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ENUMERATION OF HAMILTONIAN CYCLES AND PATHS IN A GRAPH

C. J. LIU

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ABSTRACT. First, we show that the determinant of a given matrix can be expanded by its principal minors together with a set of arbitrary parameters. The enumeration of Hamiltonian cycles and paths in a graph is then carried out by an algebraic method. Three types of nonalgebraic representation are formulated. The first type is given in terms of the determinant and permanent of a parametrized adjacent matrix. The second type is presented by a determinantal function of multivariables, each variable having domain $\{0, 1\}$. Formulas of the third type are expressed by spanning trees of subgraphs. When applying the formulas to a complete multipartite graph, one can easily find the results.

INTRODUCTION

Let $\mathbf{A} = (a_{ij})$ be the adjacency matrix of graph G. The corresponding Kirchhoff matrix $\mathbf{K} = (k_{ij})$ is obtained from $\mathbf{A}$ by replacing in $-\mathbf{A}$ each diagonal entry by the degree of its corresponding vertex; i.e., the ith diagonal entry is identified with the degree of the ith vertex. It is well known that

$$\det \mathbf{K}(i|i) = \text{number of spanning trees of } G, \quad i = 1, \ldots, n \tag{1}$$

where $\mathbf{K}(i|i)$ is the ith principal submatrix of $\mathbf{K}$.

Let $C_{i(j)}$ be the set of graphs obtained from G by attaching edge $(v_i v_j)$ to each spanning tree of G. Denote by $C_i = \bigcup_j C_{i(j)}$. It is obvious that the collection of Hamiltonian cycles is a subset of C_i. Note that the cardinality of C_i is $k_{ii} \det \mathbf{K}(i|i)$. Let $\widehat{X} = \{\hat{x}_1, \ldots, \hat{x}_n\}$. Define multiplication for the elements of $\widehat{X}$ by

$$\hat{x}_i \hat{x}_j = \hat{x}_j \hat{x}_i, \qquad \hat{x}_i^2 = 0, \qquad i, j = 1, \ldots, n. \tag{2}$$

Let $\hat{k}_{ij} = k_{ij}\hat{x}_j$ and $\hat{k}_{ii} = -\sum_{j \neq i} \hat{k}_{ij}$. Then the number of Hamiltonian cycles

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H_c is given by the relation [1]

$$\left(\prod_{j=1}^{n} \hat{x}_j\right) H_c = \frac{1}{2}\hat{k}_{ii} \det \widehat{\mathbf{K}}(i|i), \qquad i = 1, \ldots, n. \tag{3}$$

The task here is to express (3) in a form free of any $\hat{x}_i$, $i = 1, \ldots, n$. The result also leads to the resolution of enumeration of Hamiltonian paths in a graph.

It is well known that the enumeration of Hamiltonian cycles and paths in a complete graph K_n and in a complete bipartite graph $K_{n_1 n_2}$ can only be found from *first combinatorial principles* [2]. One wonders if there exists a formula which can be used very efficiently to produce K_n and $K_{n_1 n_2}$. Recently, using Lagrangian methods, Goulden and Jackson have shown that H_c can be expressed in terms of the determinant and permanent of the adjacency matrix [3]. However, the formula of Goulden and Jackson determines neither K_n nor $K_{n_1 n_2}$ effectively. In this paper, using an algebraic method, we parametrize the adjacency matrix. The resulting formula also involves the determinant and permanent, but it can easily be applied to K_n and $K_{n_1 n_2}$. In addition, we eliminate the permanent from H_c and show that H_c can be represented by a determinantal function of multivariables, each variable with domain $\{0, 1\}$. Furthermore, we show that H_c can be written by number of spanning trees of subgraphs. Finally, we apply the formulas to a complete multipartite $K_{n_1 \cdots n_p}$.

The conditions $a_{ij} = a_{ji}$, $i, j = 1, \ldots, n$, are not required in this paper. All formulas can be extended to a digraph simply by multiplying H_c by 2.

Main theorem

Let $\mathbf{B} = (b_{ij})$ be an $n \times n$ matrix. Let $\mathbf{n} = \{1, \ldots, n\}$. Using the properties of (2), it is readily seen that

Lemma 1.

$$\prod_{i \in \mathbf{n}} \left(\sum_{j \in \mathbf{n}} b_{ij}\hat{x}_j\right) = \left(\prod_{i \in \mathbf{n}} \hat{x}_i\right) \operatorname{per} \mathbf{B} \tag{4}$$

where per $\mathbf{B}$ *is the permanent of* $\mathbf{B}$.

Let $\widehat{Y} = \{\hat{y}_1, \ldots, \hat{y}_n\}$. Define multiplication for the elements of $\widehat{Y}$ by

$$\hat{y}_i\hat{y}_j + \hat{y}_j\hat{y}_i = 0, \qquad i, j = 1, \ldots, n. \tag{5}$$

Then, it follows that

Lemma 2.

$$\prod_{i \in \mathbf{n}} \left(\sum_{j \in \mathbf{n}} b_{ij}\hat{y}_j\right) = \left(\prod_{i \in \mathbf{n}} \hat{y}_i\right) \det \mathbf{B}. \tag{6}$$

Note that all basic properties of determinants are direct consequences of Lemma 2.

Write

$$\sum_{j\in\mathbf{n}} b_{ij}\hat{y}_j = \sum_{j\in\mathbf{n}} b_{ij}^{(\lambda)}\hat{y}_j + (b_{ii}-\lambda_i)\hat{y}_i \tag{7}$$

where

$$b_{ii}^{(\lambda)} = \lambda_i, \qquad b_{ij}^{(\lambda)} = b_{ij}, \qquad i \neq j. \tag{8}$$

Let $\mathbf{B}^{(\lambda)} = (b_{ij}^{(\lambda)})$. By (6) and (7), it is straightforward to show the following result:

Theorem 1.

$$\det \mathbf{B} = \sum_{l=0}^{n}\sum_{I_l\subseteq\mathbf{n}}\prod_{i\in I_l}(b_{ii}-\lambda_i)\det \mathbf{B}^{(\lambda)}(I_l|I_l), \tag{9}$$

where $I_l = \{i_1, \ldots, i_l\}$ *and* $\mathbf{B}^{(\lambda)}(I_l|I_l)$ *is the principal submatrix obtained from* $\mathbf{B}^{(\lambda)}$ *by deleting its* $i_1, \ldots, i_l$ *rows and columns.*

Remark. Let $\mathbf{M}$ be an $n\times n$ matrix. The convention $\mathbf{M}(\mathbf{n}|\mathbf{n}) = 1$ has been used in (9) and hereafter.

Before proceeding with our discussion, we pause to note that Theorem 1 yields immediately a fundamental formula which can be used to compute the coefficients of a characteristic polynomial [4]:

Corollary. *Write* $\det(\mathbf{B}-x\mathbf{I}) = \sum_{l=0}^{n}(-1)^l b_l x^l$. *Then*

$$b_l = \sum_{I_l\subseteq\mathbf{n}} \det \mathbf{B}(I_l|I_l). \tag{10}$$

Let

$$\mathbf{K}(t, t_1, \ldots, t_n) = \begin{pmatrix} D_1 t & -a_{12}t_2 & \cdots & -a_{1n}t_n \\ -a_{21}t_1 & D_2 t & \cdots & -a_{2n}t_n \\ \vdots & \vdots & \vdots & \vdots \\ -a_{n1}t_1 & -a_{n2}t_2 & \cdots & D_n t \end{pmatrix}, \tag{11}$$

where

$$D_i = \sum_{j\in\mathbf{n}} a_{ij}t_j, \quad i = 1, \ldots, n. \tag{12}$$

Set

$$D(t_1, \ldots, t_n) = \tfrac{\partial}{\partial t}\det \mathbf{K}(t, t_1, \ldots, t_n)|_{t=1}.$$

Then

$$D(t_1, \ldots, t_n) = \sum_{i\in\mathbf{n}} D_i \det \mathbf{K}(t=1, t_1, \ldots, t_n; i|i), \tag{13}$$

where $\mathbf{K}(t = 1, t_1, \ldots, t_n; i|i)$ is the ith principal submatrix of $\mathbf{K}(t = 1, t_1, \ldots, t_n)$.

Theorem 1 leads to

$$(14)\quad \det \mathbf{K}(t, t_1, \ldots, t_n) = \sum_{I\subseteq \mathbf{n}} (-1)^{|I|} t^{n-|I|} \prod_{i\in I} t_i \prod_{j\in I} (D_j + \lambda_j t_j) \det \mathbf{A}^{(\lambda t)}(\bar{I}|\bar{I}).$$

Note that

$$(15)\quad \det \mathbf{K}(t=1, t_1, \ldots, t_n) = \sum_{I\subseteq \mathbf{n}} (-1)^{|I|} \prod_{i\in I} t_i \prod_{j\in I} (D_j + \lambda_j t_j) \det \mathbf{A}^{(\lambda)}(\bar{I}|\bar{I}) = 0.$$

It follows from (13), (14), and (15) that

$$(16)\qquad D(t_1, \ldots, t_n) = \sum_{I\subseteq \mathbf{n}} (-1)^{|I|-1} |I| \prod_{i\in I} t_i \prod_{j\in I} (D_j + \lambda_j t_j) \det \mathbf{A}^{(\lambda)}(\bar{I}|\bar{I}).$$

Let $t_i = \hat{x}_i$, $i = 1, \ldots, n$. Lemma 1 leads to

$$(17)\qquad D(\hat{x}_1, \ldots, \hat{x}_n) = \prod_{i\in \mathbf{n}} \hat{x}_i \sum_{I\subseteq \mathbf{n}} (-1)^{|I|-1} |I| \operatorname{per} \mathbf{A}^{(\lambda)}(I|I) \det \mathbf{A}^{(\lambda)}(\bar{I}|\bar{I}).$$

By (3), (13), and (17), we have the following result:

Theorem 2.

$$(18)\qquad H_c = \frac{1}{2n} \sum_{l=1}^{n} l(-1)^{l-1} A_l^{(\lambda)},$$

where

$$(19)\qquad A_l^{(\lambda)} = \sum_{I_l\subseteq \mathbf{n}} \operatorname{per} \mathbf{A}^{(\lambda)}(I_l|I_l) \det \mathbf{A}^{(\lambda)}(\bar{I}_l|\bar{I}_l),\ |I_l| = l.$$

It is worth noting that $A_l^{(\lambda)}$ of (19) is similar to the coefficients b_l of the characteristic polynomial of (10). It is well known in graph theory that the coefficients b_l can be expressed as a sum over certain subgraphs. It is interesting to see whether A_l^0, $\lambda = 0$, have the structural properties of a graph.

We may call (18) a parametric representation of H_c. In computation, the parameter λ_i plays very important roles. The choice of the parameter usually depends on the properties of the given graph. For a complete graph K_n, let $\lambda_i = 1$, $i = 1, \ldots, n$. It follows from (19) that

$$(20)\qquad A_l^{(1)} = \begin{cases} n!, & \text{if } l = 1 \\ 0, & \text{otherwise.} \end{cases}$$

By (18)

$$(21)\qquad H_c = \tfrac{1}{2}(n-1)!.$$

For a complete bipartite graph $K_{n_1 n_2}$, let $\lambda_i = 0$, $i = 1, \ldots, n$. By (19),

$$(22)\qquad A_l^0 = \begin{cases} -n_1! n_2! \delta_{n_1 n_2}, & \text{if } l = 2 \\ 0, & \text{otherwise .} \end{cases}$$

Theorem 2 leads to

$$H_c = \frac{1}{n_1 + n_2} n_1! n_2! \delta_{n_1 n_2}. \tag{23}$$

Now, we consider an asymmetrical approach. Theorem 1 leads to

$$\begin{aligned} (24) \quad & \det \mathbf{K}(t = 1, t_1, \ldots, t_n; l|l) \\ & = \sum_{I \subseteq \mathbf{n} - \{l\}} (-1)^{|I|} \prod_{i \in I} t_i \prod_{j \in I} (D_j + \lambda_j t_j) \det \mathbf{A}^{(\lambda)}(\bar{I} \cup \{l\} | \bar{I} \cup \{l\}). \end{aligned}$$

Let $t_i = \hat{x}_i$, $i = 1, \ldots, n$. Lemma 1 yields

$$\begin{aligned} (25) \quad & \left(\sum_{i \in \mathbf{n}} a_{l_i} \hat{x}_i \right) \det \mathbf{K}(t = 1, \hat{x}_1, \ldots, \hat{x}_n; l|l) \\ & = \left(\prod_{i \in \mathbf{n}} \hat{x}_i \right) \sum_{I \subseteq \mathbf{n} - \{l\}} (-1)^{|I|} \operatorname{per} \mathbf{A}^{(\lambda)}(I|I) \det \mathbf{A}^{(\lambda)}(\bar{I} \cup \{l\} | \bar{I} \cup \{l\}). \end{aligned}$$

By (3) and (25) we have the following asymmetrical result:

Theorem 3.

$$H_c = \frac{1}{2} \sum_{I \subseteq \mathbf{n} - \{l\}} (-1)^{|I|} \operatorname{per} \mathbf{A}^{(\lambda)}(I|I) \det \mathbf{A}^{(\lambda)}(\bar{I} \cup \{l\} | \bar{I} \cup \{l\}) \tag{26}$$

which reduces to Goulden–Jackson's formula when $\lambda_i = 0$, $i = 1, \ldots, n$ [4].

Note that Theorem 3 fails to provide the simple relations of (20) or (22) when the graph K_n or $K_{n_1 n_2}$ is treated.

In what follows, we shall formulate the enumeration of the Hamiltonian cycle in an alternative setting to the one (Theorem 2 or 3) that involves permanents.

It follows from (15) that

$$\det \mathbf{K}(t = 1, \hat{x}_1, \ldots, \hat{x}_n) = \prod_{i \in \mathbf{n}} \hat{x}_i \sum_{I \subseteq \mathbf{n}} (-1)^{|I|} \operatorname{per} \mathbf{A}^{(\lambda)}(I|I) \det \mathbf{A}^{(\lambda)}(\bar{I}|\bar{I}) = 0. \tag{27}$$

Theorem 2 and (27) lead to the result

$$H_c = \frac{1}{2n} \sum_{I \subseteq \mathbf{n}} (-1)^{n - |I|} |I| \operatorname{per} \mathbf{A}^{(\lambda)}(\bar{I}|\bar{I}) \det \mathbf{A}^{(\lambda)}(I|I). \tag{28}$$

To enumerate a permanent, we use Ryser's formula [5]

$$\operatorname{per} \mathbf{A}^{(\lambda)}(\bar{I}|\bar{I}) = \sum_{J \subseteq I} (-1)^{|J|} \prod_{j \in J} d_{j,J} \prod_{i \in I - J} (d_{i,J} + \lambda_i), \tag{29}$$

where

$$d_{i,I} = \sum_{j \in I} a_{ij}. \tag{30}$$

Note that (16) yields

$$D(t_1, \ldots, t_n) = \sum_{I \subseteq \mathbf{n}} (-1)^{n - |I|} |I| \prod_{i \in I} (D_i + \lambda_i t_i) \prod_{j \in I} t_j \det \mathbf{A}^{(\lambda)}(I|I). \tag{31}$$

By (28), (29), and (31), we have

Theorem 4.

$$H_c = \frac{1}{2n}\sum_{l=0}^{n}(-1)^l \Delta_l, \tag{32}$$

where

$$\Delta_l = \sum_{I_l \subseteq \mathbf{n}} D(t_1, \ldots, t_n)\Big|_{t_i = \begin{cases} 0, & \text{if } i \in I_l \\ 1, & \text{otherwise} \end{cases},\ i=1,\ldots,n.} \tag{33}$$

Similarly, we have the asymmetrical case:

Theorem 5.

$$H_c = \frac{1}{2}\sum_{l=0}^{n-1}(-1)^l \Delta_l^{(n)}, \tag{34}$$

where

(35)
$\Delta_l^{(n)} =$

$$\sum_{I_l \subseteq n-\{n\}} d_{n,I_l}\left[D_n \det \mathbf{K}(t=1, t_1, \ldots, t_n; n|n)\Big|_{t_i = \begin{cases} 0, & \text{if } i \in I_l \\ 1, & \text{otherwise} \end{cases},\ i=1,\ldots,n}\right].$$

It is interesting to note that Δ_l of (33) has the structural properties of a graph. Let G_I be the subgraph obtained from G by deleting all vertices $i \in I$. It is straightforward to show that

Theorem 6.

$$\Delta_l = \sum_{I_l \subseteq \mathbf{n}} \prod_{i \in I_l} d_{i,I_l} \sum_{j \in \overline{I}_l} d_{j,I_l} T_{I_l}, \tag{36}$$

where

$$d_{i,I} = (\textit{degree of vertex } i \textit{ in } G) - (\textit{degree of vertex } i \textit{ in } G_I) \tag{37}$$

and

$$T_I = \textit{number of spanning trees in } G_I. \tag{38}$$

Similarly, $\Delta_l^{(n)}$ of (37) may be written

Theorem 7.

$$\Delta_l^{(n)} = \sum_{I_l \subseteq \mathbf{n}} d_{n,I_l} \prod_{i \in I_l} d_{i,I_l} T_{I_l}. \tag{39}$$

We now encounter enumeration of Hamiltonian paths in G. Let G^+ be the graph obtained from G by adding an $(n+1)$th vertex together with an edge to each vertex of G. It is readily seen that each Hamiltonian path in G can be converted to one and only one Hamiltonian cycle in G^+; therefore we have

Theorem 8. *Let H_p be the number of Hamiltonian paths of a given graph. Then*

$$H_p \text{ in } G = H_c \text{ in } G^+. \tag{40}$$

Application. We consider here the applications of Theorem 6 and 7 to a complete multipartite graph $K_{n_1 \cdots n_p}$. It can be shown that the number of spanning trees of $K_{n_1 \cdots n_p}$ may be written

$$T = n^{p-2} \prod_{i=1}^{p} (n - n_i)^{n_i - 1} \tag{41}$$

where

$$n = n_1 + \cdots + n_p. \tag{42}$$

It follows from Theorems 6 and 7 that

$$\begin{aligned} H_c = \frac{1}{2n} \sum_{l=0}^{n} (-1)^l (n-l)^{p-2} \sum_{l_1 + \cdots + l_p = l} \prod_{i=1}^{p} \binom{n_i}{l_i} \\ \times [(n-l) - (n_i - l_i)]^{n_i - l_i} \cdot \left[(n-l)^2 - \sum_{j=1}^{p} (n_i - l_j)^2 \right] \end{aligned} \tag{43}$$

and

$$\begin{aligned} H_c = \frac{1}{2} \sum_{l=0}^{n-1} (-1)^l (n-l)^{p-2} \sum_{l_1 + \cdots + l_p = l} \prod_{i=1}^{p} \binom{n_i}{l_i} \\ \times [(n-l) - (n_i - l_i)]^{n_i - l_i} \left(1 - \frac{l_p}{n_p} \right) [(n-l) - (n_p - l_p)]. \end{aligned} \tag{44}$$

The enumeration of H_c in a $K_{n_1 \cdots n_p}$ graph can also be carried out by Theorem 2 or 3 together with the algebraic method of (2). Some elegant representations may be obtained. For example, H_c in a $K_{n_1 n_2 n_3}$ graph may be written

$$\begin{aligned} H_c = \frac{n_1! n_2! n_3!}{n_1 + n_2 + n_3} \sum_i \left[\binom{n_1}{i} \binom{n_2}{n_3 - n_1 + i} \binom{n_3}{n_3 - n_2 + i} \right. \\ \left. + \binom{n_1 - 1}{i} \binom{n_2 - 1}{n_3 - n_1 + i} \binom{n_3 - 1}{n_3 - n_2 + i} \right]. \end{aligned} \tag{45}$$

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DEPARTMENT OF MATHEMATICS, STATISTICS, AND COMPUTER SCIENCE, MARQUETTE UNIVERSITY, MILWAUKEE, WISCONSIN 53233