The spectral theory of graphs

Mariano Suárez-Álvarez
Universidad de Buenos Aires / CONICET — GTIIT

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Graphs

A graph is a pair $G = (V, E)$ with

- V a set
- E a set of two element subsets of V

Example (A little example)

$G = (V, E)$ with

$$V = \{1, 2, 3, 4, 5\},$$
$$E = \{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 1\}, \{3, 5\}\}.$$

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Graphs

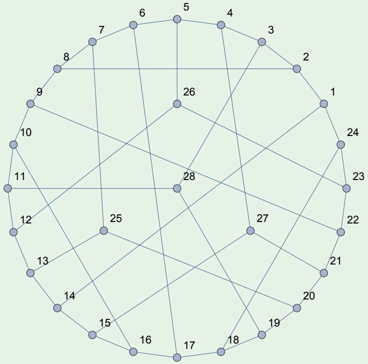
Example (The Coxeter graph)

$$V = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28\},$$

$$E = \big\{\{1, 2\}, \{1, 14\}, \{1, 24\}, \{2, 3\}, \{2, 8\}, \{3, 4\}, \{3, 28\}, \{4, 5\}, \{4, 27\}, \{5, 6\}, \{5, 26\}, \{6, 7\}, \{6, 17\}, \{7, 8\}, \{7, 25\}, \{8, 9\}, \{9, 10\}, \{9, 22\}, \{10, 11\}, \{10, 16\}, \{11, 12\}, \{11, 28\}, \{12, 13\}, \{12, 26\}, \{13, 14\}, \{13, 25\}, \{14, 15\}, \{15, 16\}, \{15, 27\}, \{16, 17\}, \{17, 18\}, \{18, 19\}, \{18, 24\}, \{19, 20\}, \{19, 28\}, \{20, 21\}, \{20, 25\}, \{21, 22\}, \{21, 27\}, \{22, 23\}, \{23, 24\}, \{23, 26\}\big\}$$

Graphs

Example (The Coxeter graph)



Graphs

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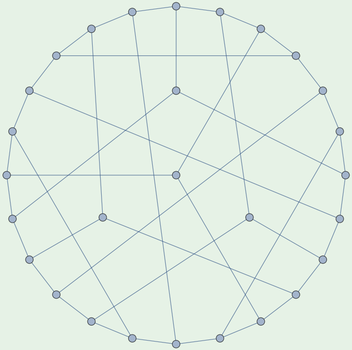

Graphs

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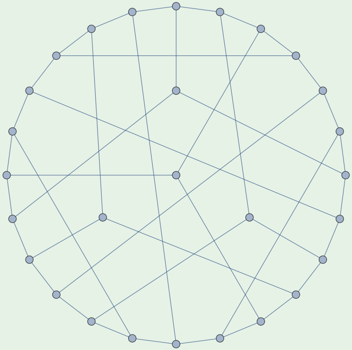

Coxeter, H. S. M. *My Graph.* Proc. London Math. Soc. **46**, 117-136, 1983.

Graphs

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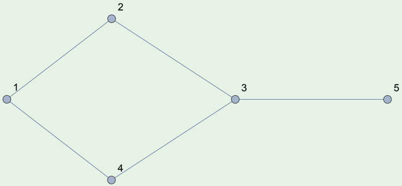
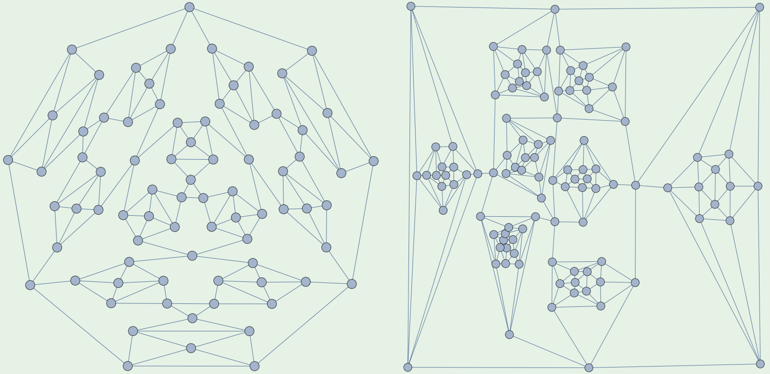


Graphs

Example (van Cleemput–Zamfirescu graphs)



van Cleemput, N. and Zamfirescu, C. T. *Regular Non-Hamiltonian Polyhedral Graphs.* Appl. Math. Comput. **338** 192-206, 2018.

Graphs

We write n for the *number of vertices* of a graph.

We will almost always suppose that the set of vertices is

$$V = \{1, 2, 3, \ldots, n\}.$$

The adjacency matrix

The *adjacency matrix* of a graph $G = (V, E)$ is the matrix

$$A = (a_{i,j}) \in \mathrm{M}_n(\mathbb{R}), \qquad a_{i,j} = \begin{cases} 1 & \text{if } \{i,j\} \in E; \\ 0 & \text{if not.} \end{cases}$$

Example

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

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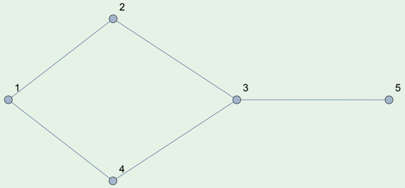


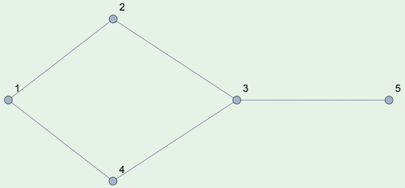
$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

The adjacency matrix

The entries of A have a very simple combinatorial interpretation:

$$a_{i,j} = \#\{\text{paths from } i \text{ to } j \text{ of length } 1\}.$$

Example



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The adjacency matrix

The observation generalizes:

Lemma

If $\ell \in \mathbb{N}_0$ *and* $A^\ell = (a_{i,j}^{(\ell)})$, *then*

$$a_{i,j}^{(\ell)} = \#\{\textit{paths from } i \textit{ to } j \textit{ of length } 1\}.$$

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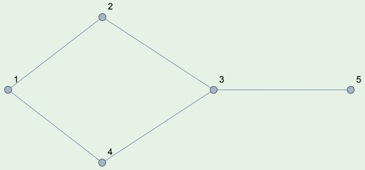

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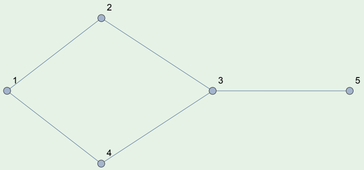

$$A^2 = \begin{pmatrix} 2 & 0 & 2 & 0 & 0 \\ 0 & 2 & 0 & 2 & 1 \\ 2 & 0 & 3 & 0 & 0 \\ 0 & 2 & 0 & 2 & 1 \\ 0 & 1 & 0 & 1 & 1 \end{pmatrix}$$

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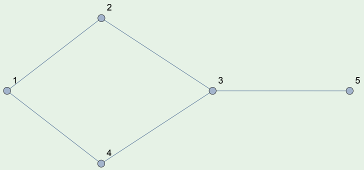

$$A^3 = \begin{pmatrix} 0 & 4 & 0 & 4 & 2 \\ 4 & 0 & 5 & 0 & 0 \\ 0 & 5 & 0 & 5 & 3 \\ 4 & 0 & 5 & 0 & 0 \\ 2 & 0 & 3 & 0 & 0 \end{pmatrix}$$

The adjacency matrix

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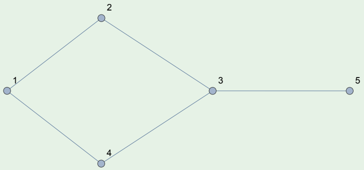

$$A^4 = \begin{pmatrix} 8 & 0 & 10 & 0 & 0 \\ 0 & 9 & 0 & 9 & 5 \\ 10 & 0 & 13 & 0 & 0 \\ 0 & 9 & 0 & 9 & 5 \\ 0 & 5 & 0 & 5 & 3 \end{pmatrix}$$

The adjacency matrix

Lemma

The number C_ℓ of closed paths of length ℓ is

$$\operatorname{tr} A^\ell = a_{1,1}^{(\ell)} + a_{2,2}^{(\ell)} + \cdots + a_{n,n}^{(\ell)}.$$

The adjacency matrix

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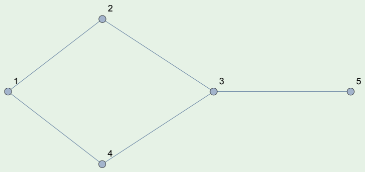

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$$\operatorname{tr} A^2 = 10$$

The adjacency matrix

Lemma

The number C_ℓ *of* *closed* *paths of length* ℓ *is*

$$\operatorname{tr} A^\ell = a_{1,1}^{(\ell)} + a_{2,2}^{(\ell)} + \cdots + a_{n,n}^{(\ell)}.$$

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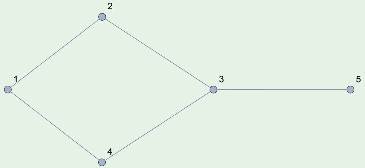

$$A^3 = \begin{pmatrix} 0 & 4 & 0 & 4 & 2 \\ 4 & 0 & 5 & 0 & 0 \\ 0 & 5 & 0 & 5 & 3 \\ 4 & 0 & 5 & 0 & 0 \\ 2 & 0 & 3 & 0 & 0 \end{pmatrix}$$

$$\operatorname{tr} A^3 = 0$$

The adjacency matrix

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The number C_ℓ of closed paths of length ℓ is

$$\operatorname{tr} A^\ell = a_{1,1}^{(\ell)} + a_{2,2}^{(\ell)} + \cdots + a_{n,n}^{(\ell)}.$$

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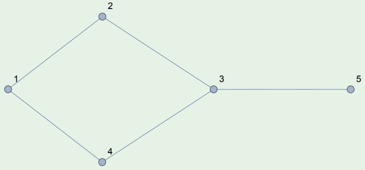

$$A^4 = \begin{pmatrix} 8 & 0 & 10 & 0 & 0 \\ 0 & 9 & 0 & 9 & 5 \\ 10 & 0 & 13 & 0 & 0 \\ 0 & 9 & 0 & 9 & 5 \\ 0 & 5 & 0 & 5 & 3 \end{pmatrix}$$

$$\operatorname{tr} A^4 = 42$$

The adjacency matrix

Linear algebra enters the picture

Since $A = (a_{i,j})$ has

$$a_{i,j} = \begin{cases} 1 & \text{if } \{i, j\} \in E; \\ 0 & \text{if not,} \end{cases}$$

it is a *symmetric* real matrix and therefore

- it is diagonalizable over $\mathbb{R}$ with real eigenvalues, and
- there is a orthonormal basis of $\mathbb{R}^n$ of eigenvectors of A.

Definition

We let θ_1, θ_2, ..., θ_n be the eigenvalues of A, indexed so that

$$\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n.$$

These numbers the *eigenvalues* of the graph G.

The adjacency matrix

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The adjacency matrix

Linear algebra enters the picture

We know there is an orthogonal matrix P such that

$$A = PDP^{-1}, \qquad D = \begin{pmatrix} \theta_1 & & & \\ & \theta_2 & & \\ & & \ddots & \\ & & & \theta_n \end{pmatrix}.$$

In particular, for all ℓ we have

$$\operatorname{tr} A^\ell = \operatorname{tr} D^\ell = \operatorname{tr} \begin{pmatrix} \theta_1^\ell & & & \\ & \theta_2^\ell & & \\ & & \ddots & \\ & & & \theta_n^\ell \end{pmatrix}$$

The adjacency matrix

Linear algebra enters the picture

Proposition

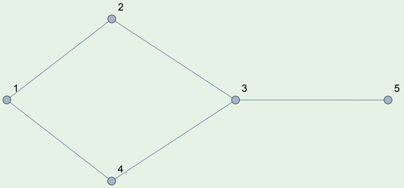
If $\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n$ are the eigenvalues of G, then the number of closed paths of length ℓ is

$$\theta_1^\ell + \theta_2^\ell + \cdots + \theta_n^\ell.$$

The adjacency matrix

Linear algebra enters the picture

Example



$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

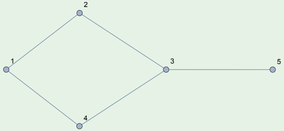
$$\chi_A(t) = t^5 - 5t^3 + 2t,$$

$$-\sqrt{\frac{1}{2}\left(5+\sqrt{17}\right)}, -\sqrt{\frac{1}{2}\left(5-\sqrt{17}\right)}, 0, \sqrt{\frac{1}{2}\left(5-\sqrt{17}\right)}, \sqrt{\frac{1}{2}\left(5+\sqrt{17}\right)}$$

The adjacency matrix

Linear algebra enters the picture

Example



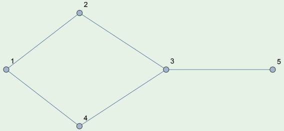
$$C_\ell = (1 + (-1)^\ell)\left(\left(\frac{1}{2}\left(5+\sqrt{17}\right)\right)^{\ell/2} + \left(\frac{1}{2}\left(5-\sqrt{17}\right)\right)^{\ell/2}\right)$$

$$C_{2\ell} \sim 2\left(\frac{1}{2}\left(5+\sqrt{17}\right)\right)^{\ell/2} \sim 2 \cdot 1.46143^\ell$$

The adjacency matrix

Linear algebra enters the picture

Example



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Linear algebra enters the picture

Proposition

The number of closed paths of length ℓ *is*

$$C_\ell \sim \rho^\ell$$

with $\rho := \max\{|\theta_1|, \ldots, |\theta_n|\}$.

The spectral theory of graphs

Our subject is the following problem:

Problem

Study the graph G by looking at properties of the sequence

$$\sigma(G) = (\theta_1, \theta_2, \ldots, \theta_n)$$

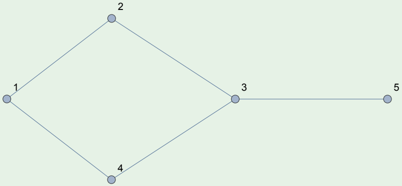
of its eigenvalues and the corresponding eigenvectors.

The part of mathematics that deals with this is the

spectral theory of graphs.

Spectra

Example



$$\begin{pmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

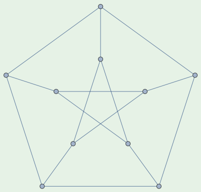
$$\chi(X) = t^5 - 5t^3 + 2t$$

$$\sigma = \left\{0, \pm\sqrt{\frac{1}{2}\left(5 \pm \sqrt{17}\right)}\right\}$$

$$= \{-2.135\ldots, -0.662\ldots, 0, 0.662\ldots, 2.135\ldots\}$$

Spectra

Example (The Petersen graph)

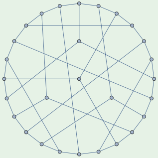


$$\chi(X) = t^{10} - 15t^8 + 75t^6 - 24t^5 - 165t^4 + 120t^3 + 120t^2 - 160t + 48$$

$$\sigma = \{-2, -2, -2, -2, 1, 1, 1, 1, 1, 3\}$$

Spectra

Example (The Coxeter graph)



$$\chi(X) = t^{28} - 42t^{26} + 777t^{24} - 8344t^{22} - 48t^{21} + 57666t^{20} + 1232t^{19} - 268716t^{18} - 13104t^{17} + 860314t^{16} + 74256t^{15} - 1893960t^{14} - 239568t^{13} + 2827965t^{12} + 433776t^{11} - 2790970t^{10} - 396816t^{9} + 1772925t^{8} + 118192t^{7} - 719376t^{6} + 44352t^{5} + 170464t^{4} - 37632t^{3} - 16128t^{2} + 7168t - 768$$

$$\sigma = \{-1-\sqrt{2}, -1-\sqrt{2}, -1-\sqrt{2}, -1-\sqrt{2}, -1-\sqrt{2}, -1-\sqrt{2}, -1, -1, -1, -1, -1, -1, -1, \sqrt{2}-1, \sqrt{2}-1, \sqrt{2}-1, \sqrt{2}-1, \sqrt{2}-1, \sqrt{2}-1, 2, 2, 2, 2, 2, 2, 2, 2, 3\}$$

The spectral theory of graphs

The diameter

The *diameter* of a graph is the maximal distance between its vertices.

Example

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The spectral theory of graphs

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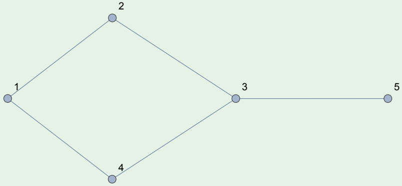

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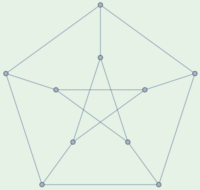

Proposition

If G is connected and d is its diameter, then G has at least $d+1$ different eigenvalues.

Proof. Let t be the number of distinct eigenvalues.

Since A is diagonalizable, its minimal polynomial has degree t, and there are real numbers α_0, ..., α_{t-1} such that

$$A^t = \alpha_0 A^0 + \alpha_1 A + \cdots + \alpha_{t-1} A^{t-1}.$$

Suppose $t \leq d$ and let i and j be two vertices such that $\operatorname{dist}(i,j) = t$. Then

$$a_{i,j}^{(t)} > 0 \qquad \text{and} \qquad a_{i,j}^{(k)} = 0 \quad \text{if } k < t.$$

This is absurd. □

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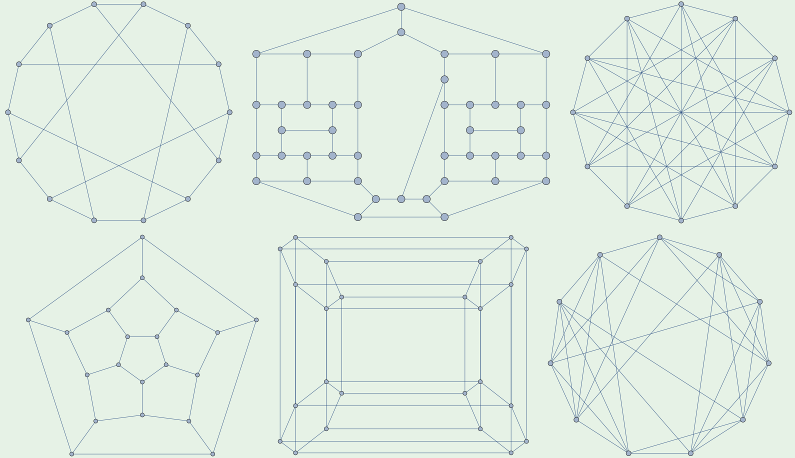
The spectral theory of graphs

Regular graphs

A graph is *regular* if all its vertices have the same number of neighbors. That number is then the *degree* of G.

Example



Proposition

Let G be a connected graph.

- *If G is regular of degree k, then $\theta_1 = k$.*
- *If G is not regular, then*

$$k_{\min} < \overline{k} < \theta_1 < k_{\max}$$

In any case, θ_1 is a simple eigenvalue.

Proof. The hypothesis means that

$$A \cdot 1 = k \cdot 1.$$

Moreover, if $t > k$, then the matrix

$$t \cdot I_n - A$$

is strictly diagonally dominant, so it is inversible. □

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G is regular if and only if $\sum_{i=1}^{n} \theta_i^2 = n \cdot \theta_1$.

Proof. If G is regular of degree k, then $\theta_1 = k$ and

$$\sum_{i=1}^{n} \theta_i^2 = \operatorname{tr} A^2 = \#\{\text{closed parths of length } 2\} = n \cdot k = n \cdot \theta_1.$$

Conversely, if the condition holds, then

$$\overline{k} = \frac{1}{n} \operatorname{tr} A^2 = \frac{1}{n} \sum_{i=1}^{n} \theta_i^2 = \theta_1$$

so the proposition tells us that the graph is regular. □

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The spectral theory of graphs

The largest eigenvalue

Since

$$\overline{k} < \theta_1$$

graphs with small θ_1 should be very simple...

Suppose G is connected.

- If $\theta_1 = 0$ then $G = K_1$.
- If $0 < \theta_1 \leq 1$, then $G = K_2$ and $\theta_1 = 1$.
- If $1 < \theta_1 \leq \sqrt{2}$, then G is a path of length 3 and $\theta_1 = \sqrt{2}$.

The spectral theory of graphs

The largest eigenvalue

Using Frobenius–Perron theory one can prove:

Proposition

If H is obtained from G by removing a vertex, then

$$\theta_1(H) < \theta_1(G).$$

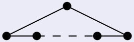
The spectral theory of graphs

The largest eigenvalue

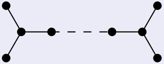
Theorem

Si G connected and $\theta_1 = 2$, then it is one of

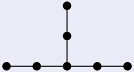
$\hat{A}_n, n \geq 2$



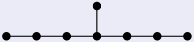
$\hat{D}_n,\ n \geq 4$



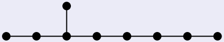
$\hat{E}_6$



$\hat{E}_7$



$\hat{E}_8$

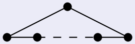


These are the *extended Dynkin diagrams*.

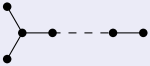
Theorem

Si G connected and $\theta_1 < 2$, then it is one of

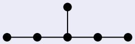
$\hat{A}_n, n \geq 2$



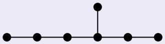
$\hat{D}_n,\ n \geq 4$



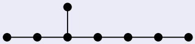
$\hat{E}_6$



$\hat{E}_7$



$\hat{E}_8$



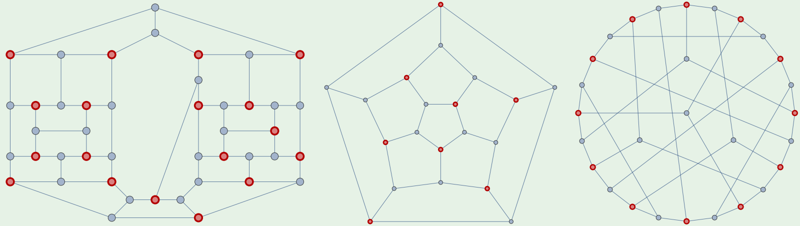
These are the *Dynkin diagrams*.

The spectral theory of graphs

The independence number

The *independence number* $\alpha(G)$ is the maximum cardinal of a set of vertices which are not neighbors of each other.

Example



Theorem

We have that

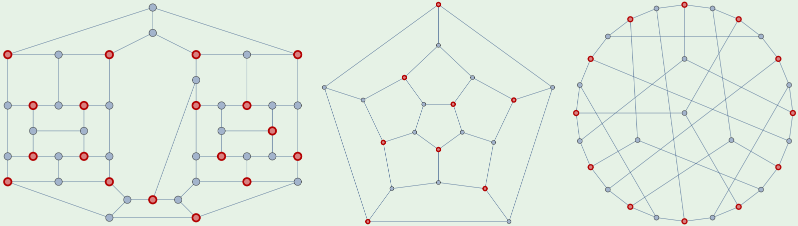
$$\alpha(G) \leq \#\{i : \theta_i \geq 0\}, \qquad \alpha(G) \leq \#\{i : \theta_i \leq 0\}$$

The spectral theory of graphs

The independence number

The *independence number* $\alpha(G)$ is the maximum cardinal of a set of vertices which are not neighbors of each other.

Example



Theorem

We have that

$$\alpha(G) \leq \#\{i : \theta_i \geq 0\}, \qquad \alpha(G) \leq \#\{i : \theta_i \leq 0\}$$

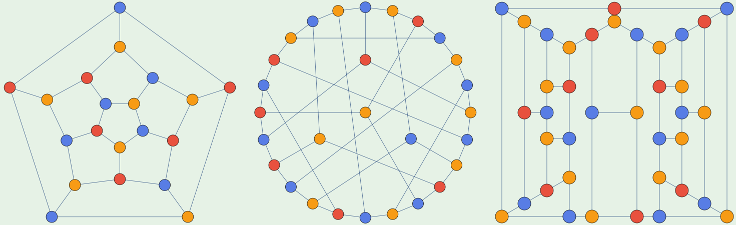
The spectral theory of graphs

The chromatic number

The *chromatic number* $\chi(G)$ is the minimum number of colors with which we can paint the vertices so that

no two neighbors have the same color

Example



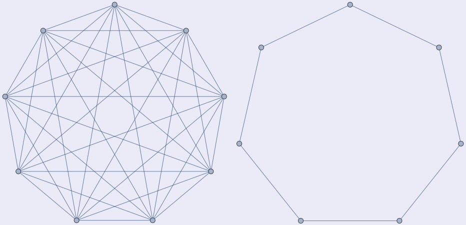
The spectral theory of graphs

The chromatic number

Theorem

Suppose G is connected with some edge.

- $\chi(G) \leq 1 + \theta_1$*, and the equality holds if and only if G is complete or an odd cycle.*



- $\chi(G) \geq 1 - \dfrac{\theta_1}{\theta_n}$.