

Hankel determinants of RNA secondary structure sequences

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ABSTRACT:- Let $(S_{n+1}^l)_{n \geq 0}$ be secondary structure sequences, S_n^l satisfy the following recurrence

$$S_{n+1}^l = S_n^l + \sum_{k=l}^{n-1} S_k^l S_{n-1-k}^l \text{ for } n \geq l+1 \text{ with } S_0^l = S_1^l = \dots = S_{l+1}^l = 1. \text{ In particular, when } l=0, S_n^0 = M_n,$$

where M_n are the Motzkin numbers. We evaluate Hankel determinant $\det(S_{i+j+l}^l)_{0 \leq i, j \leq n}$ and $\det(S_{i+j+l+1}^l)_{0 \leq i, j \leq n}$. We show that $H_{n+1}^l = (\det(S_{i+j+l+1}^l)_{0 \leq i, j \leq n}) = 1$ for $l \geq 0$. We give another proof of $\det(M_{i+j+1})_{0 \leq i, j \leq n}$.

Keywords:- RNA secondary structure; Hankel determinant; Motzkin numbers; enumeration; sequence

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I. INTRODUCTION

The secondary structure is a subset of helical structure consistent with a planar graph. The tertiary structure is the non-planar folding. Secondary and tertiary structures determine the three-dimensional shape of RNA molecule, hence determine the function of these important biological molecules [9]. Given a sequence $(a_n)_{n \geq 0}$, define its $(n+1) \times (n+1)$ Hankel determinant $\det(a_{i+j})_{0 \leq i, j \leq n}$. Hankel determinants occur naturally in diverse areas of mathematics, we refer the readers to krattenthaler [7] for an excellent survey of determinant evaluations and [8] for a complement. We state some results needed for our study [6,10]. For a fixed integer $l \geq 0$, S_{n+1}^l satisfy the following recurrence $S_{n+1}^l = S_n^l + \sum_{k=l}^{n-1} S_k^l S_{n-1-k}^l$, $S_0^l = S_1^l = \dots = S_{l+1}^l = 1$, where $(S_{n+1}^l)_{n \geq 0}$ are secondary structure sequences. The sequence $(a_n)_{n \geq 0}$ of positive numbers is log-convex if the sequence a_n/a_{n-1} is increasing. The sequences $(S_n^l)_{n \geq 0}$ are log-convex, for $l=1, 2, 3$ and 4, see [4]. In particular, when $l=0$, $S_n^0 = M_n$, where M_n are the Motzkin numbers. The Motzkin number sequence $1, 1, 2, 4, 9, 21, 51, \dots$, enumerates many different combinatorial objects and has been the subject of several studies [1]. Hankel determinants of the Motzkin numbers have occurred in the literature [1,2,3,5]. We evaluate two families of Hankel determinants. $H_{n+1}^l = \det(S_{i+j+l}^l)_{0 \leq i, j \leq n}$, $H_{n+1}^{l+1} = \det(S_{i+j+l+1}^{l+1})_{0 \leq i, j \leq n}$. In particular, when $l=0$, $H_{n+1}^0 = \det(M_{i+j})_{0 \leq i, j \leq n}$. This determinant evaluation is already known. Cameron and Yip [3] evaluate this Hankel determinant by using combinational method. We give another proof of this determinant.

II. THEOREM AND PROPOSITION

A. Theorem

$H_{n+1}^l = (\det(S_{i+j+l+1}^l)_{0 \leq i, j \leq n}) = 1$ for $l \geq 0$, where S_{n+1}^l satisfy the recurrence.

B. Proposition

$$H_{n+1}^1 = \det(M_{i+j+1})_{0 \leq i, j \leq n} = \begin{cases} 1 & n \equiv 0, 5 \pmod{6} \\ 0 & n \equiv 1, 4 \pmod{6} \\ -1 & n \equiv 2, 3 \pmod{6} \end{cases}$$

III. PROOF

All determinants in this paper will be evaluated by employing row, column operations and using the recursive relation of sequence.

A. Proof of Theorem

$$H_{n+1}^l = \begin{vmatrix} S_l^l & S_{l+1}^l & \cdots & S_{l+n}^l \\ S_{l+1}^l & S_{l+2}^l & \cdots & S_{l+n+1}^l \\ \vdots & \vdots & \ddots & \vdots \\ S_{l+n}^l & S_{l+n+1}^l & \cdots & S_{l+2n}^l \end{vmatrix}_{n+1}$$

- 1) Subtract the i th column multiplied by S_{n-1-i}^l from the $(n+1)$ th column for $i=1, 2, 3, \dots, n-1$ and subtract the n th column. Next, applying a similar procedure to the n th, $(n-1)$ th, \dots , 2nd columns by using recursion relation, we have

$$\begin{vmatrix} S_l^l S_0^l & S_l^l S_1^l & \cdots & S_l^l S_{n-1}^l \\ \sum_{i=l}^{l+1} S_i^l S_{l+1-i}^l & \sum_{i=l}^{l+1} S_i^l S_{l+2-i}^l & \cdots & \sum_{i=l}^{l+1} S_i^l S_{l+n-i}^l \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=l}^{l+n-1} S_i^l S_{l+n-1-i}^l & \sum_{i=l}^{l+n-1} S_i^l S_{l+n-i}^l & \cdots & \sum_{i=l}^{l+n-1} S_i^l S_{l+2n-2-i}^l \end{vmatrix}_n$$

- 2) Perform row operations for the above determinant. For fixed $k=2, 3, \dots, n$, we subtract i th row multiplied by S_{k+l-i}^l / S_i^l , for $i=1, 2, \dots, k-1$, from the k th row.

$$\begin{vmatrix} S_0^l & S_1^l & \cdots & S_{n-1}^l \\ S_1^l & S_2^l & \cdots & S_n^l \\ \vdots & \vdots & \ddots & \vdots \\ S_{n-1}^l & S_n^l & \cdots & S_{2n-2}^l \end{vmatrix}_n$$

From the result above, we take $l=0$.

$$\begin{vmatrix} S_0^0 & S_1^0 & \cdots & S_n^0 \\ S_1^0 & S_2^0 & \cdots & S_{n+1}^0 \\ \vdots & \vdots & \ddots & \vdots \\ S_n^0 & S_{n+1}^0 & \cdots & S_{2n-2}^0 \end{vmatrix}_{n+1}$$

Then we get

$$H_{n+1}^l = H_n^0 = \cdots = H_1^0 = S_0^0 = 1.$$

3) Next let's consider

$$H_{n+1}^{l+1} = \begin{vmatrix} S_{l+1}^l & S_{l+2}^l & \cdots & S_{l+n+1}^l \\ S_{l+2}^l & S_{l+3}^l & \cdots & S_{l+n+2}^l \\ \vdots & \vdots & \ddots & \vdots \\ S_{l+n+1}^l & S_{l+n+2}^l & \cdots & S_{l+2n+1}^l \end{vmatrix}_{n+1}$$

By using the recursion relation, applying the similar procedure above then we have

$$\begin{vmatrix} 1 & S_0^l & \cdots & S_{n-1}^l \\ S_0^l & S_1^l & \cdots & S_n^l \\ \vdots & \vdots & \ddots & \vdots \\ S_{n-1}^l & S_n^l & \cdots & S_{2n-1}^l \end{vmatrix}_{n+1}$$

In the general case, we can't get the interesting results. Noting that $S_{n+1}^0 = M_{n+1}$, by using above results, employing row and column operations for the determinants and using the recursion relation, we get the proposition.

B. Proof of Proposition

$$\begin{vmatrix} 1 & M_0 & \cdots & M_{n-1} \\ M_0 & M_1 & \cdots & M_n \\ \vdots & \vdots & \ddots & \vdots \\ M_{n-1} & M_n & \cdots & M_{2n-1} \end{vmatrix}_{n+1}$$

1) Subtract the i th column multiplied by M_{n-1-i} from the $(n+1)$ th column for $i=1,2,\dots,k-1$ and subtract the n th column. Next, applying a similar procedure to the n th, $(n-1)$ th, \dots , 2nd columns by using the recursion relation, we have

$$\begin{vmatrix} 0 & M_0 M_0 & \cdots & M_0 M_{n-2} \\ M_0 M_0 & \sum_{i=0}^1 M_i M_{1-i} & \cdots & \sum_{i=0}^1 M_i M_{n-1-i} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=0}^{n-2} M_i M_{n-2-i} & \sum_{i=0}^{n-1} M_i M_{n-1-i} & \cdots & \sum_{i=0}^{n-1} M_i M_{2n-3-i} \end{vmatrix}_n$$

2) Perform row operations for the above determinant. For fixed $k=1,2,\dots,n$, we subtract i th row multiplied by M_{k-i}/M_0 , for $i=1,2,\dots,k-1$, from the k th row, and $M_0=1$. We have

$$\begin{vmatrix} 0 & M_0 & \cdots & M_{n-2} \\ M_0 & M_1 & \cdots & M_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ M_{n-2} & M_{n-1} & \cdots & M_{2n-3} \end{vmatrix}$$

3) Subtract the i th column multiplied by M_{n-2-i} from the n th column for $i = 2, \dots, n-2$ and subtract the $(n-1)$ th column. Next, applying a similar procedure to the $(n-1)$ th, \dots , 2nd columns by using the recursion relation, we have

$$- \begin{vmatrix} M_0 & M_0 M_0 & \cdots & M_0 M_{n-3} \\ M_1 & \sum_{i=0}^1 M_i M_{1-i} & \cdots & \sum_{i=0}^1 M_i M_{n-2-i} \\ \vdots & \vdots & \ddots & \vdots \\ M_{n-2} & \sum_{i=0}^{n-2} M_i M_{n-2-i} & \cdots & \sum_{i=0}^{n-2} M_i M_{2n-5-i} \end{vmatrix}_{n-1}$$

4) For fixed $k = 2, 3, \dots, n-1$, we subtract i th row multiplied by M_{k-i}/M_0 , for $i = 1, 2, \dots, k-1$, from the k th row. we have

$$- \begin{vmatrix} M_1 & M_2 & \cdots & M_{n-2} \\ M_2 & M_3 & \cdots & M_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ M_{n-2} & M_{n-1} & \cdots & M_{2n-5} \end{vmatrix}_{n-2}$$

then we can obtain $H_{n+1}^1 = -H_{n-2}^1$. This completes the proof of proposition.

IV. FURTHERWORK

We evaluate Hankel determinants $\det(S_{i+j+l}^l + S_{i+j+l+1}^l)_{0 \leq i, j \leq n}$ and $\det(S_{i+j+l+1}^l + S_{i+j+l+2}^l)_{0 \leq i, j \leq n}$. Then, we prove the log-convexity by using a technique based on the Hankel determinants.

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