Mathematics for Computer Science (30470023) Spring 2020

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1 Overview

To start up this lecture, we reviewed what is called NP-Complete problems and approximation algorithms for these problems, including Eulerian path approach to the DNA Assembly problem and Radio Frequency Confliction problem.

Today, two famous theorems will be introduced to show how the amazing power of linear algebra can be used in algorithm design.

2 (Kirchhoff's) Matrix Tree Theorem

The theorem is introduced by the problems of counting. We have recognized that Hamiltonian cycle problem is NP-Complete which is hard to solve. Further more, if we want to count the number of Hamiltonian cycles in a given graph G, this problem becomes extraordinarily hard, even much more difficult than just finding if such cycle exists. Also, other problems including counting the number of spanning tree will also be proposed in this lecture.

2.1 Preliminaries

Definition 2.1. A spanning tree T of a graph G is a subgraph of G which connects all vertices in G and is also a tree. Define $t(G) \equiv$ *number of spanning trees of* G. Note that $t(G) = 0$ if G is disconnected.

Proposition 2.2. (Matrix Tree Theorem) For any graph $G = (V, E)$, define the Laplacian matrix $L(G) = D - A$ where $D = diag(d_1, d_2, \ldots, d_{n-1}, d_n)$ is a diagonal matrix with $d_i = degree(v_i)$. And $A = (a_{ij})$ is adjacent matrix of G, in which

$$a_{ij} = \begin{cases} 1, & \text{if } \{i, j\} \in E, \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

Define $\hat{L}^{(i)}(G) = L(G)$ deleting i-th row and i-th column (the same as minor matrix defined in linear algebra). Then, $t(G) = \det(\hat{L}^{(i)}(G))$ for any $1 \leq i \leq n$. (Kirchhoff, 1847) $\diamondsuit$

Example 2.3 (Application on complete graphs). In addition, from Calay's Theorem covered in LPV, $t(K_n) = n^{n-2}$ where K_n is the complete graph on n vertices.

$$L(K_n)_{n\times n} = \begin{pmatrix} n-1 & -1 & -1 & \cdots & -1 \\ -1 & n-1 & -1 & \cdots & -1 \\ -1 & -1 & n-1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & n-1 \end{pmatrix}$$

$$\hat{L}^{(i)}(K_n)_{(n-1)\times(n-1)} = \begin{pmatrix} n-1 & -1 & -1 & \cdots & -1 \\ -1 & n-1 & -1 & \cdots & -1 \\ -1 & -1 & n-1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & n-1 \end{pmatrix}$$

From simple derivation, we get:

$$\det(\hat{L}^{(i)}(K_n)) = n^{n-2}$$

Thus checked the theorem in this special case,

$$t(K_n) = \det(\hat{L}^{(i)}(K_n)).$$

Definition 2.4. For graph $G = (V, E)$ where $|V| = n$ and $|E| = m$, $E = \{e_1, e_2, \ldots, e_m\}$, define $n \times m$ matrix B_G as follows:

$$B_G = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & -1 \end{pmatrix}$$

As shown in Figure 1, consider column i of matrix B_G, edge e_i connects vertex a with vertex b, then $(B_G)_{ai} = 1$ and $(B_G)_{bi} = -1$ (swapping 1 with -1 in this column is also okay), the other items in column i all equal 0.

Lemma 2.5. Laplacian matrix $L_G = B_G B_G^T$ ♢

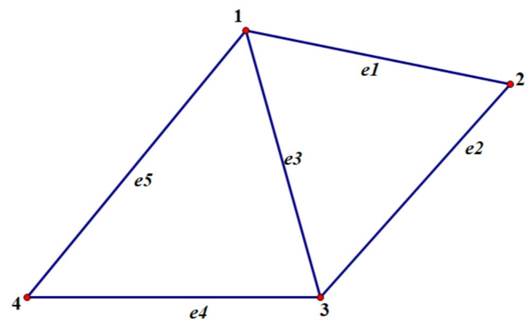


Figure 1: Example for B_G

Proof. From the definition of Laplacian matrix $L_G = D - A$. $(L_G)_{ii} = d_i$ by definition, and $(B_G B_G^T)_{ii} = \sum_{j=1}^{m}(B_G)_{ij}(B_G^T)_{ji} = \sum_{j=1}^{m}(B_G)_{ij}^2 = d_i$. So $(L_G)_{ii} = (B_G B_G^T)_{ii}$. In addition,

$$(B_G B_G^T)_{ij} = \sum_{k=1}^{m}(B_G)_{ik}(B_G^T)_{kj} = \sum_{k=1}^{m}(B_G)_{ik}(B_G)_{jk} = \begin{cases} -1, & \text{if } \{i,j\} \in E, \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

This is because the inner product will get -1 when e_k connects i and j, and get 0 otherwise. From definition of L_G, $(L_G)_{ij} = (B_G B_G^T)_{ij}$. Thus, proved the lemma. □

Lemma 2.6. Minor Laplacian matrix $\hat{L_G}^{(i)} = \hat{B_G}^{(i)}(\hat{B_G}^{(i)})^T$, where $\hat{B_G}^{(i)}$ is an $(n-1)\times m$ matrix gotten from erasing the i-th row from B_G. ♢

Proof. This lemma can be simply deduced from the previous lemma by straight calculation. □

Lemma 2.7.

$$\det(\hat{B}^{(i)}_{j_1 j_2 \dots j_{n-1}}) = \begin{cases} \pm 1, & \text{if } e_{j_1}, e_{j_2}, \dots, e_{j_{n-1}} \text{ forms a spanning tree of } G, \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

♢

Proof. If $e_{j_1}, e_{j_2}, \dots, e_{j_{n-1}}$ do not form a spanning tree, then there exists a cycle, say edges $f_1, f_2, \dots, f_k$ form a cycle. There exists an i with vertex i not in the cycle, the k column vectors of $\hat{B}^{(i)}_{j_1 j_2 \dots j_{n-1}}$ corresponding to $f_1, f_2, \dots, f_k$ are linear dependent. Thus, $\det(\hat{B}^{(i)}_{j_1 j_2 \dots j_{n-1}}) = 0$.

If $e_{j_1}, e_{j_2}, \dots, e_{j_{n-1}}$ form a spanning tree, then just consider the $(n-1)\times(n-1)$ matrix $\hat{B}^{(1)}_{j_1 j_2 \dots j_{n-1}}$. There exists a column in B_G whose first row is not equal to 0, say column j_k satisfies. Then, there is exactly one nonzero element in the column corresponding to j_i in $\hat{B}^{(1)}_{j_1 j_2 \dots j_{n-1}}$. Deleting both the row and column containing the nonzero element, we get a $(n-2)\times(n-2)$ matrix B', and $\det(\hat{B}^{(1)}_{j_1 j_2 \dots j_{n-1}}) = \pm\det(B')$. Let G' be the tree obtained from G by contracting the edge e to a single vertex, i.e., remove e and two ends of e contract to become one point. Then matrix B' can be derived by the same method as before, i.e., $B' = \hat{B_{G'}}^{(1)}_{k_1 k_2 \dots k_{n-2}}$. Similar to the above analysis, lemma is proved by mathematical induction on n. □

2.2 Cauchy-Binet Formula

Theorem 2.8. Let A be an $m \times n$ matrix and B an $n \times m$ matrix. Let $[n] = \{1, 2, 3, \ldots, n\}$, and $\binom{[n]}{m}$ be the set of all the subsets of size m in $[n]$. For $S \in \binom{[n]}{m}$, write $A_{[m],S}$ for the $m \times m$ matrix whose columns are the columns of A at indices from S, and $B_{S,[m]}$ for the $m \times m$ matrix whose rows are the rows of B at indices from S. Then we have

$$\det(AB) = \sum_{S \in \binom{[n]}{m}} \det(A_{[m],S}) \det(B_{S,[m]}) \tag{4}$$

$\diamondsuit$

Example 2.9. When $m = 1$, let $A = (a_1, a_2, \ldots, a_n), B = (b_1, b_2, \ldots, b_n)$. Then we have

$$\det(AB^T) = \sum_{j=1}^{m} a_j b_j \tag{5}$$

When $m = 2$, let $A = \begin{pmatrix} a_{11} & \ldots & a_{1n} \\ a_{21} & \ldots & a_{2n} \end{pmatrix}$, $B = \begin{pmatrix} b_{11} & \ldots & b_{1n} \\ b_{21} & \ldots & b_{2n} \end{pmatrix}$. Then we have

$$\det(AB^T) = \sum_{1 \le i < j \le n} \det \begin{pmatrix} a_{1i} & a_{1j} \\ a_{2i} & a_{2j} \end{pmatrix} \det \begin{pmatrix} b_{1i} & b_{1j} \\ b_{2i} & b_{2j} \end{pmatrix} \tag{6}$$

If $A = B$, then

$$\det(AA^T) = \sum_{i<j} \det \begin{pmatrix} a_{1i} & a_{1j} \\ a_{2i} & a_{2j} \end{pmatrix}^2 \tag{7}$$

Proof. Let A be an $m \times n$ matrix and B an $n \times m$ matrix ($m \le n$). The Weinstein–Aronszajn identity (sometimes attributed to Sylvester) is

$$\det(I_m + AB) = \det(I_n + BA) \tag{8}$$

The extension of it is

$$z^{n-m} \det(zI_m + AB) = \det(zI_n + BA) \tag{9}$$

There are many ways to prove this. Consider $(m+n) \times (m+n)$ matrix $C = \begin{pmatrix} I_m & -A \\ B & zI_n \end{pmatrix}, D = \begin{pmatrix} zI_m & -A \\ B & I_n \end{pmatrix}, E = \begin{pmatrix} zI_m & -zA \\ B & zI_n \end{pmatrix}$. Then we have

$$\det(C) = \det \begin{pmatrix} I_m & -A \\ B & zI_n \end{pmatrix} = \det \begin{pmatrix} I_m & 0 \\ B & zI_n + BA \end{pmatrix} = \det(zI_n + BA) \tag{10}$$

$$\det(D) = \det \begin{pmatrix} zI_m & -A \\ B & I_n \end{pmatrix} = \det \begin{pmatrix} zI_m + AB & 0 \\ B & I_n \end{pmatrix} = \det(zI_m + AB) \tag{11}$$

Since $z^m \det(C) = \det(E), z^n \det(D) = \det(E)$, we have $z^{n-m} \det(zI_m + AB) = \det(zI_n + BA)$.

Now consider the coefficient of z^{n-m} in the equation $z^{n-m} \det(zI_m + AB) = \det(zI_n + BA)$. The left side gives $\det(AB)$. Consider the right side. The coefficient of z^{n-m} is the sum of the determinants after deleting $n-m$ diagonal elements. Then the right side gives $\sum_{S \in \binom{[n]}{m}} \det((BA)_{S,S}) = \sum_{S \in \binom{[n]}{m}} \det(A_{[m],S}) \det(B_{S,[m]})$. Thus $\det(AB) = \sum_{S \in \binom{[n]}{m}} \det(A_{[m],S}) \det(B_{S,[m]})$. □

2.3 Proof of Matrix Tree Theorem

Theorem 2.10. (Matrix Tree Theorem, Kirchhoff, 1847) For any graph $G = (V, E)$, $t(G) = \det(\hat{L}^{(i)}(G))$ for any $1 \le i \le n$.

Remind that Laplacian matrix $L(G) = D - A$. $D = diag(d_1, d_2, \dots d, d_n)$ is a diagonal matrix with $d_i = degree(v_i)$, and $A = (a_{ij})$ is adjacent matrix of G, in which

$$a_{ij} = \begin{cases} 1, & \text{if } \{i, j\} \in E, \\ 0, & \text{otherwise.} \end{cases} \tag{12}$$

♢

Proof. According to Cauchy-Binet Formula and the lemmas proved in the previous subsection,

$$t(G) = \sum_{j_1 < \dots < j_{n-1}} (\det(\hat{B}^{(i)}_{j_1 j_2 \dots j_{n-1}})^2) = \det(\hat{B_G}^{(i)} (\hat{B_G}^{(i)})^T) = \det(\hat{L_G}^{(i)})$$

□

Corollary 2.11. L_G is symmetric, and also semi-definite. ♢

Proof. This corollary can be proved by:

$$x^T L_G x = x^T B_G B_G^T x = \|B_G^T x\|^2 \ge 0$$

□

Corollary 2.12. All eigenvalues of L_G are greater or equal to 0, and the smallest eigenvalue λ_1 is exactly 0. ♢

Proof. The first result comes directly from the previous corollary. In addition, notice that rank$(L_G) \le n-1$ because each row of L_G sums up to the same constant number 0, so the determination of L_G equals 0, thus proved the result. □

Corollary 2.13. $t(G) = \frac{1}{n} \lambda_2 \lambda_3 \dots \lambda_n$. ♢

Proof.

$$f(x) = \det(L_G - xI) = (-1)^n x(x - \lambda_2)(x - \lambda_3) \dots (x - \lambda_n)$$

Think of another expression of the coefficient of x in $f(x)$ and compare two expressions can then prove this corollary. The details are left to readers. □

Corollary 2.14. Graph G is disconnected if and only if $\lambda_2 = 0$. ♢

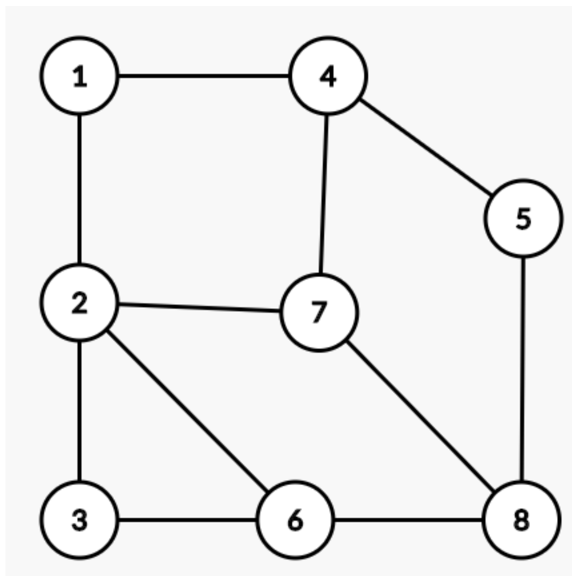
Proof. This result can be directed derived from the previous corollary. □

3 FKT Theorem

3.1 Preliminaries

Definition 3.1. Let $G = (V, E)$ and $M \subseteq E$. If $\forall e_1, e_2 \in M$, e_1, e_2 are disjoint, then M is called a matching. If M covers all the vertices, then M is called a perfect matching. ♢

Definition 3.2. If a graph G can be drawn on the plane in such a way that its edges intersect only at their endpoints, then G is called a planar graph. For example,



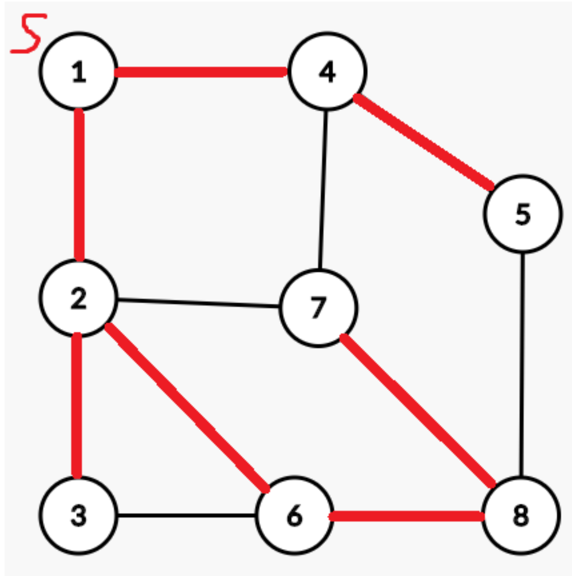
♢

3.2 FKT algorithm

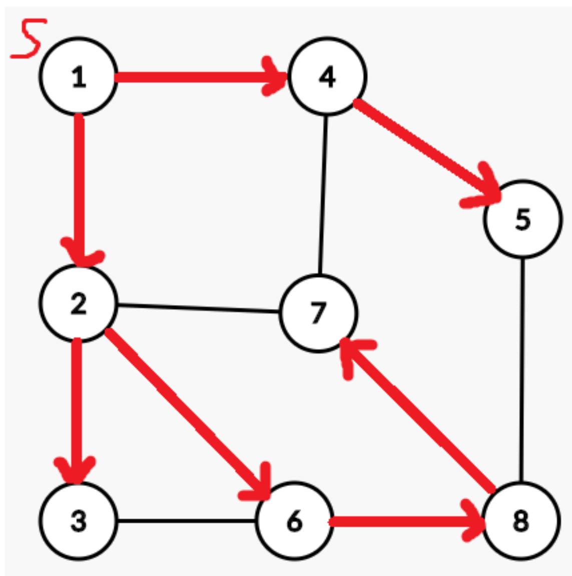
It's difficult to count the number of matchings in general graphs, even for planar graphs (they are #P-Complete exactly). But we have a algorithm to count the number of perfect matchings in planar graphs in polynomial time. It's called FKT algorithm, named after Fisher, Kasteleyn, and Temperley.

Now, we want to count the number of perfect matchings in G in 3.1.

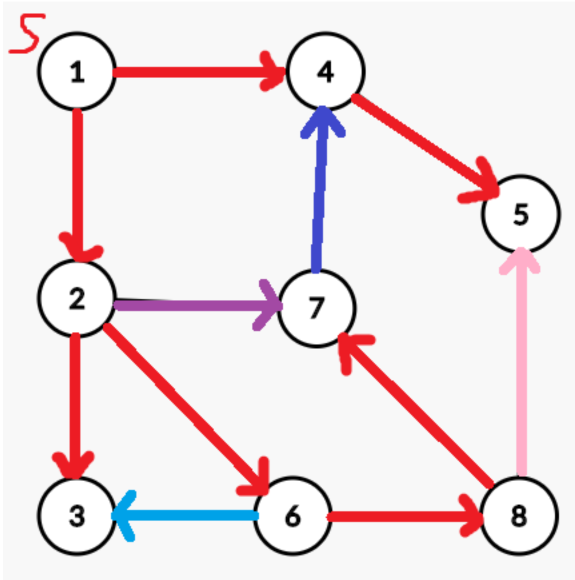
First, find a spanning tree in G.



Then, give an arbitrary orientation to each edge in the spanning tree.



Then, choose a direction (clockwise or counterclockwise). Choose counterclockwise. Orient the edges so that in every face, the number of edges oriented counterclockwise is odd. Since G is a planar graph, there's only one way to orient these edges.



Let A be $n \times n$ matrix, and $A_{ij} = \begin{cases} 1, & \text{if the direction of } (i,j) \text{ is } i \to j, \\ -1, & \text{if the direction of } (i,j) \text{ is } j \to i, \\ 0, & \text{if } i = j \end{cases}$. Then we have

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 & 1 & 0 \end{pmatrix} \tag{13}$$

The number of perfect matchings in G is $\sqrt{\det(A)} = 3$.