all length in form of vertex pairs (start, finish). That is a NP-hard problem because any of its solutions will include a solution of the Hamiltonian path/cycle problems [5]. This presentation uses set matrices to realize the following plan to solve the generalized problem: present the walk length dynamics with a generative grammar, but include in the grammar’s production rules some path/cycle filters in order to deplete the resulting walk language to the indication of path/cycle’s presence/absence, only.

The design’s idea may be traced back through the dynamic programming, the Ramsey theory, the formal language theory, and to the icosian calculus [16, 17]. Realization of the design requires to maintain a set of visited/unvisited vertices and to use that set as a filter in production of the next generation of walks. Set matrices satisfy the requirements. Sorting/factoring of the visited/unvisited vertices into vertex pairs (start, finish) creates a set matrix analog of the adjacency matrix. And the especially designed powers of the set matrix create an analytic path/cycle filter. The path/cycle language’s specification gets a realization in form of the easy-to-check properties of the elements of the adjacency set matrix’s powers.

The factoring of the set of visited/unvisited vertices into vertex pairs (start, finish) may be seen as a walk coloring where colors are the factor-sets. Then, the family of algorithms realizing the design can be parametrized with the following four extreme strategies: to color the walks with sets of the visited/unvisited start/finish vertices. Work [18] describes a walk coloring with the unvisited vertices. This work deploys walk coloring with the visited vertices. The worst case for the algorithms is a complete graph. For a complete graph with \( n \) vertices, the algorithms perform \( n \) iterations and, on each of these iterations, \( O(n^2) \)-time processing for each of the \( n^2 \) vertex pairs. That totals in time \( O(n^5) \) needed for the algorithms to find all paths and all cycles of all length in the form of vertex pairs (start, finish).

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1. Set Matrices

Let $V$ be a universal set. Set matrices are matrices whose elements are sets. All set operations can be defined on the set matrices. For example, if $A = (a_{ij})$ and $B = (b_{ij})$ are set matrices of the appropriate sizes, then

Compliment:

$$A^c = (a^c_{ij});$$

Join:

$$A \cup B = (a_{ij} \cup b_{ij});$$

Intersection:

$$A \cap B = (a_{ij} \cap b_{ij}),$$

Multiplication:

$$AB = \left( \bigcup_{\mu} a_{i\mu} \times b_{\mu j} \right),$$

- where “$\times$” is Cartesian product of sets, etc. More operations can be found in [13].

For the path/cycle problem, the most interesting operation is the set matrix multiplication. The operation can be redefined in different ways. In this presentation, let us use the following multiplication: for set matrices $A = (a_{ij})_{n \times m}$ and $B = (b_{ij})_{m \times k}$, product $AB$ is the $n \times k$ set matrix whose elements are

$$\begin{align*}
(AB)_{ij} &= \left\{ \bigcap_{\mu=1}^{n} a_{i\mu} \cup b_{\mu j}, \quad i \neq j \right\} \\
&\bigcup \left\{ V, \quad i = j \right\}
\end{align*}$$

(1.1)

Here and further, symbol $(X)_{ij}$ means $(i, j)$-element of matrix $X$.

Formula (1.1) is the formula of the number matrix multiplication, except “$+$” is replaced with “$\cap$”, “$\times$” is replaced with “$\cup$”, and some special cases are taken care of. The special cases treatment makes multiplication (1.1) a non-associative operation:

**Exercise 1.1.**

$$\begin{align*}
\left[ \begin{pmatrix} \emptyset & \emptyset \\ \emptyset & \{a\} \end{pmatrix} \right] \left[ \begin{pmatrix} \emptyset & \emptyset \\ \emptyset & \{b\} \end{pmatrix} \right] &= \left[ \begin{pmatrix} V & \emptyset \\ \emptyset & V \end{pmatrix} \right] \left[ \begin{pmatrix} \emptyset & \{c\} \\ \emptyset & \emptyset \end{pmatrix} \right] = \left[ \begin{pmatrix} V & \emptyset \\ \emptyset & V \end{pmatrix} \right], \\
\left[ \begin{pmatrix} \emptyset & \emptyset \\ \emptyset & \{a\} \end{pmatrix} \right] \left[ \begin{pmatrix} \emptyset & \emptyset \\ \emptyset & \{b\} \end{pmatrix} \right] &= \left[ \begin{pmatrix} \emptyset & \emptyset \\ \emptyset & \{a\} \end{pmatrix} \right] \left[ \begin{pmatrix} V & \emptyset \\ \emptyset & V \end{pmatrix} \right] = \left[ \begin{pmatrix} V & \emptyset \\ \emptyset & V \end{pmatrix} \right].
\end{align*}$$

Let $A$ be a square set matrix. The following iterations define the left and right $k$-th powers of the matrix, $k \geq 1$:

$$R^1 = T^1 = A$$

$$\begin{align*}
(R^{k+1})_{ij} &= \left\{ \bigcap_{\mu} (R^1)_{i\mu} \cup (R^k)_{\mu j}, \quad i \neq j \right\} \\
&\bigcup \left\{ V, \quad i = j \right\}
\end{align*}$$

(1.2)

$$\begin{align*}
(T^{k+1})_{ij} &= \left\{ \bigcap_{\mu} (T^k)_{i\mu} \cup (T^1)_{\mu j}, \quad i \neq j \right\} \\
&\bigcup \left\{ V, \quad i = j \right\}
\end{align*}$$

Let us estimate the computational complexity of formula (1.2). Multiplication (1.1) requires $O(n^3)$ operations “$\cap$” and “$\cup$”. Thus, if $t_{k-1}$ is the number of operations needed to calculate $(k - 1)$-th power, then the number of operations needed to calculate $k$-th power is

$$t_k = t_{k-1} + O(n^3) = O(kn^3).$$
Thus, the time needed to calculate $k$-th power can be estimated as
\begin{equation}
O(kn^3|V|).
\end{equation}

The list of set matrix operations and properties can be continued. But let us start and demonstrate some benefits.

2. Path problem

Let $g = (V, A)$ be a given (multi) digraph: $V$ is the vertex set and $A$ is the arc set of $g$. Let the vertex set $V$ be the universal set. Let’s enumerate it:

$$V = \{v_1, v_2, \ldots, v_n\}.$$ 

Let $G$ be the adjacency matrix of $g$ appropriate to this enumeration. Then the positive elements of powers of $G$ indicate the presence of walks: vertex pairs (start, finish) of $k$-walks are indexes of positive elements of matrix $G^k$. The powers of this adjacency matrix can detect a shortest path but not a path of a specific length. Also, calculating the powers involves magnitudes of

$$O(n^{k-1}(\max_{ij}(G)_{ij})^k).$$

Although, the last problem can be solved with the Boolean adjacency matrices [13].

Let $T$ be the following set matrix of size $n \times n$:

\begin{equation}
(T)_{ij} = \begin{cases} 
\{v_j\}, & (G)_{ij} > 0 \land i \neq j \\
V, & (G)_{ij} \leq 0 \lor i = j 
\end{cases}
\end{equation}

Matrix $T$ may be seen as an adjacency set matrix. Let $T^k$ be the $k$-th right power of matrix $T$, defined with formulas 1.2.

**Lemma 2.1.** In digraph $g$ for $k < n$, if set $(T^k)_{ij} \neq V$, then the set is equal to

$$(T^k)_{ij} = \bigcap_{\mu} \{v_{\mu_1}, v_{\mu_2}, \ldots, v_{\mu_{k-1}}, v_{\mu_k}\},$$

where the intersection is taken over all ordered number samples

$$\mu = (\mu_1, \mu_2, \ldots, \mu_{k-1}, \mu_k)$$

which satisfy the following constrains:

\begin{align*}
1 \leq \mu_x &\leq n, \ x = 1, 2, \ldots, k \\
(v_i, v_{\mu_i}) &\in A, \ (v_{\mu_x}, v_{\mu_{x+1}}) \in A, \ x = 1, 2, \ldots, k - 1 \\
\mu_k &\neq j \\
\mu_x &\neq \mu_y \iff x \neq y
\end{align*}

- where set $A$ is the arc set of digraph $g$.

**Proof.** Due to definitions 1.2 and 2.1 if

$$(T^k)_{ij} = \bigcap_{\mu} (T^1)_{\mu_1} \cup (T^1)_{\mu_1, \mu_2} \cup \ldots \cup (T^1)_{\mu_{k-2}, \mu_{k-1}} \cup (T^1)_{\mu_{k-1}, \mu_k} \neq V,$$

then there are number samples $\mu = (\mu_1, \mu_2, \ldots, \mu_{k-1}, \mu_k)$ which satisfy the first four constrains, and

\begin{equation}
(T^k)_{ij} = \bigcap_{\mu} \{v_{\mu_1}\} \cup \{v_{\mu_2}\} \cup \ldots \cup \{v_{\mu_{k-1}}\} \cup \{v_{\mu_k}\},
\end{equation}
where the intersection is taken over all those number samples. Proving the last constrain will prove the lemma. To do so, let's use mathematical induction over \( k \).

For \( k = 1 \), due to definitions 1.2 and 2.1, \((T^1)_{ij} \neq V\) if there are arcs from vertex \( v_i \) into vertex \( v_j \) and the arcs are not loops \((i \neq j)\). Then, \((T^1)_{ij} = \{v_j\}\) and \((v_i, v_j) \in A\). Thus, the lemma holds for \( k = 1 \).

Because of an irregularity in the powers definition, the induction has to start from \( k = 2 \). In this case, due to definitions 1.2 and 2.1, if \((T^k)_{ij} = \bigcap \gamma (T^1)_{i\gamma} \cup (T^1)_{\gamma j} \neq V\), then there are such indexes \( \gamma \) that \((T^k)_{ij} = \bigcap i \neq \gamma, \gamma \neq j, i \neq j, (v_i, v_{\gamma}) \in A, (v_{\gamma}, v_j) \in A\). Thus, the lemma holds for \( k = 2 \).

Let's assume that the lemma holds for all \( k \leq m - 1 < n - 1 \), and let \((T^m)_{ij} \neq V\). Then, due to decomposition 2.2, 
\[
(T^m)_{ij} = \bigcap_{\mu} \{v_{\mu_1}\} \cup \{v_{\mu_2}\} \cup \ldots \cup \{v_{\mu_{m-1}}\} \cup \{v_{\mu_m}\} \neq V,
\]
then there are such indexes \( \gamma \) that 
\[
(T^k)_{ij} = \bigcap_{i \neq \gamma, \gamma \neq j, i \neq j, (v_i, v_{\gamma}) \in A, (v_{\gamma}, v_j) \in A}\{v_{\gamma}, v_j\},
\]
where \( A \) is the arc set of digraph \( g \). Thus, the lemma holds for \( k = 2 \).

Let's assume that the lemma holds for all \( k \leq m - 1 < n - 1 \), and let \((T^m)_{ij} \neq V\). Then, due to decomposition 2.2, for any of such number samples \( \mu \), the following holds:
\[
(T^{m-1})_{i\mu_{m-1}} \subseteq \{v_{\mu_1}\} \cup \{v_{\mu_2}\} \cup \ldots \cup \{v_{\mu_{m-1}}\} \subseteq Z \neq V,
\]
and
\[
(T^{m-1})_{\mu_1,\mu_{m-1}} \subseteq \{v_{\mu_2}\} \cup \{v_{\mu_2}\} \cup \ldots \cup \{v_{\mu_{m-1}}\} \subseteq Z \neq V.
\]
Then, due to the induction hypothesis, both number samples
\[
(\mu_1, \mu_2, \ldots, \mu_{m-2}, \mu_{m-1})
\]
and
\[
(\mu_2, \mu_3, \ldots, \mu_{m-1}, \mu_m)
\]
satisfy all five constrains. Particularly,
\[
\mu_x \neq \mu_y, \Leftrightarrow x \neq y, x, y = 1, 2, \ldots, m - 1;
\]
\[
\mu_x \neq \mu_y, \Leftrightarrow x \neq y, x, y = 2, 3, \ldots, m;
\]
and, due to the third constrain for \((T^{m-1})_{\mu_1,\mu_m} \neq V\),
\[
\mu_1 \neq \mu_m = j.
\]
Thus, the whole number sample \( \mu \) satisfies the fifth constrain. That concludes the induction and proves the lemma for all \( k < n \).

Lemma 2.1 allows the following interpretation:

**Lemma 2.2.** In digraph \( g \), if \((T^k)_{ij} \neq V\), then there is a \( k \)-path from vertex \( v_i \) into vertex \( v_j \).

**Proof.** The constrains in lemma 2.1 are the definition of a path from \( v_i \) into \( v_j \).
Lemmas 2.1 and 2.2 show that matrices $T^k$ collect the vertex-bridges. That may be interesting for the graph toughness theory [6, 15].

**Lemma 2.3.** In digraph $g$, if there is a $k$-path from vertex $v_i$ into vertex $v_j$ then $(T^k)_{ij} \neq V$.

**Proof.** Let the following vertices constitute a $k$-path from vertex $v_i$ into vertex $v_j$:

$$v_{\mu_1}=i, v_{\mu_2}, \ldots, v_{\mu_{k+1}}=j.$$ 

Indexes of these vertices satisfy the constrains in lemma 2.1. Then, due to definitions 1.2 and 2.1,

$$(T^k)_{ij} = \bigcap_{\mu} (T^1)_{i\mu_1} \cup (T^1)_{\mu_1\mu_2} \cup \ldots \cup (T^1)_{\mu_{k-2}\mu_{k-1}} \cup (T^1)_{\mu_{k-1}\mu_k} \subseteq \{v_i\} \cup \{v_{\mu_2}\} \cup \ldots \cup \{v_{\mu_k}\} \cup \{v_{\mu_{k+1}}\} \subseteq V - \{v_i\} \neq V.$$ 

□

**Theorem 2.4.** In digraph $g$ for $k \geq 1$, there are $k$-paths from vertex $v_i$ into vertex $v_j$ iff $(T^k)_{ij} \neq V$.

**Proof.** The theorem aggregates lemmas 2.2 and 2.3. Let us notice that case $k \geq n$ is covered by lemmas 2.1 and 2.3:

$$k \geq n \Rightarrow T^k = (V)_{n\times n}.$$ 

□

Estimation 1.3 shows the computational complexity to detect the $k$-paths with theorem 2.3. Particularly, when $k = n - 1$, the theorem detects the existence or absence of Hamiltonian paths in time $O(n^5)$.

All the results can be repeated with the left powers of matrix $T$. Also, definition 2.4 uses the arc finish vertices. Obviously, the results can be repeated with the start vertices using the following set matrix instead of matrix 2.1

$$(R)_{ij} = \begin{cases} \{v_i\}, & (G)_{ij} > 0 \land i \neq j \\ V, & (G)_{ij} \leq 0 \lor i = j \end{cases}$$

Colorings 2.1 and 2.3 cover two of the four extreme strategies of walk coloring: to color walks with the visited start/finish vertices. Another two extreme strategies are discussed in [18]. They produce the same results but in terms of the compliment sets.

3. Cycle problem

Obviously, the solution of the path problem described in section 2 solves the cycle problem, as well. Let us formalize that analytically.

Let’s define another set matrix multiplication: if $A$ and $B$ are set matrices of appropriate sizes, then

$$(AB)_{ij} = \begin{cases} \bigcap_{\nu} (A)_{i\nu} \cup (B)_{\nu j}, & i = j \\ V, & i \neq j \end{cases}$$

$$(3.1)$$
And let us define the following walk coloring:

$$(S)_{ij} = \begin{cases} \{\text{"Loop"}\}, & (G)_{ij} > 0 \land i = j \\ V, & (G)_{ij} \leq 0 \lor i \neq j \end{cases}$$

(3.2)

$S^1 = S$, $S^{k+1} = T^k R^1$, $k \geq 1$,

- where set matrices $T^k$ and $R^1$ were defined in section 2, and matrix multiplication $3.1$ is used.

**Theorem 3.1.** In digraph $g$ for $k \geq 1$, there are $k$-cycles attached to vertex $v_i$ iff

$$(S^k)_{ii} \neq V.$$ 

**Proof.** Case when $k = 1$ is obvious. Let $k > 1$.

Necessity. Let a $k$-cycle be attached to vertex $v_i$, and let the cycle visit the following vertices in the order shown:

$v_{\mu_1} = i, v_{\mu_2}, \ldots, v_{\mu_k}, v_{\mu_{k+1}} = i.$

Then, the last $k$ vertices in the row constitute a $(k-1)$-path from $v_{\mu_2}$ into $v_i$. Thus, due to lemma 2.1 and theorem 2.4,

$v_i \in (T^{k-1})_{\mu_2 i} \neq V.$

On the other hand, due to definition 2.3,

$$(R^1)_{i\mu_2} = \{v_1\} \neq V.$$ 

Thus, due to definition 3.1,

$$(S^k)_{ii} = ((T^{k-1})_{\mu_2 i} \cup \{v_i\}) \cap \ldots \subseteq (T^{k-1})_{\mu_2 i} \cup \{v_i\} = (T^{k-1})_{\mu_2 i} \neq V.$$ 

Sufficiency. Let

$$(S^k)_{ii} = \bigcap_{\nu}(T^{k-1})_{i\nu} \cup (R^1)_{i\nu} \neq V.$$ 

Then, there is such number $\nu$ that

$$(T^{k-1})_{i\nu} \cup (R^1)_{i\nu} \neq V.$$ 

Then, due to theorem 2.3 there is a $(k - 1)$-path from $v_i$ into $v_\nu$; and, due to definition 2.3 there is an arc from $v_\nu$ into $v_i$. The path and arc create a $k$-cycle attached to $v_i$. □

**Estimation 1.3** gives the computational complexity of theorem 3.1. Particularly, when $k = n$, the theorem detects the existence/absence of Hamiltonian cycles in time $O(n^5)$. But some simplifications are possible. The existence/absence of Hamiltonian cycles can be detected by only calculating any one string of matrix $T^{n-1}$. That reduces the time needed to solve the Hamiltonian cycle problem to $O(n^4)$. 


Conclusion

The paper presented set matrices as an efficient tool for solving the combinatorial problems. The matrices were used to solve the path/cycle problem in polynomial time:

- **k-path**: Calculate set matrix $T^k$ with formulas 2.1 and 1.2. Use theorem 2.3 to detect all $k$-paths in form vertex pair (start, finish);

- **k-cycle**: Calculate set matrix $S^k$ with formulas 2.1, 1.2, 2.3, 3.1, and 3.2. Use theorem 3.1 to detect all vertices which have a $k$-cycle attached.

Boolean property “It is equal to the vertex set” of the elements of matrices $T^k$ and $S^k$ fulfill the path/cycle language’s specification: indicate the presence/absence of paths/cycles. For a graph with $n$ vertices, it will take $O(n^5)$-time to write down the whole language in form of $O(n)$ matrices of size $n \times n$ filled with 1 and 0: 1 will mean the existence of appropriate paths/cycles and 0 will mean their absence.

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