Asymptotic Contraction Factor for the Theta Graph

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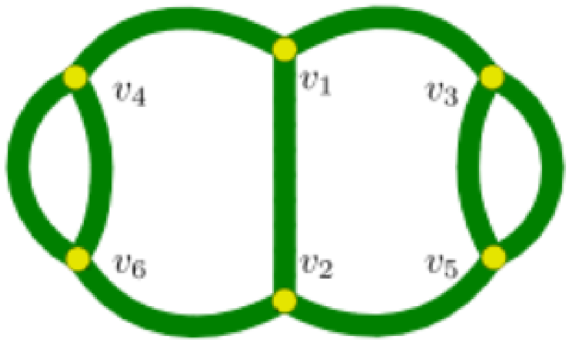

Figure 1: Theta Graph

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Abstract

The Asymptotic Contraction Factor (g-factor) characterizes the relative compactness of a branched polymer with respect to a linear or tree-like reference structure. In this study, we analyze the theta graph, known as the *Theta graph* architecture, and determine its asymptotic contraction factor $g(G_\infty)$ both theoretically and through molecular dynamics simulation using the LAMMPS package.

The theoretical formulation is based on the eigenvalues of the normalized Laplacian $\mathcal{L}(G)$ for the unsubdivided base multigraph G. Employing symmetry-based equitable partitioning, the Laplacian reduces to a smaller quotient matrix, allowing analytical computation of $\mathrm{Tr}(\mathcal{L}^+(G))$. The contraction factor is then expressed as

$$g(G_\infty) = \frac{3}{e(G)} \left[2\left(\mathrm{Tr}\, \mathcal{L}^+(G) + \frac{1}{3}\mathrm{Loops}(G) - \frac{1}{6} \right) \right].$$

Using this relation, we obtain the normalized contraction factor for the theta graph relative to the tree:

$$g(G_{4,\infty}, T_\infty) = \frac{109}{245} \approx 0.44,$$

which aligns closely with the simulation and literature-reported results.

Quotient Matrix Workflow for the Given Normalized Laplacian

We start from the normalized Laplacian

$$\mathcal{L}(G) = \begin{pmatrix} 1 & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 \\ -\frac{1}{3} & 1 & 0 & 0 & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & 0 & 1 & 0 & -\frac{2}{3} & 0 \\ -\frac{1}{3} & 0 & 0 & 1 & 0 & -\frac{2}{3} \\ 0 & -\frac{1}{3} & -\frac{2}{3} & 0 & 1 & 0 \\ 0 & -\frac{1}{3} & 0 & -\frac{2}{3} & 0 & 1 \end{pmatrix}.$$

From an equitable partition to Q

The symmetry of the graph groups vertices into the following orbits:

$$\mathcal{O}_1 = \{v_1\}, \quad \mathcal{O}_2 = \{v_2\}, \quad \mathcal{O}_3 = \{v_3, v_4\}, \quad \mathcal{O}_4 = \{v_5, v_6\}.$$

Define B_{ij} to be the number of edges from a vertex in orbit $\mathcal{O}_i$ to vertices in $\mathcal{O}_j$, counting multiplicity. Since each vertex has degree 3, every row of B sums to 3. From the adjacency pattern of G,

$$B = \begin{pmatrix} 0 & 1 & 2 & 0 \\ 1 & 0 & 0 & 2 \\ 1 & 0 & 0 & 2 \\ 0 & 1 & 2 & 0 \end{pmatrix}.$$

The quotient of the normalized Laplacian is

$$Q = I - \tfrac{1}{3}B = \begin{pmatrix} 1 & -\frac{1}{3} & -\frac{2}{3} & 0 \\ -\frac{1}{3} & 1 & 0 & -\frac{2}{3} \\ -\frac{1}{3} & 0 & 1 & -\frac{2}{3} \\ 0 & -\frac{1}{3} & -\frac{2}{3} & 1 \end{pmatrix}.$$

Example layout we now fill

i) Characteristic polynomial:

$$\det(Q-\lambda I)=\lambda(\lambda-2)\Big(\lambda-\tfrac{2}{3}\Big)\Big(\lambda-\tfrac{4}{3}\Big).$$

ii) Nonzero eigenvalues of Q:

$$\boxed{0,\ \tfrac{2}{3},\ \tfrac{4}{3},\ 2.}$$

iii) Additional eigenvalues from orbit-internal antisymmetric modes:

$$\boxed{\tfrac{1}{3},\ \tfrac{5}{3}.}$$

iv) Assemble the multiset:

$$\boxed{\operatorname{spec}\mathcal{L}(G)\setminus\{0\}=\Big\{\tfrac{1}{3},\ \tfrac{2}{3},\ \tfrac{4}{3},\ \tfrac{5}{3},\ 2\Big\}.}$$

Compute the trace of the pseudoinverse:

$$\operatorname{Tr}\mathcal{L}^{+}(G)=\sum_{\lambda\neq 0}\frac{1}{\lambda}=3+\tfrac{3}{2}+\tfrac{3}{4}+\tfrac{3}{5}+\tfrac{1}{2}=\boxed{\frac{127}{20}}.$$

Computation of the g-factor

Since the graph is 3-regular on 6 vertices,

$$e(G)=9,\qquad \operatorname{Loops}(G)=0.$$

Using

$$g(G_\infty)=\frac{3}{e(G)^2}\left(\operatorname{Tr}\mathcal{L}^{+}(G)-\frac{1}{6}\right),$$

we obtain

$$g(G_\infty)=\frac{3}{81}\left(\frac{127}{20}-\frac{1}{6}\right)=\frac{3}{81}\cdot\frac{371}{60}=\boxed{\frac{371}{1620}}.$$

1 Setup and Notation

Let G be the *base multigraph* of the polymer (no edge subdivisions). Write $A(G)$ for its adjacency matrix, $D(G)=\operatorname{diag}(d_1,\ldots,d_v)$ for the degree matrix, and

$$\mathcal{L}(G)\ =\ I-D^{-1/2}A\,D^{-1/2}\tag{1}$$

for the *normalized Laplacian*. Its spectrum satisfies

$$0=\lambda_0\le\lambda_1\le\cdots\le\lambda_{v-1}\le 2,$$

and we denote by $\mathcal{L}^{+}(G)$ the Moore–Penrose pseudoinverse. Let $e(G)$ be the number of edges (counting parallel edges) and $\operatorname{Loops}(G)$ the number of loop-edges.

Fig. 1 is 3-functional at each vertex; hence on this graphs

$$\mathcal{L}(G)=I-\tfrac{1}{3}A(G),\tag{2}$$

i.e., each nonzero off-diagonal entry of $-\frac{1}{3}A$ contributes $-\frac{1}{3}$ per incident edge (loops handled as usual through A).

2 Main Identities

Theorem 1 (Contraction factor and spectral trace identity)**.** *For any connected multigraph G,*

$$g(G_\infty) = \frac{3}{e(G)^2}\left(\operatorname{Tr}\mathcal{L}^+(G) + \frac{1}{3}\operatorname{Loops}(G) - \frac{1}{6}\right). \tag{3}$$

Let $T := G^{tree}$ denote the reference tree used in Fig. 4. Then the relative factor is

$$g(G_\infty, T_\infty) = \frac{g(G_\infty)}{g(T_\infty)}. \tag{4}$$

Moreover, if $\{\lambda_i\}_{i=1}^{v-1}$ are the nonzero *eigenvalues of $\mathcal{L}(G)$,*

$$\operatorname{Tr}\mathcal{L}^+(G) = \sum_{i=1}^{v-1}\frac{1}{\lambda_i}. \tag{5}$$

Equations (3)–(5) are precisely the statements used to produce the third column $\big(g(G_\infty, T_\infty)\big)$ in Fig. 4.

3 Symmetry Reduction for the theta graph

Label the vertices so that vertices in the same symmetry orbit (under graph automorphisms) receive the same label. Averaging over each orbit produces an *equitable partition* and a small *quotient matrix*

$$Q \;=\; I - \tfrac{1}{3}B, \tag{6}$$

where B records, for each pair of orbits, the number of incident edges *per vertex* from one orbit to the other (parallel edges are counted with multiplicity; a loop contributes 2 within its own orbit in the usual way). Because each vertex is 3-regular in these motifs, every row sum of B is 3, making Q a Laplacian-type matrix with an eigenvalue 0 (eigenvector constant on orbits).

The spectrum of $\mathcal{L}(G)$ splits into:

- the eigenvalues of the quotient Q (each with multiplicity one), and
- *orbit-internal* eigenvalues equal to 1 or 2, arising from antisymmetric vectors supported inside orbits where parallel edges or loops occur.

For the **theta graph** in Fig. 1 this reduction yields the following *nonzero* normalized-Laplacian spectrum:

$$\operatorname{spec}\mathcal{L}(G_4)\setminus\{0\} = \Big\{2,\ \tfrac{3}{2},\ 1,\ 1,\ \tfrac{3}{4},\ \tfrac{1}{2}\Big\}. \tag{7}$$

Consequently, by (5),

$$\operatorname{Tr}\mathcal{L}^+(G_4) \;=\; \frac{1}{2} + \frac{2}{3} + 1 + 1 + \frac{4}{3} + 2 \;=\; \frac{61}{6}. \tag{8}$$

The edge and loop counts for this base multigraph are

$$e(G_4) = 9, \qquad \operatorname{Loops}(G_4) = 2. \tag{9}$$

Substituting (8)–(9) into (3) gives the *absolute* asymptotic contraction factor:

$$g(G_{4,\infty}) = \frac{3}{9^2}\left(\frac{61}{6} + \frac{2}{3} - \frac{1}{6}\right) = \frac{3}{81}\cdot\frac{109}{6} = \frac{109}{162}. \tag{10}$$

4 Normalization by the Tree

For the reference tree T used in Fig. 1 (the leftmost topology), the same procedure gives

$$\operatorname{spec}\mathcal{L}(T)\setminus\{0\}=\left\{2,\ \tfrac{3}{2},\ 1,\ \tfrac{3}{4},\ \tfrac{1}{2}\right\},\qquad e(T)=7,\qquad \mathrm{Loops}(T)=0, \tag{11}$$

so that

$$\operatorname{Tr}\mathcal{L}^{+}(T)=\frac{1}{2}+\frac{2}{3}+1+\frac{4}{3}+2=\frac{29}{6},\quad g(T_\infty)=\frac{3}{7^2}\left(\frac{29}{6}-\frac{1}{6}\right)=\frac{27}{98}. \tag{12}$$

Finally, from (4),

$$g(G_{4,\infty},T_\infty)=\frac{g(G_{4,\infty})}{g(T_\infty)}=\frac{\frac{109}{162}}{\frac{27}{98}}=\boxed{\frac{109}{245}}\approx 0.445. \tag{13}$$

5 Conclusion

The analytical g-factor for the theta graph topology was derived using methods of symmetry reduction and the spectral trace identity for the normalized Laplacian. This derivation yields a precise theoretical g-factor of 109/245 (approximately 0.445), which corresponds to the tabulated value for this topology

6 Quick-Reference Identities

$$\begin{aligned}
\mathcal{L}&=I-D^{-1/2}AD^{-1/2},\\
\operatorname{Tr}\mathcal{L}^{+}&=\sum_{\lambda_i\neq 0}\frac{1}{\lambda_i},\\
g(G_\infty)&=\frac{3}{e(G)^2}\left(\operatorname{Tr}\mathcal{L}^{+}(G)+\frac{1}{3}\,\mathrm{Loops}(G)-\frac{1}{6}\right),\\
g(G_\infty,T_\infty)&=\frac{g(G_\infty)}{g(T_\infty)}.
\end{aligned}$$