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四叶图距离矩阵 2 个最大特征值和的变化

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摘 要:为了能够在任何情况下准确得到四叶图在 2 种图变换下距离特征值的极值,运用行列式的性质、韦达定理及不等式的放缩,给出了四叶图的 2 种图变换及上述问题的结果。首先分别给出变换前后 3 种四叶图距离矩阵、距离拉普拉斯矩阵及距离无符号拉普拉斯矩阵,利用行列式的性质计算得出其特征多项式,由韦达定理判断出 3 种距离特征多项式正负根的个数,通过不等式的放缩估计出特征值的范围,从而求出 2 个最大特征值和的范围;其次对变化前后四叶图的 3 种距离矩阵 2 个最大特征值的和进行比较。结果显示,四叶图在经过 2 种变换后 2 个最大特征值的和是增加的。所得结果为特殊图类距离特征值极值问题提供了研究方法,对分子稳定性问题的研究具有一定的借鉴价值。

关键词:图论;四叶图;距离矩阵;特征值;图变换

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Variation of sum of two largest eigenvalues of the distance matrices of four-leaf graph

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Abstract: In order to accurately obtain the extremum of the distance eigenvalues of four-leaf graphs under two graph transformations in any case, two graph transformations of four-leaf graphs and the results of the above problems were given by using the properties of the determinant, the Vieta theorem and the reduction of inequality. Firstly, the distance matrices, the distance Laplacian matrices and the distance signless Laplacian matrices of three kinds of four-leaf graphs before and after the transformation were given. The characteristic polynomials were obtained by using the properties of the determinant. The number of positive and negative roots of three kinds of distance characteristic polynomials was determined by the Vieta theorem. The range of eigenvalues was estimated by the reduction of inequality. Thus, the range of the sum of the two maximum eigenvalues was obtained. Finally, the two maximum eigenvalues of three kinds of distance matrices of four-leaf graphs before and after the transformations were compared. The comparison shows that the sum of the two maximum eigenvalues of four-leaf graph increases after two transformations. The results provide a research method for the extremum problems of distance eigenvalues of special graphs, and have certain reference value for the research of molecular stability.

Keywords: graph theory; four-leaf graph; distance matrix; eigenvalue; graph transformation

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1 问题的提出

多年来,图距离矩阵特征值的研究一直是热点问题。GRAHAM 等^[1]证明了树的距离矩阵的行列式仅是顶点数的函数,之后国内外学者对距离矩阵的谱进行了研究。HAKIMI 等^[2]提出了距离矩阵的可实现性问题,RUZIEH 等^[3]找到了路的所有特征值和特征向量,FOWLER 等^[4]给出了圈 C_n 的所有距离特征值,文献^[5]给出了萤火虫图距离矩阵 2 个最大特征值的下界,杨若松等^[6]得出了 5 类特殊图的距离矩阵的多项式。关于图的拉普拉斯矩阵特征值的研究有很多^[7-11]。文献^[12]给出了距离拉普拉斯矩阵和无符号拉普拉斯矩阵的定义,文献^[13]得到了简单图拉普拉斯矩阵第一大与第二大特征值和的上界及树的前 k 大特征值和的上界,文献^[14]研究了单圈图距离拉普拉斯矩阵的 2 个最大特征值。对于特殊图类距离矩阵特征值的相关研究见文献^[15-19]。

设简单图 G 的点集为 $V = \{v_1, v_2, \dots, v_n\}$, G 的距离矩阵定义为 $\mathbf{D}(G) = (d_{ij})_{n \times n}$, 其中 d_{ij} 表示 v_i 与 v_j 之间的距离,其特征值 $\lambda_1(\mathbf{D}(G)) \geq \lambda_2(\mathbf{D}(G)) \geq \dots \geq \lambda_i(\mathbf{D}(G)) \geq \dots \geq \lambda_n(\mathbf{D}(G))$ 被称为图 G 的距离谱。图 G 中一个点 v 的迹 $Tr(v)$ 表示点 v 到图 G 中所有点的距离和, $\mathbf{diag}(Tr)$ 表示 (i, i) 位置上的元素为 $Tr(v_i)$ 的对角矩阵; $\mathbf{L}_D(G) = \mathbf{diag}(Tr) - \mathbf{D}(G)$ 为图 G 的距离拉普拉斯矩阵,其特征值 $\mu_1(\mathbf{L}_D(G)) \geq \mu_2(\mathbf{L}_D(G)) \geq \dots \geq \mu_i(\mathbf{L}_D(G)) \geq \dots \geq \mu_n(\mathbf{L}_D(G))$ 被称为图 G 的距离拉普拉斯谱。 $\mathbf{Q}_D(G) = \mathbf{diag}(Tr) + \mathbf{D}(G)$ 为图 G 的距离无符号拉普拉斯矩阵,其特征值 $q_1(\mathbf{Q}_D(G)) \geq q_2(\mathbf{Q}_D(G)) \geq \dots \geq q_i(\mathbf{Q}_D(G)) \geq \dots \geq q_n(\mathbf{Q}_D(G))$ 被称为图 G 的距离无符号拉普拉斯谱。

若图 G 中有一块是树,其他块是圈,且所有圈都粘在这颗树的根节点上,则称 G 为仙人掌图,用 $G(n, r)$ 表示含有 r 个圈的 n 阶仙人掌图。当 $r=4$ 且每个圈为三角形时称为四叶图^[20]。笔者主要研究四叶图在 2 种变换下的距离矩阵、距离拉普拉斯矩阵和距离无符号拉普拉斯矩阵的 2 个最大特征值的和。由于确定上述矩阵的 2 个最大特征值和的问题比较困难,所以本文给出四叶图的 2 种变换,估计了变换前后四叶图的距离矩阵、距离拉普拉斯矩阵和距离无符号拉普拉斯矩阵的 2 个最大特征值的和,进而得出经过这 2 种变换,上述矩阵 2 个特征值的和是增加的。

2 主要结果

为了书写方便,把 $\lambda_i(\mathbf{D}(G)), \mu_i(\mathbf{L}_D(G))$ 和 $q_i(\mathbf{Q}_D(G))$ 分别记为 $\lambda_i(G), \mu_i(G)$ 和 $q_i(G)$, 记 $S_2(\mathbf{D}(G)), S_2(\mathbf{L}_D(G))$ 和 $S_2(\mathbf{Q}_D(G))$ 为图 G 的 $\mathbf{D}(G), \mathbf{L}_D(G)$ 和 $\mathbf{Q}_D(G)$ 的 2 个最大特征值的和。

下面定义 2 种变换,如图 1 和图 2 所示。笔者主要讨论四叶图在这 2 种变换下,距离矩阵、距离拉普拉斯矩阵和距离无符号拉普拉斯矩阵 2 个最大特征值和的变化。

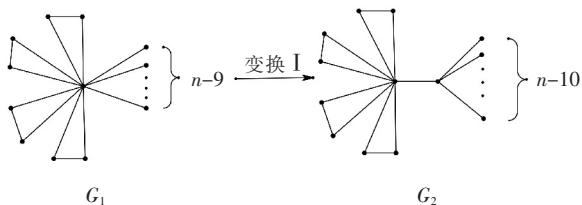


图 1 四叶图 G_1 到 G_2 的变换
Fig.1 Transformation from G_1 to G_2

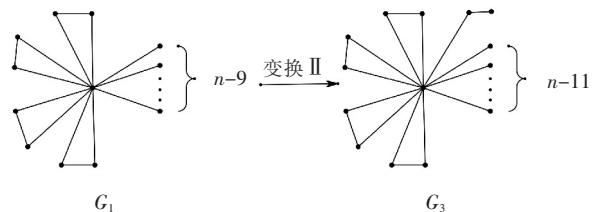


图 2 四叶图 G_1 到 G_3 的变换
Fig.2 Transformation from G_1 to G_3

2.1 距离矩阵 2 个最大特征值的和

定理 1 设 $n > 18$, 则 $2n - 5 < S_2(\mathbf{D}(G_1)) < 2n - 3$ 。

证明 显然可得,图 G_1 的距离矩阵为

$$D(G_1) = \begin{pmatrix} 0 & 1 & \cdots & 2 & 2 & \cdots & 2 & 2 & \cdots & 2 & 1 \\ 1 & 0 & \cdots & 2 & 2 & \cdots & 2 & 2 & \cdots & 2 & 1 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots \\ 2 & 2 & \cdots & 0 & 1 & \cdots & 2 & 2 & \cdots & 2 & 1 \\ 2 & 2 & \cdots & 1 & 0 & \cdots & 2 & 2 & \cdots & 2 & 1 \\ \hline 2 & 2 & \cdots & 2 & 2 & \cdots & 0 & 2 & \cdots & 2 & 1 \\ 2 & 2 & \cdots & 2 & 2 & \cdots & 2 & 0 & \cdots & 2 & 1 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots \\ 2 & 2 & \cdots & 2 & 2 & \cdots & 2 & 2 & \cdots & 0 & 1 \\ 1 & 1 & \cdots & 1 & 1 & \cdots & 1 & 1 & \cdots & 1 & 0 \end{pmatrix},$$

通过简单计算,可以确定矩阵 $D(G_1)$ 的特征多项式为

$$|\lambda E - D(G_1)| =$$

$$(\lambda + 2)^{n-10} (\lambda + 1)^4 (\lambda + 3)^3 \begin{vmatrix} \lambda - 2n + 5 & -2n + 18 & -1 \\ -\lambda - 3 & \lambda + 2 & 0 \\ -8 & -1 & \lambda \end{vmatrix} =$$

$$(\lambda + 2)^{n-10} (\lambda + 1)^4 (\lambda + 3)^3 [\lambda^3 - (2n - 7)\lambda^2 - (7n - 29)\lambda - 3n + 11]. \tag{1}$$

令 $p(\lambda) = \lambda^3 - (2n - 7)\lambda^2 - (7n - 29)\lambda - 3n + 11$, 可以观察到 $p(-3) = -40 < 0, p(-2) = 3n - 27 > 0, p(-1) = 2n - 23 > 0, p(0) = -3n + 11 < 0, p(2n - 4) = -2n^2 + 4n - 67 < 0, p(2n - 3) = 26n^2 + 4n - 40 > 0$.

由以上过程可以得出 $2n - 4 < \lambda_1(G_1) < 2n - 3, -1 < \lambda_2(G_1) < 0$, 这表明 $2n - 5 < S_2(D(G_1)) < 2n - 3$.

定理 2 设 $n > 18$, 则 $2n - 1 < S_2(D(G_2)) < 4n$.

证明 显然可得, 图 G_2 的距离矩阵为

$$D(G_2) = \begin{pmatrix} 0 & 1 & \cdots & 2 & 2 & \cdots & 3 & 3 & \cdots & 3 & \cdots & 2 & 1 \\ 1 & 0 & \cdots & 2 & 2 & \cdots & 3 & 3 & \cdots & 3 & \cdots & 2 & 1 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & & \vdots & \vdots \\ 2 & 2 & \cdots & 0 & 1 & \cdots & 3 & 3 & \cdots & 3 & \cdots & 2 & 1 \\ 2 & 2 & \cdots & 1 & 0 & \cdots & 3 & 3 & \cdots & 3 & \cdots & 2 & 1 \\ \hline 3 & 3 & \cdots & 3 & 3 & \cdots & 0 & 2 & \cdots & 2 & \cdots & 1 & 2 \\ 3 & 3 & \cdots & 3 & 3 & \cdots & 2 & 0 & \cdots & 2 & \cdots & 1 & 2 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & & \vdots & \vdots \\ 3 & 3 & \cdots & 3 & 3 & \cdots & 2 & 2 & \cdots & 0 & \cdots & 1 & 2 \\ \hline 2 & 2 & \cdots & 2 & 2 & \cdots & 1 & 1 & \cdots & 1 & \cdots & 0 & 1 \\ 1 & 1 & \cdots & 1 & 1 & \cdots & 2 & 2 & \cdots & 2 & \cdots & 1 & 0 \end{pmatrix},$$

通过简单计算可以得到图 G_2 距离矩阵的特征多项式为

$$|\lambda E - D(G_2)| =$$

$$(\lambda + 2)^{n-11} (\lambda + 1)^4 (\lambda + 3)^3 \begin{vmatrix} \lambda - 13 & -3n + 30 & -2 & -1 \\ -24 & \lambda - 2n + 22 & -1 & -2 \\ -16 & -n + 10 & \lambda & -1 \\ -8 & -2n + 20 & -1 & \lambda \end{vmatrix} =$$

$$(\lambda + 2)^{n-11}(\lambda + 1)^4(\lambda + 3)^3[\lambda^4 + (9 - 2n)\lambda^3 + (443 - 51n)\lambda^2 + (389 - 49n)\lambda + 22 - 6n], \quad (2)$$

令 $p(\lambda) = \lambda^4 + (9 - 2n)\lambda^3 + (443 - 51n)\lambda^2 + (389 - 49n)\lambda + 22 - 6n$, 假设 $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ 是 $p(\lambda)$ 的根, 则 $\sum_i \lambda_i = 2n - 9 > 0, \lambda_1 \lambda_2 \lambda_3 \lambda_4 = 22 - 6n < 0$ 。即多项式 $p(\lambda)$ 有 1 个正根或 3 个正根。由于 $p(-2) = 9.7n - 63 > 0, p(-1) = -6n + 68 < 0, p(-\frac{1}{2}) > 9.7n - 63 > 0, p(0) = 22 - 6n < 0$, 所以多项式 $p(\lambda)$ 仅有 1 个正根, 且最小的负根一定小于 -1 。

$$p(2n - \frac{1}{2}) = -136n^3 + \frac{3\ 597}{2}n^2 - \frac{179}{2}n - \frac{4\ 691}{4} < 0,$$

$$p(4n) = 128n^4 + 496n^3 + 6\ 892n^2 + 1\ 556n + 22 > 0,$$

可得 $2n - \frac{1}{2} < \lambda_1(G_2) < 4n, -\frac{1}{2} < \lambda_2(G_2) < 0$, 即 $2n - 1 < S_2(\mathbf{D}(G_2)) < 4n$ 。

定理 3 设 $n > 18$, 则 $2n - \frac{5}{2} < S_2(\mathbf{D}(G_3)) < 2n - 1$ 。

证明 图 G_3 的距离矩阵为

$$\mathbf{D}(G_3) = \begin{pmatrix} 0 & 1 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 2 & 1 & 3 \\ 1 & 0 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 2 & 1 & 3 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 2 & 2 & \cdots & 0 & 1 & 2 & 2 & \cdots & 2 & 2 & 1 & 3 \\ 2 & 2 & \cdots & 1 & 0 & 2 & 2 & \cdots & 2 & 2 & 1 & 3 \\ \hline 2 & 2 & \cdots & 2 & 2 & 0 & 2 & \cdots & 2 & 2 & 1 & 3 \\ 2 & 2 & \cdots & 2 & 2 & 2 & 0 & \cdots & 2 & 2 & 1 & 3 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 2 & 2 & \cdots & 2 & 2 & 2 & 2 & \cdots & 0 & 2 & 1 & 3 \\ 2 & 2 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 0 & 1 & 1 \\ \hline 1 & 1 & \cdots & 1 & 1 & 1 & 1 & \cdots & 1 & 1 & 0 & 2 \\ 3 & 3 & \cdots & 3 & 3 & 3 & 3 & \cdots & 3 & 1 & 2 & 0 \end{pmatrix},$$

经过简单计算得到矩阵 $\mathbf{D}(G_3)$ 的特征多项式为

$$|\lambda E - \mathbf{D}(G_3)| =$$

$$(\lambda + 2)^{n-12}(\lambda + 1)^4(\lambda + 3)^3 \begin{vmatrix} \lambda - 13 & -2n + 22 & -2 & -1 & -3 \\ -16 & \lambda - 2n + 24 & -2 & -1 & -3 \\ -16 & -2n + 22 & \lambda & -1 & -1 \\ -8 & -n + 11 & -1 & \lambda & -2 \\ -24 & -3n + 33 & -1 & -2 & \lambda \end{vmatrix} =$$

$$(\lambda + 2)^{n-12}(\lambda + 1)^4(\lambda + 3)^3[\lambda^5 + (11 - 2n)\lambda^4 + (76 - 20n)\lambda^3 + (252 - 58n)\lambda^2 + (228 - 52n)\lambda + 44 - 12n]. \quad (3)$$

令 $p(\lambda) = \lambda^5 + (11 - 2n)\lambda^4 + (76 - 20n)\lambda^3 + (252 - 58n)\lambda^2 + (228 - 52n)\lambda + 44 - 12n$, 假设 $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \lambda_5$ 是 $p(\lambda)$ 的根, 则 $\sum_i \lambda_i = 2n - 11 > 0, \lambda_1 \lambda_2 \lambda_3 \lambda_4 \lambda_5 = 12n - 44 > 0$, 所以多项式 $p(\lambda)$ 有 1 个正根或 3 个正根。

由于

$$\begin{aligned}
 p(60-10n) < 0, \quad p(-3) = 224 > 0, \quad p(-2) = 132 - 12n < 0, \quad p\left(-\frac{1}{2}\right) = \frac{15}{8}n - \frac{507}{32} > 0, \\
 p(0) = 44 - 12n < 0, \quad p(2n-1) = 296n^3 + 106n^2 - 174n + 2 > 0, \\
 p(2n-2) = -16n^4 + 208n^3 - 72n^2 - 758n + 132 < 0,
 \end{aligned}$$

即 $2n-2 < \lambda_1(G_3) < 2n-1, -\frac{1}{2} < \lambda_2(G_3) < 0$, 这表明 $2n - \frac{5}{2} < S_2(\mathbf{D}(G_3)) < 2n-1$ 。

定理 4 设 $n > 18$, 则 $S_2(\mathbf{D}(G_1)) < S_2(\mathbf{D}(G_3)) < S_2(\mathbf{D}(G_2))$ 。

2.2 距离拉普拉斯矩阵 2 个最大特征值的和

定理 5 当 $n > 25$ 时, 有 $S_2(\mathbf{L}_D(G_1)) = 4n-4$ 。

证明 图 G_1 的距离拉普拉斯矩阵为

$$\mathbf{L}_D(G_1) = \begin{pmatrix} 2n-4 & -1 & \cdots & -2 & -2 & -2 & -2 & \cdots & -2 & -1 \\ -1 & 2n-4 & \cdots & -2 & -2 & -2 & -2 & \cdots & -2 & -1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ -2 & -2 & \cdots & 2n-4 & -1 & -2 & -2 & \cdots & -2 & -1 \\ -2 & -2 & \cdots & -1 & 2n-4 & -2 & -2 & \cdots & -2 & -1 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -2 & -2 & \cdots & -2 & -2 & 2n-3 & -2 & \cdots & -2 & -1 \\ -2 & -2 & \cdots & -2 & -2 & -2 & 2n-3 & \cdots & -2 & -1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ -2 & -2 & \cdots & -2 & -2 & -2 & -2 & \cdots & 2n-3 & -1 \\ -1 & -1 & \cdots & -1 & -1 & -1 & -1 & \cdots & -1 & n-1 \end{pmatrix},$$

计算可得:

$$\begin{aligned}
 |\mu E - \mathbf{L}_D(G_1)| = & (\mu - 2n + 1)^{n-7} (\mu - 2n + 3)^4 \begin{vmatrix} \mu - 2n + 17 & 2n - 18 & 1 \\ 16 & \mu - 17 & 1 \\ 8 & n - 9 & \mu - n + 1 \end{vmatrix} = \\
 & (\mu - 2n + 1)^{n-7} (\mu - 2n + 3)^4 [\mu^3 + (1 - 3n)\mu^2 + (2n^2 - n)\mu]. \tag{4}
 \end{aligned}$$

令 $p(\mu) = \mu^3 + (1 - 3n)\mu^2 + (2n^2 - n)\mu$, 其根为 $2n-1, n$ 和 0 , 所以 $\mu_1(G_1) = 2n-3, \mu_2(G_1) = 2n-1$, 这表明 $S_2(\mathbf{L}_D(G_1)) = 4n-4$ 。

定理 6 当 $n > 25$ 时, 有 $6n-21 < S_2(\mathbf{L}_D(G_2)) < 6n-11$ 。

证明 由

$$\mathbf{L}_D(G_2) = \begin{pmatrix} 3n-14 & -1 & \cdots & -2 & -2 & -3 & -3 & \cdots & -3 & -2 & -1 \\ -1 & 3n-14 & \cdots & -2 & -2 & -3 & -3 & \cdots & -3 & -2 & -1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ -2 & -2 & \cdots & 3n-14 & -1 & -3 & -3 & \cdots & -3 & -2 & -1 \\ -2 & -2 & \cdots & -1 & 3n-14 & -3 & -3 & \cdots & -3 & -2 & -1 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -3 & -3 & \cdots & -3 & -3 & 2n+5 & -2 & \cdots & -2 & -1 & -2 \\ -3 & -3 & \cdots & -3 & -3 & -2 & 2n+5 & \cdots & -2 & -1 & -2 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ -3 & -3 & \cdots & -3 & -3 & -2 & -2 & \cdots & 2n+5 & -1 & -2 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -2 & -2 & \cdots & -2 & -2 & -1 & -1 & \cdots & -1 & 2n-11 & -1 \\ -1 & -1 & \cdots & -1 & -1 & -2 & -2 & \cdots & -2 & -1 & n+7 \end{pmatrix},$$

计算可得:

$$|\mu E - \mathbf{L}_D(G_2)| = (\mu - 2n + 13)^4 (\mu - 2n - 7)^{n-11} (\mu - 3n + 11)^3 \begin{vmatrix} \mu - 3n + 27 & 3n - 30 & 1 & 2 \\ 24 & \mu - 27 & 2 & 1 \\ 8 & 2n - 20 & \mu - 2n + 11 & 1 \\ 16 & n - 10 & 1 & \mu - n - 7 \end{vmatrix} = \mu(\mu - 2n + 13)^4 (\mu - 2n - 7)^{n-11} (\mu - 3n + 11)^3 [\mu^3 + (4 - 6n)\mu^2 + (11n^2 - 5n - 77)\mu + (-6n^3 - 15n^2 + 237n)]. \tag{5}$$

令 $p(\mu) = \mu^3 + (4 - 6n)\mu^2 + (11n^2 - 5n - 77)\mu + (-6n^3 - 15n^2 + 237n)$, 由于 $p(n) = -16n^2 + 160n < 0$, $p(2n - 25) = 11n^2 - 192n + 1300 > 0$, $p(2n) = -9n^2 + 83n < 0$, $p(3n - 10) = -4n^2 - 424n + 170 < 0$, $p(3n) = 6n^2 + 6n > 0$,

则 $3n - 10 < \mu_1(G_2) < 3n, \mu_2(G_2) = 3n - 11$, 可知 $6n - 21 < S_2(\mathbf{L}_D(G_2)) < 6n - 11$.

定理 7 当 $n > 25$ 时, 有 $6n - 4 < S_2(\mathbf{L}_D(G_3)) < 6n + 9$.

证明 图 G_3 的距离拉普拉斯矩阵为

$$\mathbf{L}_D(G_3) = \begin{pmatrix} 2n-3 & -1 & \cdots & -2 & -2 & -2 & -2 & \cdots & -2 & -1 & -2 & -3 \\ -1 & 2n-3 & \cdots & -2 & -2 & -2 & -2 & \cdots & -2 & -1 & -2 & -3 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ -2 & -2 & \cdots & 2n-3 & -1 & -2 & -2 & \cdots & -2 & -1 & -2 & -3 \\ -2 & -2 & \cdots & -1 & 2n-3 & -2 & -2 & \cdots & -2 & -1 & -2 & -3 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -2 & -2 & \cdots & -2 & -2 & 2n-3 & -2 & \cdots & -2 & -1 & -2 & -3 \\ -2 & -2 & \cdots & -2 & -2 & -2 & 2n-3 & \cdots & -2 & -1 & -2 & -3 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ -2 & -2 & \cdots & -2 & -2 & -2 & -2 & \cdots & 2n-3 & -1 & -2 & -3 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -1 & -1 & \cdots & -1 & -1 & -1 & -1 & \cdots & -1 & n & -1 & -2 \\ -2 & -2 & \cdots & -2 & -2 & -2 & -2 & \cdots & -2 & -1 & 2n-4 & -1 \\ -3 & -3 & \cdots & -3 & -3 & -3 & -3 & \cdots & -3 & -2 & -1 & 3n+6 \end{pmatrix},$$

经过计算可得:

$$|\mu E - \mathbf{L}_D(G_3)| = (\mu - 2n + 2)^4 (\mu + 2n + 1)^{n-12} (\mu - 2n)^3 \begin{vmatrix} \mu - 2n + 6 & 2n - 22 & 1 & 2 & 3 \\ 16 & \mu - 21 & 1 & 2 & 3 \\ 8 & n - 11 & \mu - n & 1 & 2 \\ 16 & 2n - 22 & 1 & \mu - 2n + 4 & 1 \\ 24 & 3n - 33 & 2 & 2 & \mu - 3n + 6 \end{vmatrix} =$$

$$\begin{aligned}
 & (\mu-2n+2)^4(\mu+2n+1)^{n-12}(\mu-2n)^3[\mu^5+(5-8n)\mu^4+(23n^2-28n+26)\mu^3+ \\
 & (-28n^3+53n^2-144n+66)\mu^2+(12n^4-40n^3+256n^2-208n-66)\mu+ \\
 & 12n^4-144n^3+120n^2+132n]= \\
 & (\mu-2n+2)^4(\mu+2n+1)^{n-12}(\mu-2n)^3 p(\mu), \tag{6}
 \end{aligned}$$

由于

$$\begin{aligned}
 p(-1) &= -132n^3-106n^2+136n+110 < 0, & p(1) &= 24n^4-212n^3+452n^2-176n+32 > 0, \\
 p(2n-9) &= -130n^3+1584n^2+4122n-39258 < 0, & p(2n) &= 128n^2 > 0, \\
 p(3n-4) &= -6n^4+54n^3+269n^2-3096n+2984 < 0, \\
 p(3n+8) &= 12n^4+1470n^3+2314n^2+64030n+70256 > 0,
 \end{aligned}$$

则 $3n-4 < \mu_1(G_3) < 3n+8, 2n < \mu_2(G_3) < 2n+1$, 可知 $6n-4 < S_2(L_D(G_3)) < 6n+9$.

定理 8 设 $n > 25$ 时, 有 $S_2(L_D(G_1)) < S_2(L_D(G_2)) < S_2(L_D(G_3))$ 。

2.3 距离无符号拉普拉斯矩阵 2 个最大特征值的和

定理 9 若 $n > 35$, 则 $S_2(Q_D(G_1)) < 6n-11$ 。

证明 显然可得:

$$Q_D(G_1) = \begin{pmatrix} 2n-4 & 1 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 1 \\ 1 & 2n-4 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 2 & 2 & \cdots & 2n-4 & 1 & 2 & 2 & \cdots & 2 & 1 \\ 2 & 2 & \cdots & 1 & 2n-4 & 2 & 2 & \cdots & 2 & 1 \\ \hline 2 & 2 & \cdots & 2 & 2 & 2n-3 & 2 & \cdots & 2 & 1 \\ 2 & 2 & \cdots & 2 & 2 & 2 & 2n-3 & \cdots & 2 & 1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 2 & 2 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2n-3 & 1 \\ 1 & 1 & \cdots & 1 & 1 & 1 & 1 & \cdots & 1 & n-1 \end{pmatrix},$$

通过计算可得:

$$\begin{aligned}
 |qE - Q_D(G_1)| &= \\
 & (q-2n+5)^{n-6}(q-2n+7)^3 \begin{vmatrix} q-2n-9 & -2n+18 & -1 \\ -16 & q-4n+23 & -1 \\ -8 & -n+9 & q-n+1 \end{vmatrix} = \\
 & (q-2n+5)^{n-6}(q-2n+7)^3 [q^3+(15-7n)q^2+(14n^2-63n+96)q-8n^3+52n^2-132n+104] = \\
 & (q-2n+5)^{n-6}(q-2n+7)^3 p(q), \tag{7}
 \end{aligned}$$

计算可得 $p(n-3) = -5n^2 - 351n - 76 < 0, p(n-1) = n^2 - 7n + 7 > 0, p(4n-6) = 4n^2 + 90n - 148 > 0,$
 $p(4n-10) = -20n^2 - 538n + 1644 < 0, p(2n-5) = -4n^2 + 50n - 126 < 0$ 。由函数的性质可知, $p(q)$ 的一个根在 $(4n-10, 4n-6)$ 内, 另一个根在 $(n-1, 4n-10)$ 内, 而 $p(2n-5) < 0$, 所以 $p(q)$ 的另一个根小于 $2n-5$ 。

综上可得 $q_1(G_1) < 4n - 6, q_2(G_1) = 2n - 5$, 即 $S_2(Q_D(G_1)) < 6n - 11$ 。

定理 10 若 $n > 35$, 则 $7n + 3 < S_2(Q_D(G_2)) < 13n - 17$ 。

证明

$$Q_D(G_2) = \begin{pmatrix} 3n-14 & 1 & \cdots & 2 & 2 & 3 & 3 & \cdots & 3 & 2 & 1 \\ 1 & 3n-14 & \cdots & 2 & 2 & 3 & 3 & \cdots & 3 & 2 & 1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 2 & 2 & \cdots & 3n-14 & 1 & 3 & 3 & \cdots & 3 & 2 & 1 \\ 2 & 2 & \cdots & 1 & 3n-14 & 3 & 3 & \cdots & 3 & 2 & 1 \\ \hline 3 & 3 & \cdots & 3 & 3 & 2n+5 & 2 & \cdots & 2 & 1 & 2 \\ 3 & 3 & \cdots & 3 & 3 & 2 & 2n+5 & \cdots & 2 & 1 & 2 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 3 & 3 & \cdots & 3 & 3 & 2 & 2 & \cdots & 2n+5 & 1 & 2 \\ \hline 2 & 2 & \cdots & 2 & 2 & 1 & 1 & \cdots & 1 & 2n-11 & 1 \\ 1 & 1 & \cdots & 1 & 1 & 2 & 2 & \cdots & 2 & 1 & n+7 \end{pmatrix},$$

由上式计算可得:

$$\begin{aligned} |qE - Q_D(G_2)| &= \\ &= (q-3n+15)^4 (q-2n-3)^{n-11} (q-3n+17)^3 \begin{vmatrix} q-3n+1 & -3n+30 & -1 & -2 \\ -24 & q-4n+17 & -2 & -1 \\ -8 & -2n+20 & q-2n+11 & -1 \\ -16 & -n+10 & -1 & q-n-7 \end{vmatrix} \\ &= (q-3n+15)^4 (q-2n-3)^{n-11} (q-3n+17)^3 [q^4 + (22-10n)q^3 + (35n^2-211n+741)q^2 + \\ &\quad (-50n^3+465n^2-2\ 281n+2\ 376)q + 24n^4 - 236n^3 + 304n^2 + 11\ 564n - 57\ 672] = \\ &= (q-3n+15)^4 (q-2n-3)^{n-11} (q-3n+17)^3 p(q), \end{aligned} \tag{8}$$

由于

$$p(1) > 24n^4 - 286n^3 + n^2 > 0, \quad p(n) = -210n^4 + 40n^3 - 1\ 230n^2 + 13\ 940n - 57\ 672 < 0,$$

$$p(2n-1) = 304n^3 - 1\ 180n^2 + 15\ 556n - 59\ 328 > 0,$$

$$p(2n+20) = -574n^3 - 634n^2 + 142\ 376n + 622\ 248 < 0,$$

$$p(4n+10) = -224n^3 - 14\ 904n^2 + 76\ 808n + 622\ 248 < 0,$$

$$p(10n) = 3\ 024n^4 + 5\ 314n^3 + 51\ 594n^2 + 35\ 324n - 57\ 672 > 0,$$

则 $4n + 20 < q_1(G_2) < 10n, q_2(G_2) = 3n - 17$, 可知 $7n + 3 < S_2(Q_D(G_2)) < 13n - 17$ 。

定理 11 若 $n > 35$, 则 $7n - 15 < S_2(Q_D(G_3)) < 7n - 5$ 。

证明 图 G_3 的距离无符号拉普拉斯矩阵为

$$Q_D(G_3) = \begin{pmatrix} 2n-3 & 1 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 1 & 2 & 3 \\ 1 & 2n-3 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 1 & 2 & 3 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 2 & 2 & \cdots & 2n-3 & 1 & 2 & 2 & \cdots & 2 & 1 & 2 & 3 \\ 2 & 2 & \cdots & 1 & 2n-3 & 2 & 2 & \cdots & 2 & 1 & 2 & 3 \\ \hline 2 & 2 & \cdots & 2 & 2 & 2n-3 & 2 & \cdots & 2 & 1 & 2 & 3 \\ 2 & 2 & \cdots & 2 & 2 & 2 & 2n-3 & \cdots & 2 & 1 & 2 & 3 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 2 & 2 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2n-3 & 1 & 2 & 3 \\ \hline 1 & 1 & \cdots & 1 & 1 & 1 & 1 & \cdots & 1 & n & 1 & 2 \\ 2 & 2 & \cdots & 2 & 2 & 2 & 2 & \cdots & 2 & 1 & 2n-4 & 1 \\ 3 & 3 & \cdots & 3 & 3 & 3 & 3 & \cdots & 3 & 2 & 1 & 3n+6 \end{pmatrix},$$

计算可得:

$$|qE - Q_D(G_3)| = (q-2n+4)^4 (q-2n+5)^{n-12} (q-2n+6)^3 \begin{vmatrix} q-2n-10 & -2n+22 & -1 & -2 & -3 \\ -16 & q-4n+27 & -1 & -2 & -3 \\ -8 & -n+11 & q-n & -1 & -2 \\ -16 & -2n+22 & -1 & q-2n+4 & -1 \\ -24 & -3n+33 & -2 & -1 & q-3n+6 \end{vmatrix} = (q-2n+4)^4 (q-2n+5)^{n-12} (q-2n+6)^3 [q^5 + (27-2n)q^4 + (55n^2 - 256n + 312)q^3 + (847n^2 - 2060n + 1758 - 120n^3)q^2 + (3906 - 6592n + 4102n^2 - 1156n^3 + 124n^4)q + 676 - 4516n + 5048n^2 - 2388n^3 + 59n^4 - 48n^5] = (q-2n+4)^4 (q-2n+5)^{n-12} (q-2n+6)^3 p(q), \tag{9}$$

因为

$$\begin{aligned} p(-1) &= -48n^5 + 425n^4 - 1325n^3 + 1738n^2 + 260n - 1758 < 0, \\ p(n) &= 11n^4 - 34n^3 + 214n^2 - 610n + 676 > 0, \\ p(2n-20) &< -n^4 - n^3 < 0, \\ p(2n-4) &> n^4 + 8n^3 + 26248n^2 > 0, \\ p(3n-5) &= 94n^4 - 103n^3 + 13914n^2 - 503n - 154 > 0, \\ p(3n) &= -21n^4 - 198n^3 + 1094n^2 + 720n + 676 < 0, \\ p(4n-10) &< -n < 0, \\ p(4n-5) &> 405n^4 + n^2 + n > 0, \end{aligned}$$

则 $4n-10 < q_1(G_3) < 4n-5, 3n-5 < q_2(G_3) < 3n$, 可知 $7n-15 < S_2(Q_D(G_3)) < 7n-5$ 。

定理 12 设 $n > 35$ 时, 有 $S_2(Q_D(G_1)) < S_2(Q_D(G_3)) < S_2(Q_D(G_2))$ 。

3 结 论

笔者对四叶图 3 种距离矩阵 2 个最大特征值的和进行了研究。结论如下:对于图 G_1, G_2, G_3 的距离矩阵特征值,当 $n > 18$ 时,有 $S_2(\mathbf{D}(G_1)) < S_2(\mathbf{D}(G_3)) < S_2(\mathbf{D}(G_2))$;对于图 G_1, G_2, G_3 的距离拉普拉斯矩阵特征值,当 $n > 25$ 时,有 $S_2(\mathbf{L}_D(G_1)) < S_2(\mathbf{L}_D(G_2)) < S_2(\mathbf{L}_D(G_3))$;对于图 G_1, G_2, G_3 的距离无符号拉普拉斯矩阵特征值,当 $n > 35$ 时,有 $S_2(\mathbf{Q}_D(G_1)) < S_2(\mathbf{Q}_D(G_3)) < S_2(\mathbf{Q}_D(G_2))$ 。四叶图经过 2 种变换后,3 种距离矩阵 2 个最大特征值的和都是增加的。

鉴于四叶图结构的复杂性,确定矩阵的 2 个最大特征值和的问题是比较困难的。笔者只研究了四叶图的 2 种图变换下 3 种距离矩阵 2 个最大特征值和的变化。研究方法可为继续研究四叶图 3 种距离矩阵 2 个最大特征值和的极值问题开拓思路。

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