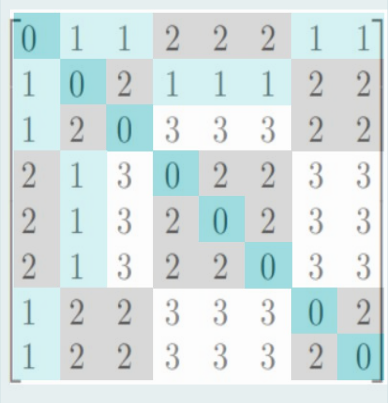
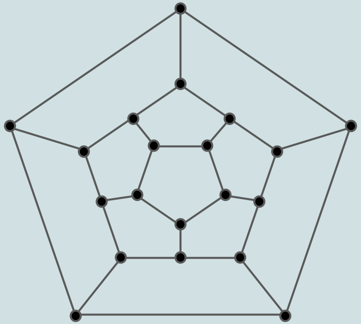
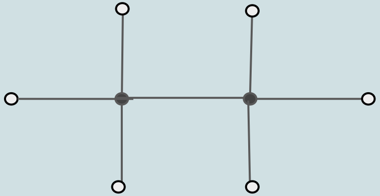


$$\begin{bmatrix} 0&1&1&2&2&2&1&1\\ 1&0&2&1&1&1&2&2\\ 1&2&0&3&3&3&2&2\\ 2&1&3&0&2&2&3&3\\ 2&1&3&2&0&2&3&3\\ 2&1&3&2&2&0&3&3\\ 1&2&2&3&3&3&0&2\\ 1&2&2&3&3&3&2&0 \end{bmatrix}$$

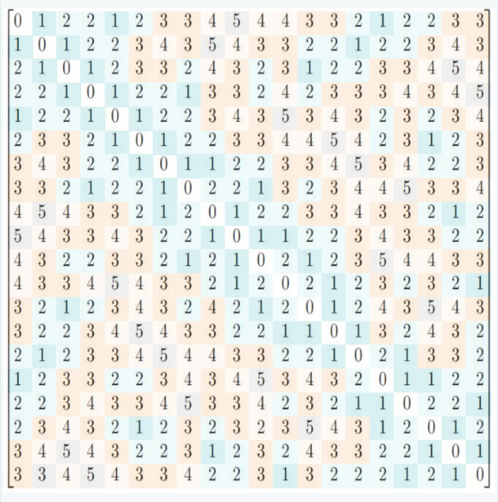
Bounds on the Largest Eigenvalue a of Distance Matrix





Natalie Denny

Advisor: John Caughman
Second Reader: Derek Garton



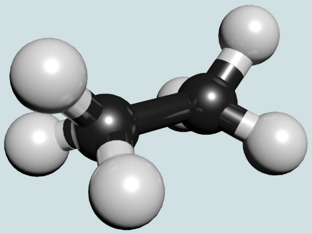
$$\begin{bmatrix}
0&1&2&2&1&2&3&3&4&5&4&4&3&3&2&1&2&2&3&3\\
1&0&1&2&2&3&4&3&5&4&3&3&2&2&1&2&2&3&4&3\\
2&1&0&1&2&3&3&2&4&3&2&3&1&2&2&3&3&4&5&4\\
2&2&1&0&1&2&2&1&3&3&2&4&2&3&3&3&4&3&4&5\\
1&2&2&1&0&1&2&2&3&4&3&5&3&4&3&2&3&2&3&4\\
2&3&3&2&1&0&1&2&2&3&3&4&4&5&4&2&3&1&2&3\\
3&4&3&2&2&1&0&1&1&2&2&3&3&4&5&3&4&2&2&3\\
3&3&2&1&2&2&1&0&2&2&1&3&2&3&4&4&5&3&3&4\\
4&5&4&3&3&2&1&2&0&1&2&2&3&3&4&3&3&2&1&2\\
5&4&3&3&4&3&2&2&1&0&1&1&2&2&3&4&3&3&2&2\\
4&3&2&2&3&3&2&1&2&1&0&2&1&2&3&5&4&4&3&3\\
4&3&3&4&5&4&3&3&2&1&2&0&2&1&2&3&2&3&2&1\\
3&2&1&2&3&4&3&2&4&2&1&2&0&1&2&4&3&5&4&3\\
3&2&2&3&4&5&4&3&3&2&2&1&1&0&1&3&2&4&3&2\\
2&1&2&3&3&4&5&4&4&3&3&2&2&1&0&2&1&3&3&2\\
1&2&3&3&2&2&3&4&3&4&5&3&4&3&2&0&1&1&2&2\\
2&2&3&4&3&3&4&5&3&3&4&2&3&2&1&1&0&2&2&1\\
2&3&4&3&2&1&2&3&2&3&2&3&5&4&3&1&2&0&1&2\\
3&4&5&4&3&2&2&3&1&2&3&2&4&3&3&2&2&1&0&1\\
3&3&4&5&4&3&3&4&2&2&3&1&3&2&2&2&1&2&1&0
\end{bmatrix}$$

Overview

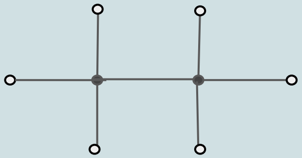
- "On the Largest Eigenvalue of the Distance Matrix of a Connected Graph" by Bo Zhou and Nenad Trinajstic
- Application to Chemistry/Chemical Graph Theory
- The Distance Matrix of a Graph
- Bounds on the Largest Eigenvalue
- Nordhaus-Gaddum type result

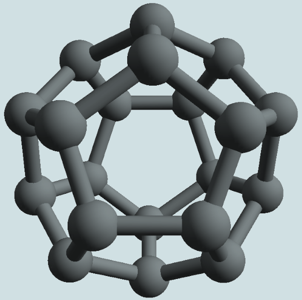
Application to Chemistry

Eigenvalues of distance matrices are used in chemical QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) modeling.

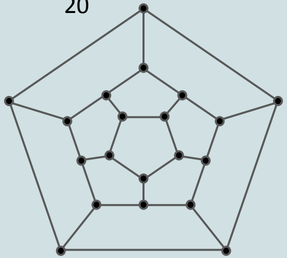


C_2H_6 (Ethane)





C_{20} Fullerene



The Wiener Index

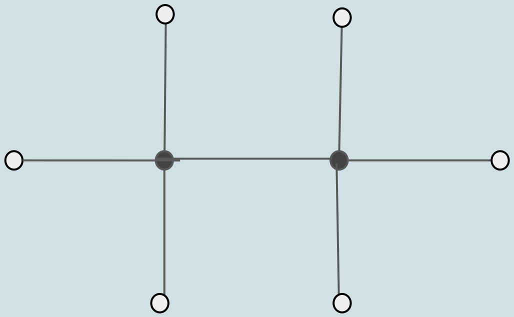
- Named for Harry Wiener (Chemist, Medical Doctor, Pharmaceutical Executive, Psychiatry Researcher)

- The First Topological Index (1947): originally called “The Path Number”

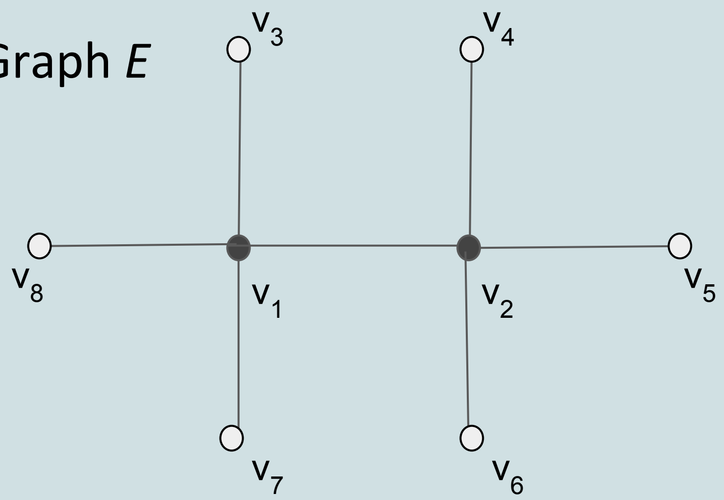
- Was the seed to further molecular descriptors such as using eigenvalues of distance matrices (Bonchev & Trinajstic, 1977)

0	1	1	2	2	2	1	1
1	0	2	1	1	1	2	2
1	2	0	3	3	3	2	2
2	1	3	0	2	2	3	3
2	1	3	2	0	2	3	3
2	1	3	2	2	0	3	3
1	2	2	3	3	3	0	2
1	2	2	3	3	3	2	0

C_2H_6



Graph *E*



$$D_E = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \end{array} \begin{array}{c} \begin{array}{cccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 2 & 2 & 2 & 1 & 1 \\ 1 & 0 & 2 & 1 & 1 & 1 & 2 & 2 \\ 1 & 2 & 0 & 3 & 3 & 3 & 2 & 2 \\ 2 & 1 & 3 & 0 & 2 & 2 & 3 & 3 \\ 2 & 1 & 3 & 2 & 0 & 2 & 3 & 3 \\ 2 & 1 & 3 & 2 & 2 & 0 & 3 & 3 \\ 1 & 2 & 2 & 3 & 3 & 3 & 0 & 2 \\ 1 & 2 & 2 & 3 & 3 & 3 & 2 & 0 \end{bmatrix} \end{array}$$

The Distance Matrix

$D_E =$

	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
v_1	0	1	1	2	2	2	1	1
v_2	1	0	2	1	1	1	2	2
v_3	1	2	0	3	3	3	2	2
v_4	2	1	3	0	2	2	3	3
v_5	2	1	3	2	0	2	3	3
v_6	2	1	3	2	2	0	3	3
v_7	1	2	2	3	3	3	0	2
v_8	1	2	2	3	3	3	2	0

- Real
- Symmetric
- Non-Negative
- Irreducible

Also uniquely determines a graph up to isomorphism!

The Wiener Index

Definition 2.2. *Let G be a connected graph with n vertices. Define*

$$W(G) = \sum_{1 \leq i < j \leq n} \boldsymbol{D}_{ij}.$$

In other words, $W(G)$ is the sum of the distances between all unordered pairs of vertices. We refer to $W(G)$ as the ***Wiener index*** *of G.*

D_E =

	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
v_1	0	1	1	2	2	2	1	1
v_2	1	0	2	1	1	1	2	2
v_3	1	2	0	3	3	3	2	2
v_4	2	1	3	0	2	2	3	3
v_5	2	1	3	2	0	2	3	3
v_6	2	1	3	2	2	0	3	3
v_7	1	2	2	3	3	3	0	2
v_8	1	2	2	3	3	3	2	0

$\Rightarrow$ **W(E) = 58**

S(G)

Definition 2.3. *Let G be a connected graph with n vertices. We define $S(G)$ to be the sum:*

$$S(G) = \sum_{u,v \in V(G)} dist(u,v)^2.$$

$D_E =$

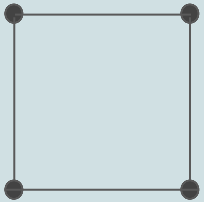
	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
v_1	0	1	1	2	2	2	1	1
v_2	1	0	2	1	1	1	2	2
v_3	1	2	0	3	3	3	2	2
v_4	2	1	3	0	2	2	3	3
v_5	2	1	3	2	0	2	3	3
v_6	2	1	3	2	2	0	3	3
v_7	1	2	2	3	3	3	0	2
v_8	1	2	2	3	3	3	2	0

$\Rightarrow$ **S(E) = 136**

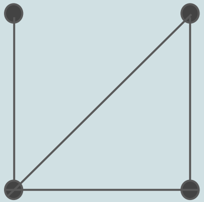
The Wiener Index & S(G) limitations

The Wiener index & S(G) do not uniquely determine a graph (and hence the underlying structure of the molecule).

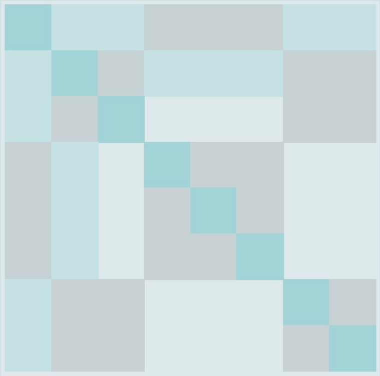
For example, consider the two graphs below.



$W(G_1) = 8$
$S(G_1) = 12$



$W(G_2) = 8$
$S(G_2) = 12$



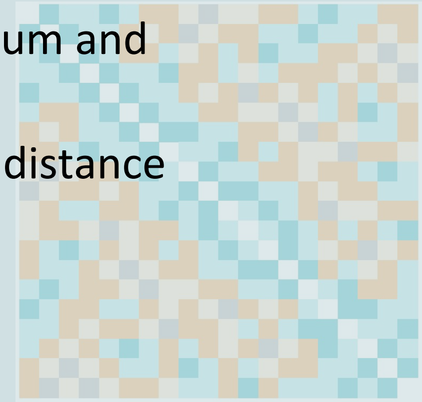
Bounds on the Largest Eigenvalue

$$0 < D_{min} \leq \lambda_{max} \leq D_{max}$$

Since distance matrices are real and non-negative, then by the Perron-Frobenius theorem we know that the largest eigenvalue is unique and positive. It is called the Perron root or the Perron-Frobenius eigenvalue.

Perron-Frobenius also gives us that λ_{max} is bounded by the minimum and maximum row sum.

Let D_{min} and D_{max} be the minimum and maximum row sum of the distance matrix respectively.



Bounds on the Largest Eigenvalue

$$D_{min} \leq \Lambda(G) \leq D_{max}$$

$$D_E = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \end{array} \begin{array}{c} \begin{array}{cccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 2 & 2 & 2 & 1 & 1 \\ 1 & 0 & 2 & 1 & 1 & 1 & 2 & 2 \\ 1 & 2 & 0 & 3 & 3 & 3 & 2 & 2 \\ 2 & 1 & 3 & 0 & 2 & 2 & 3 & 3 \\ 2 & 1 & 3 & 2 & 0 & 2 & 3 & 3 \\ 2 & 1 & 3 & 2 & 2 & 0 & 3 & 3 \\ 1 & 2 & 2 & 3 & 3 & 3 & 0 & 2 \\ 1 & 2 & 2 & 3 & 3 & 3 & 2 & 0 \end{bmatrix} \end{array}$$

$$\Rightarrow 10 \leq \Lambda(E) \leq 16$$

Bounds on the Largest Eigenvalue

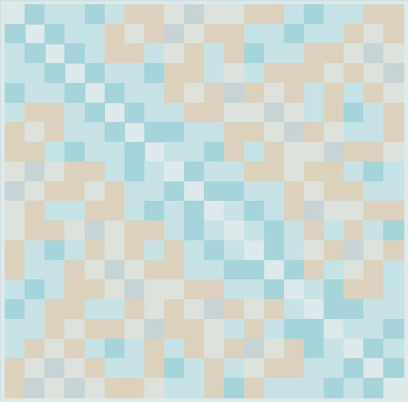
$$D_{min} \leq \mathbf{\Lambda}(G) \leq n(n-1)/2$$

$$D_{max}$$

What about that maximum row sum?

$$D_G = \begin{bmatrix} 0 & 1 & 2 & 3 & \cdots & n-1 \\ & & & & & \\ & & & & & \end{bmatrix}$$

$\Rightarrow D_M \leq n(n-1)/2$



Bounds on the Largest Eigenvalue

$$D_{min} \leq \mathbf{\Lambda}(G) \leq n(n-1)/2$$

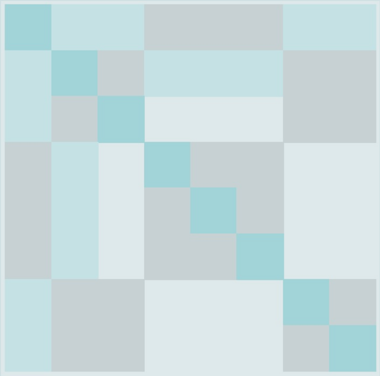
Lemma 4.3. *Let D_M be the maximum row sum of the distance matrix $\mathbf{D}$. Let G be a connected graph with n vertices and diameter d. Then*

$$D_M \leq \sum_{i=1}^{d-1} i + (n-d)(d) \leq \frac{n(n-1)}{2}$$

and equality holds if and only if G is a path of length $n-1$.

$D_M(E) \leq 1 + 2 + (8-3)(3) = 18$

And we saw that actually, $D_M(E) = 16$.

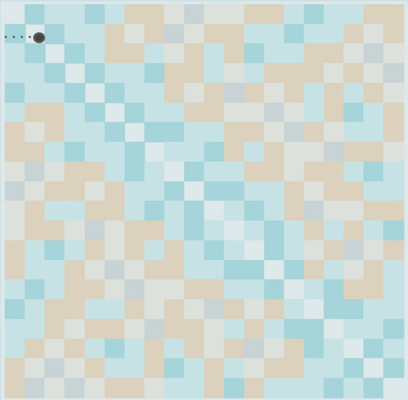


Bounds on the Largest Eigenvalue

$$D_{min} \leq \mathbf{\Lambda}(G) \leq n(n-1)/2$$

Corollary 4.3.1. *Let G be a path with n vertices, then the row sums of the distance matrix are not equal.*

$$D_G = \begin{bmatrix} 0 & 1 & 2 & 3 & & \cdots & n-1 \\ 1 & 0 & 1 & 2 & 3 & \cdots & n-2 \\ & & & & & & \\ & & & & & & \end{bmatrix}$$

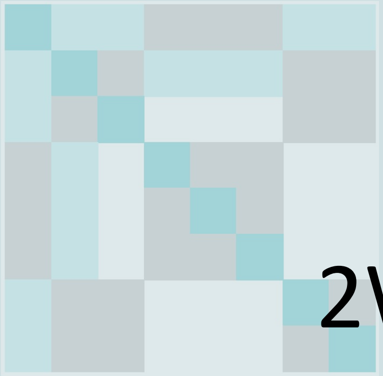


Bounds on the Largest Eigenvalue

$$D_{min} \leq \Lambda(G) < n(n-1)/2$$

Using the Rayleigh Quotient, we can deduce that the upper bound is only equal to the largest row sum when the row sums are equivalent. So for $n \geq 3$, you have a strict less than $n(n-1)/2$.

$$D_G = \begin{bmatrix} 0 & 1 & 2 & 3 & & \dots & n-1 \\ 1 & 0 & 1 & 2 & 3 & \dots & n-2 \\ & & & & & & \\ & & & & & & \end{bmatrix}$$



Bounds on the Largest Eigenvalue

$2W(G)/n \leq \mathbf{\Lambda}(G) < n(n-1)/2$

D_{min}

Lemma 5.3. *[6, Cor.7] Let Λ be the largest eigenvalue of the distance matrix, $\boldsymbol{D}$. Then*

$$\Lambda \geq \frac{2}{n} W(G)$$

with equality if and only if the row sums of $\boldsymbol{D}$ are all equal.

Previously, $10 \leq \mathbf{\Lambda}(E) < 16$.

Now by Lemma 5.3, $14.5 \leq \mathbf{\Lambda}(E) < 16$.

Bounds on the Largest Eigenvalue

$$2W(G)/n \leq \boldsymbol{\Lambda}(G) < n(n-1)/2$$

Lemma 5.4. *[6, Cor.8] Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$\Lambda \geq 2(n-1) - \frac{2m}{n}$$

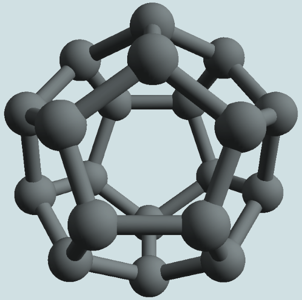
with equality if and only if $G = K_n$ or G is a regular graph of diameter two.

This lower bound is always at most 2W(G)/n. But gives a way to express the lower bound in terms of edges of the graph.

Wiener Index still wins!

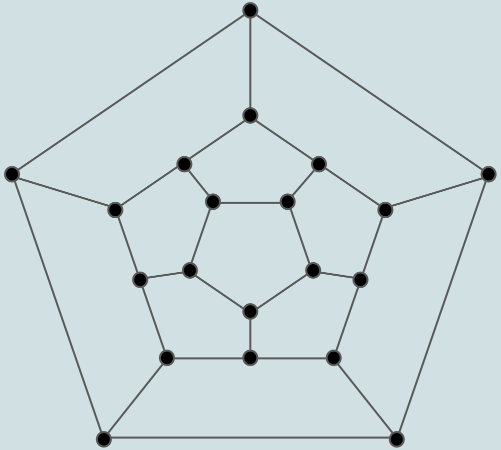
Previously, $14.5 \leq \boldsymbol{\Lambda}(E) < 16$.

By Lemma 5.4, $12.25 \leq \boldsymbol{\Lambda}(E)$.



Another Example: C_{20}

Graph C:



C is distance-regular with diameter 5 and valency 3

$$D_C=\begin{bmatrix}
0&1&2&2&1&2&3&3&4&5&4&4&3&3&2&1&2&2&3&3\\
1&0&1&2&2&3&4&3&5&4&3&3&2&2&1&2&2&3&4&3\\
2&1&0&1&2&3&3&2&4&3&2&3&1&2&2&3&3&4&5&4\\
2&2&1&0&1&2&2&1&3&3&2&4&2&3&3&3&4&3&4&5\\
1&2&2&1&0&1&2&2&3&4&3&5&3&4&3&2&3&2&3&4\\
2&3&3&2&1&0&1&2&2&3&3&4&4&5&4&2&3&1&2&3\\
3&4&3&2&2&1&0&1&1&2&2&3&3&4&5&3&4&2&2&3\\
3&3&2&1&2&2&1&0&2&2&1&3&2&3&4&4&5&3&3&4\\
4&5&4&3&3&2&1&2&0&1&2&2&3&3&4&3&3&2&1&2\\
5&4&3&3&4&3&2&2&1&0&1&1&2&2&3&4&3&3&2&2\\
4&3&2&2&3&3&2&1&2&1&0&2&1&2&3&5&4&4&3&3\\
4&3&3&4&5&4&3&3&2&1&2&0&2&1&2&3&2&3&2&1\\
3&2&1&2&3&4&3&2&4&2&1&2&0&1&2&4&3&5&4&3\\
3&2&2&3&4&5&4&3&3&2&2&1&1&0&1&3&2&4&3&2\\
2&1&2&3&3&4&5&4&4&3&3&2&2&1&0&2&1&3&3&2\\
1&2&3&3&2&2&3&4&3&4&5&3&4&3&2&0&1&1&2&2\\
2&2&3&4&3&3&4&5&3&3&4&2&3&2&1&1&0&2&2&1\\
2&3&4&3&2&1&2&3&2&3&2&3&5&4&3&1&2&0&1&2\\
3&4&5&4&3&2&2&3&1&2&3&2&4&3&3&2&2&1&0&1\\
3&3&4&5&4&3&3&4&2&2&3&1&3&2&2&2&1&2&1&0
\end{bmatrix}$$

$$\begin{bmatrix}
0&1&2&2&1&2&3&3&4&5&4&4&3&3&2&1&2&2&3&3\\
1&0&1&2&2&3&4&3&5&4&3&3&2&2&1&2&2&3&4&3\\
2&1&0&1&2&3&3&2&4&3&2&3&1&2&2&3&3&4&5&4\\
2&2&1&0&1&2&2&1&3&3&2&4&2&3&3&3&4&3&4&5\\
1&2&2&1&0&1&2&2&3&4&3&5&3&4&3&2&3&2&3&4\\
2&3&3&2&1&0&1&2&2&3&3&4&4&5&4&2&3&1&2&3\\
3&4&3&2&2&1&0&1&1&2&2&3&3&4&5&3&4&2&2&3\\
3&3&2&1&2&2&1&0&2&2&1&3&2&3&4&4&5&3&3&4\\
4&5&4&3&3&2&1&2&0&1&2&2&3&3&4&3&3&2&1&2\\
5&4&3&3&4&3&2&2&1&0&1&1&2&2&3&4&3&3&2&2\\
4&3&2&2&3&3&2&1&2&1&0&2&1&2&3&5&4&4&3&3\\
4&3&3&4&5&4&3&3&2&1&2&0&2&1&2&3&2&3&2&1\\
3&2&1&2&3&4&3&2&4&2&1&2&0&1&2&4&3&5&4&3\\
3&2&2&3&4&5&4&3&3&2&2&1&1&0&1&3&2&4&3&2\\
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1&2&3&3&2&2&3&4&3&4&5&3&4&3&2&0&1&1&2&2\\
2&2&3&4&3&3&4&5&3&3&4&2&3&2&1&1&0&2&2&1\\
2&3&4&3&2&1&2&3&2&3&2&3&5&4&3&1&2&0&1&2\\
3&4&5&4&3&2&2&3&1&2&3&2&4&3&3&2&2&1&0&1\\
3&3&4&5&4&3&3&4&2&2&3&1&3&2&2&2&1&2&1&0
\end{bmatrix}$$

Another Example: C_{20}

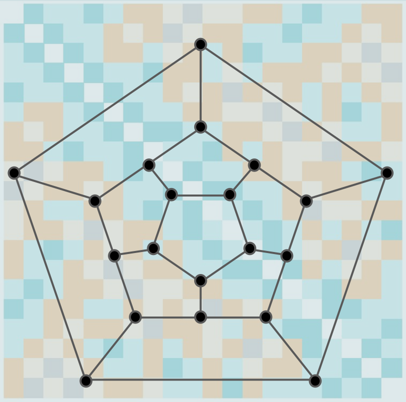
Distance-Regular gives us Equal Row Sums

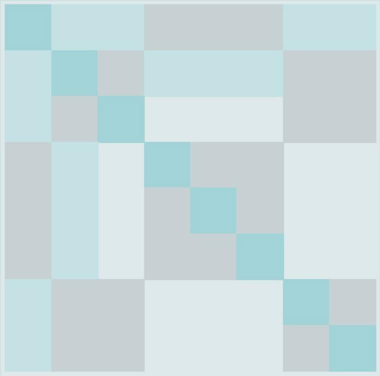
(D_i = 50 for all i)

So, W(C) =½ (20)(50) = 500

So by the Perron-Frobenius theorem,

Λ(C) = 50.



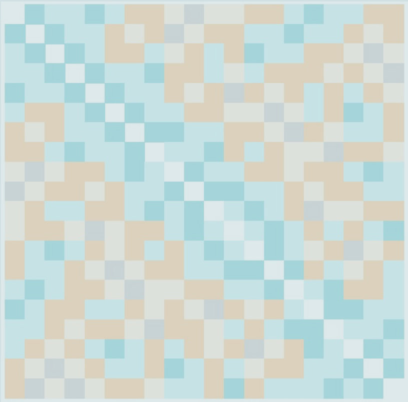


Bounds on the Largest Eigenvalue of Graphs in Class $\mathbb{G}$

The previous two examples also belong to a special class of graphs that have *exactly one* positive eigenvalue for the distance matrix. We denote this class with $\mathbb{G}$.

$\mathbb{G}$ includes:

- Infinite families such as:
  - Trees, C_n (cycles), Johnson, Hamming, Cocktail Party, Double Half Cubes
- Dodecahedron & Icosahedron
- Petersen graph



Bounds on the Largest Eigenvalue of Graphs in Class $\mathbb{G}$

Lemma 5.1. *[6, Eqn (1)], Let G be a connected graph with $n \geq 2$ vertices and let λ_i $(1 \leq i \leq n)$ be the eigenvalues of the distance matrix $\mathbf{D}$ of G. Then*

$$\sum_{i=1}^{n} \lambda_i = 0.$$

Lemma 5.2. *[6, Eqn (2)] Let G be a connected graph with $n \geq 2$ vertices and let λ_i $(1 \leq i \leq n)$ be the eigenvalues of the distance matrix $\mathbf{D}$ of G. Then*

$$\sum_{i=1}^{n} \lambda_i^2 = 2S(G)$$

Bounds on the Largest Eigenvalue of Graphs in Class $\mathbb{G}$

$$2W(G)/n \le \mathbf{\Lambda}(G) \le \sqrt{[2(n-1)/n]S(G)}$$

Theorem 6.2. *[6, Eqn(4)] Let $G \in \mathbb{G}$ with $n \ge 2$ vertices. Then*

$$\Lambda \le \sqrt{\frac{2(n-1)}{n} S(G)},$$

with equality if and only if $G = K_n$.

Previously, $14.5 \le \mathbf{\Lambda}(E) < 16$.
By Thm 6.2, $14.5 \le \mathbf{\Lambda}(E) < 15.427$.

Compare to $\mathbf{\Lambda}(C) = 50$.
Thm 6.2 gives $\mathbf{\Lambda}(C) < 54.093$.

Nordhaus-Gaddum Type Results

Theorem 7.2. *[6, Eqn (11)] Let G be a connected graph on $n \geq 4$ vertices with a connected complement $\overline{G}$. Then*

$$3(n-1) \leq \Lambda(G) + \Lambda(\overline{G}) < \frac{n(n+3)}{2} - 3,$$

with left equality if and only if G and $\overline{G}$ are both regular graphs of diameter two.

~~**Theorem**~~ Conjecture? **7.3.** *[6, Eqn (12)] Let G be a connected graph on $n \geq 4$ vertices with a connected complement $\overline{G}$. If $G \in \mathbb{G}$ or $\overline{G} \in \mathbb{G}$, then*

$$\Lambda(G) + \Lambda(\overline{G}) < \sqrt{\frac{(n+1)n(n-1)^2}{6}} + 2n - 3.$$

Questions

(as long as they aren't about chemistry :)

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References

[1] Ghodratollah Aalipour, Aida Abiad, Zhanar Berikkyzy, Jay Cummings, Jessica De Silva, Wei Gao, Kristin Heysse, Leslie Hogbend, Franklin H.J. Kenter, Jephian C.-H.Lin, and Michael Taite. On the distance spectra of graphs. *Linear Algebra and its Applications*, 497:66–87, 2016.

[2] D. Cao, V. Chvatal, A.J. Hoffman, and A. Vince. Variations on a theorem of ryser. *Linear Algebra and its Applications*, 260:215–222, 1997.

[3] James Devillers and Alexandru T Balaban. *Topological Indices and Related Descriptors in QSAR and QSPR*. CRC Press, 2000.

[4] K Roy, S Kar, and RN Das. *A primer on QSAR/QSPR modeling: Fundamental Concepts*. Springer-Verlag Inc., 2015.

[5] Bo Zhou. On the largest eigenvalue of the distance matrix of a tree. *MATCH Communications in Mathematical and Computer Chemistry*, 58:657–662, 2007.

[6] Bo Zhou and Nenad Trinajstic. On the largest eigenvalue of the distance matrix of a connected graph. *Chemical Physical Letters*, 447:384–387, 2007.