Course: ChE 209: Introduction to Soft Matters & Polymers

Final Project: Part II

Derivation for the theoretical contraction factors $g(G_\infty, G_{\text{tree}\infty})$

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1 General Formula

The asymptotic g-factor $g(G_\infty)$ is calculated using the following formula:

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

Where:

- $e(G)$ is the number of edges in graph G.
- $v(G)$ is the number of vertices in graph G.
- loops(G) is the cycle rank of graph G, given by:

$$\mathrm{loops}(G) = e(G) - v(G) + 1$$

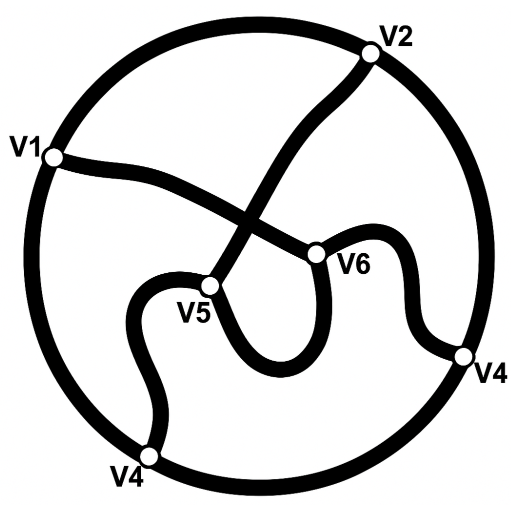
- $\mathrm{Tr}(L^+(G))$ is the trace of the Moore-Penrose pseudoinverse of the normalized graph Laplacian, $L(G)$. This is found by summing the reciprocals of all non-zero eigenvalues (λ_i) of the $L(G)$ matrix:

$$\mathrm{Tr}(L^+(G)) = \sum_{\lambda_i \neq 0} \frac{1}{\lambda_i}$$

- The normalized graph Laplacian $L(G)$ is a $v(G) \times v(G)$ matrix defined as:

$$L_{ij} = \begin{cases} 1 - \frac{2\times(\text{no. of loop edges})}{deg(i)} & \text{if } i = j \\ \frac{-R}{\sqrt{deg(i)deg(j)}} & \text{if } v_i, v_j \text{ are joined by } R \text{ edges} \\ 0 & \text{otherwise} \end{cases}$$

2 Calculation for Alpha-like Polymer (G_α)



For this graph, we have:

- Vertices: $v(G_\alpha) = 6$
- Edges: $e(G_\alpha) = 9$

All vertices have a degree of 3 ($deg(v_i) = 3$). A 6×6 matrix will be formed.

2.1 Laplacian Matrix $L(G_\alpha)$

Since this polymer has no loop edges, all diagonal entries are $L_{ii} = 1 - 0 = 1$.

$$L_{11} = L_{22} = L_{33} = L_{44} = L_{55} = L_{66} = 1$$

For the non-diagonal entries for connected vertices (with $R = 1$), the value is:

$$L_{ij} = \frac{-1}{\sqrt{deg(i)deg(j)}} = \frac{-1}{\sqrt{3 \times 3}} = -\frac{1}{3}$$

Calculating the entries for the first row (vertex v_1) as an example:

$$\begin{aligned}
L_{12} &= -1/3 \quad \text{(connected to } v_2\text{)} \\
L_{13} &= 0 \quad \text{(not connected to } v_3\text{)} \\
L_{14} &= -1/3 \quad \text{(connected to } v_4\text{)} \\
L_{15} &= 0 \quad \text{(not connected to } v_5\text{)} \\
L_{16} &= -1/3 \quad \text{(connected to } v_6\text{)}
\end{aligned}$$

Similarly, we can calculate all other entries. The full 6×6 matrix is:

$$\mathbf{L}(G_\alpha) = \begin{pmatrix} 1 & -1/3 & 0 & -1/3 & 0 & -1/3 \\ -1/3 & 1 & -1/3 & 0 & -1/3 & 0 \\ 0 & -1/3 & 1 & -1/3 & 0 & -1/3 \\ -1/3 & 0 & -1/3 & 1 & -1/3 & 0 \\ 0 & -1/3 & 0 & -1/3 & 1 & -1/3 \\ -1/3 & 0 & -1/3 & 0 & -1/3 & 1 \end{pmatrix}$$

2.2 Eigenvalues and Trace

To find the eigenvalues, we solve $|L(G_\alpha) - \lambda I| = 0$, where I is the identity matrix. After computation, the eigenvalues (λ) are:

$$\lambda = \{0, 1, 1, 1, 1, 2\}$$

Now, to find $\text{Tr}(L^+(G_\alpha))$, we sum the reciprocals of the non-zero eigenvalues:

$$\text{Tr}(L^+(G_\alpha)) = \frac{1}{1} + \frac{1}{1} + \frac{1}{1} + \frac{1}{1} + \frac{1}{2} = 1 + 1 + 1 + 1 + 0.5 = 4.5$$

2.3 g-factor $g(G_\alpha)$

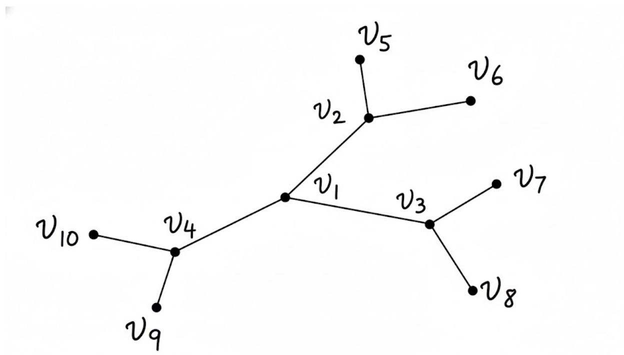
First, we find the cycle rank:

$$\text{loops}(G_\alpha) = e(G) - v(G) + 1 = 9 - 6 + 1 = 4$$

Now, we calculate the g-factor:

$$\begin{aligned}
g(G_\alpha) &= \frac{3}{e(G_\alpha)^2}\left(\text{Tr}(L^+(G_\alpha)) + \frac{1}{3}\text{loops}(G_\alpha) - \frac{1}{6}\right) \\
&= \frac{3}{9^2}\left(4.5 + \frac{1}{3}(4) - \frac{1}{6}\right) \\
&= \frac{3}{81}\left(\frac{9}{2} + \frac{7}{6}\right) \\
&= \frac{3}{81}\left(\frac{27}{6} + \frac{7}{6}\right) = \frac{3}{81}\left(\frac{34}{6}\right) \\
&= \frac{3}{81}\left(\frac{17}{3}\right) \\
&= \frac{17}{81}
\end{aligned}$$

3 Calculation for Tree Graph ($G_{\textbf{tree}}$)



For this graph, we have:

- Vertices: $v(G_{\text{tree}}) = 10$
- Edges: $e(G_{\text{tree}}) = 9$

A 10×10 matrix will be made.

3.1 Laplacian Matrix $L(G_{\mathbf{tree}})$

$$\mathbf{L}(G_{\text{tree}}) = \begin{pmatrix} 1 & -1/3 & -1/3 & -1/3 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1/3 & 1 & 0 & 0 & -1/\sqrt{3} & -1/\sqrt{3} & 0 & 0 & 0 & 0 \\ -1/3 & 0 & 1 & 0 & 0 & 0 & -1/\sqrt{3} & -1/\sqrt{3} & 0 & 0 \\ -1/3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1/\sqrt{3} & -1/\sqrt{3} \\ 0 & -1/\sqrt{3} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/\sqrt{3} & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1/\sqrt{3} & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1/\sqrt{3} & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1/\sqrt{3} & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1/\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

3.2 Eigenvalues and Trace

After computation, the 10 eigenvalues are:

$$\lambda = \Big\{0, 1, 1, 1, 1, 2, \\ 1 - \sqrt{\frac{2}{3}}, 1 + \sqrt{\frac{2}{3}}, 1 - \sqrt{\frac{2}{3}}, 1 + \sqrt{\frac{2}{3}}\Big\}$$

We sum the reciprocals of all non-zero eigenvalues to get $\text{Tr}(L^+(G_{\text{tree}}))$.

$$\text{Sum of } \frac{1}{1} \text{ (4 times)} = 4$$

$$\text{Sum of } \frac{1}{2} = 0.5$$

$$\text{Sum of reciprocal pairs:} \quad 2 \times \left(\frac{1}{1 - \sqrt{2/3}} + \frac{1}{1 + \sqrt{2/3}} \right) = 2 \times \left(\frac{(1 + \sqrt{2/3}) + (1 - \sqrt{2/3})}{(1 - 2/3)} \right)$$
$$= 2 \times \left(\frac{2}{1/3} \right) = 2 \times 6 = 12$$

Total trace (matching your note):

$$\text{Tr}(L^+(G_{\text{tree}})) = 4 + 0.5 + 12 = 16.5$$

3.3 g-factor $g(G_{\mathbf{tree}})$

The cycle rank is:

$$\text{loops}(G_{\text{tree}}) = e(G) - v(G) + 1 = 9 - 10 + 1 = 0$$

Now, we calculate the g-factor:

$$
\begin{aligned}
g(G_{\text{tree}}) &= \frac{3}{e(G_{\text{tree}})^2}\left(\text{Tr}(L^+(G_{\text{tree}})) + \frac{1}{3}\text{loops}(G_{\text{tree}}) - \frac{1}{6}\right) \\
&= \frac{3}{9^2}\left(16.5 + \frac{1}{3}(0) - \frac{1}{6}\right) \\
&= \frac{3}{81}\left(16.5 - \frac{1}{6}\right) \\
&= \frac{3}{81}\left(\frac{33}{2} - \frac{1}{6}\right) \\
&= \frac{3}{81}\left(\frac{99}{6} - \frac{1}{6}\right) \\
&= \frac{3}{81}\left(\frac{98}{6}\right) = \frac{3}{81}\left(\frac{49}{3}\right) \\
&= \frac{49}{81}
\end{aligned}
$$

4 Final Relative g-factor

The relative g-factor is the ratio of $g(G_\alpha)$ to $g(G_{\text{tree}})$:

$$
g_{\text{relative}} = \frac{g(G_\alpha)}{g(G_{\text{tree}})} = \frac{17/81}{49/81} = \boxed{\frac{17}{49}}
$$