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Algorithms for NP-hard problems (CS492)
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1 Matrix Tree Theorem

Let $G = (V, E)$ be a loopless (undirected) graph on n vertices with $V = \{v_1, \dots, v_n\}$. We identify the vertex set V with $[n]$, referring to vertex v_i by i. Fix an arbitrary ordering σ on the vertex set of a graph G. Let A_G be the adjacency matrix of G and D_G be the n by n diagonal matrix such that i-th diagonal entry of D_G equals $deg(i)$. In both A_G and D_G, the rows and columns are ordered with respect to the fixed ordering σ.

The *Laplacian* L_G of G is defined as $D_G - A_G$. We prove the next theorem, called Matrix Tree Theorem (or often called Kirchhoff's theorem), which relates the number of spanning trees of G with the determinant of L_{G-v_n}. Here the choice of v_n is arbitrary and any choice of a vertex G works.

Theorem 1. *Let G be a connected graph and v_n be a vertex of G. Then the number of spanning trees of G equals the determinant of L_{G-v_n}, the Laplacian of $G - v_n$.*

We begin with the observation that instead of a spanning tree, we can equivalently count the number of trees rooted at a fixed vertex, say v_n. A function $f : [n-1] \to [n]$ is a *pseudo-forest mapping* (with respect to G and a fixed root v_n) if for every $i \in [n-1]$, the image $f(i)$ is a neighbor of vertex i in G. A *cyclic sequence (with respect to G)* is a sequence $i_1, \dots, i_k$ of distinct elements of $[n-1]$ such that $i_2 = N(i_1)$, $i_3 = N(i_2), \cdots, i_k = N(i_{k-1})$ and $i_1 = N(i_k)$. Two cyclic sequences are considered identical if one is obtained from the other by cyclic shift of the other. An easy way to understand cyclic sequence is that it either corresponds to an edge, or it corresponds to a cycle of $G - v_n$ with a consistent orientation on the edges of the cycle. A pseudo-forest mapping is said to *produce a cyclic sequence* $C = i_1, \dots, i_k$ if $f(i_j) = i_{j+1}$ for all $j \in [k-1]$ and $i_1 = f(i_k)$. A pseudo-forest mapping is *acyclic* if it does not produce any cyclic sequence.

An *f-graph* for a pseudo-forest mapping f is the directed graph on $[n]$ whose arc set is $\{(i, f(i) : i \in [n-1]\}$. Note that a cycle of pseudo-forest mapping f corresponds to a directed cycle in the f-graph, and any cycle of pseudo-forest mapping f has length at least two because G is loopless.

Observation 1. *There is one-to-one correspondence between the set of all spanning trees of G rooted at v_n and the set of all acyclic pseudo-forest mappings.*

Proof: For each acyclic pseudo-forest mapping f, the graph on the vertex set $[n]$ and with the edge set $\{(i, f(i) : i \in [n-1]\}$ is a spanning tree of G rooted at v_n. Conversely, for any spanning tree of G rooted at v_n, one can associate a pseudo-forest mapping f by setting $f(i)$ to be the parent of i in the rooted tree. $\square$

Let $\mathcal{C} = \{C_1, \dots, C_M\}$ be the collection of all cyclic sequences with respect to G. We define the universe U and the set A_ℓ for $\ell \in [M]$ as follows.

- U is the set of all pseudo-forest mappings.
- A_ℓ is the set of all pseudo-forest mappings each of which produces the cyclic sequence C_ℓ.

By Observation 1, the number of spanning trees rooted at v_n equals the number of all acyclic pseudo-forest mappings. As the set of all acyclic pseudo-forest mappings is $\bigcap_{\ell \in [M]} (U \setminus A_\ell)$, by the intersection version of Inclusion-Exclusion formula, the cardinality of it can be expressed as

$$(\star) \qquad |\bigcap_{\ell \in [M]} (U \setminus A_\ell)| = \sum_{X \subseteq [M]} (-1)^{|X|} |\bigcap_{\ell \in X} A_\ell|.$$

For $X \subseteq [M]$, let $\mathcal{C}_X \subseteq \mathcal{C}$ be the subcollection $\{C_i : i \in X\}$ of cyclic sequences. The next claim is essential.

Lemma 1. *For $X \subseteq [M]$, the following holds.*

$$|\bigcap_{\ell \in X} A_\ell| = \begin{cases} \prod_{i \notin \cup_{x \in X} C_x} deg(i) & \text{if the cyclic sequences in } \mathcal{C}_X \text{ are pairwise disjoint} \\ 0 & \text{otherwise.} \end{cases}$$

Proof: Notice that the collection of cyclic sequences produced by a pseudo-forest mapping f are pairwise disjoint, which implies the equality in the second case. Suppose the cyclic sequences in $\mathcal{C}_X$ are pairwise disjoint. Observe that pseudo-forest mapping f produces $\mathcal{C}_X$ if and only if only if f satisfies the following.

- if i appears in some cyclic sequence $C \in \mathcal{C}_X$, then $f(i)$ is the succeeding element of i on C, and
- i does not appear in any cyclic sequence of $\mathcal{C}_X$, then $f(i) \in N(i)$.

This implies that the number of pseudo-forest mappings producing $\mathcal{C}_X$ is exactly $\prod_{i \notin \cup \mathcal{C}_X} deg(i)$, where $\cup \mathcal{C}_X$ denotes the set $\bigcup_{C \in \mathcal{C}_X} C$. This completes the proof. $\square$

Let $X \subseteq [M]$ be (the indices of) a pairwise disjoint cyclic sequences of $\mathcal{C}$. We define a function π_X on $[n-1]$ as follows.

$$\pi_X(i) = \begin{cases} \text{the succeeding element of } i \text{ on } C & \text{if } i \in C \in \mathcal{C}_X \\ i & \text{otherwise.} \end{cases}$$

It is clear that π_X is a permutation on $[n-1]$ for every $X \subseteq [M]$ such that the cyclic sequences in $\mathcal{C}_X$ are pairwise disjoint. Conversely, every permutation π on $[n-1]$ produces a (possibly empty) set of pairwise disjoint cyclic sequences. This is summarized in the next observation.

Observation 2.

$$\{\pi_X : X \subseteq [M] \text{ and the cyclic sequences in } \mathcal{C}_X \text{ are pairwise disjoint}\} = S_{n-1}.$$

Note that for $X \subseteq [M]$ such that the cyclic sequences in $\mathcal{C}_X$ are pairwise disjoint, π_X is precisely the permutation whose cycle representation is $\mathcal{C}_X$. The next statement is a folklore.

Observation 3. *Let $X \subseteq [M]$ be such that the cyclic sequences in $\mathcal{C}_X$ are pairwise disjoint. We have* $\mathsf{sgn}(\pi_X) = (-1)^{\sum_{x \in X}(|C_x|-1)}$.

We are ready to rewrite $(\star)$:

$$
\begin{aligned}
|\bigcap_{\ell\in[M]}(U\setminus A_\ell)| &= \sum_{X\subseteq[M]}(-1)^{|X|}|\bigcap_{\ell\in X}A_\ell| \\
&= \sum_{\substack{X\subseteq[M]\\ \mathcal{C}_X \text{ pairwise disjoint}}}(-1)^{|X|}\prod_{i\notin\cup\mathcal{C}_X}deg(i) \qquad \because \text{Lemma 1} \\
&= \sum_{\substack{X\subseteq[M]\\ \mathcal{C}_X \text{ pairwise disjoint}}}(-1)^{\sum_{x\in X}(|C_x|-1)}\cdot(-1)^{\sum_{x\in X}|C_x|}\prod_{i\notin\cup\mathcal{C}_X}deg(i) \\
&= \sum_{\substack{X\subseteq[M]\\ \mathcal{C}_X \text{ pairwise disjoint}}}\mathsf{sgn}(\pi_X)\cdot\prod_{i\in\cup\mathcal{C}_X}(-1)\cdot\prod_{i\notin\cup\mathcal{C}_X}deg(i) \qquad \because \text{Observation 3} \\
&= \sum_{\pi\in S_{n-1}}\mathsf{sgn}(\pi)\cdot\prod_{i:\pi(i)\neq i}(-1)\cdot\prod_{i:\pi(i)=i}deg(i) \qquad \because \text{Observation 2} \\
&= \sum_{\pi\in S_{n-1}}\mathsf{sgn}(\pi)\cdot\prod_{i\in[n-1]}L_{i,\pi(i)},
\end{aligned}
$$

where L is the Laplacian of $G-v_n$.