

# **Eigenvalues of Graphs and Their Applications: Survey and New Results**

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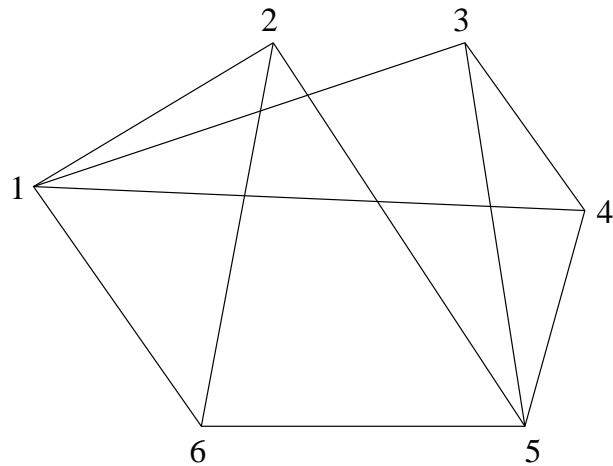
# 1. Introduction and Definitions

All graphs or digraphs considered here are simple unless otherwise specified. (This is just for simplicity, we may allow them to contain multiple edges or arcs).

**Definition 1.1.** Let  $G = (V, E)$  be a graph with vertex set  $V = \{v_1, v_2, \dots, v_n\}$  and edge set  $E = \{(v_i, v_j) | i, j = 1, 2, \dots, n; i \neq j\}$ . Its **adjacency matrix**  $A(G)$  is an  $n \times n$   $(0, 1)$ -matrix  $(a_{ij})$ , where

$$a_{ij} = \begin{cases} 1, & \text{if } (v_i, v_j) \text{ is an edge;} \\ 0, & \text{otherwise.} \end{cases}$$

**Example 1.1.** A graph  $G$  and its adjacency matrix



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

Note that, if  $G$  is a graph of  $n$  vertices,  $A(G)$  is an  $n \times n$  symmetric  $(0, 1)$ -matrix with zero diagonal entries .

**Definition 1.2.** The **eigenvalues of  $G$**  are the eigenvalues of its adjacency matrix  $A(G)$ . The collection of eigenvalues of  $G$  is called the **spectrum of  $G$** .

**Note 1:** Since  $A(G)$  is symmetric, the eigenvalues of  $G$ ,  $\lambda_i(G)$ ,  $i = 1, 2, \dots, n$ , are real numbers, so we may order them as

$$\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_k(G) \geq \lambda_{k+1}(G) \geq \dots \geq \lambda_n(G).$$

There is another kind of graph spectra, called *Laplacian spectra* [Chung, 1997]. We will not be involving here.

**Definition 1.3.**  $G_1 = (V_1, E_1)$  is called the *complement* of  $G_2 = (V_2, E_2)$  if  $V_1 = V_2$  and an edge  $e \in E_1$  iff  $e \notin E_2$ . The *complement* of  $G$  is written as  $G^c$ .

## Outline of the Presentation

1. Introduction, Definitions, and Applications
2. Some Recent Results on Graph Spectra
3. Spectra of Graphs with  $\lambda_3(G) < 0$
4. Graphs Characterized by  $\lambda_{n-2}(G)$
5. Two Conjectures

## 1.1. Why Eigenvalues of Graphs?

(1) Eigenvalues of graphs appear frequently in the mathematical sciences, physics and chemistry etc..

(2) The spectral techniques are useful in graph theory, combinatorics and the related areas in applied sciences (e.g. the dimer problem, Ice-type model, Ising model in Statistical Physics).

An **Open Problem**, which has recently been paid much attention:

*Which graphs have distinct eigenvalues?*

posed by Harary and Schwenk in 1974.

Representatives: [Cvetkovic et al., 95], [Biggs, 95], [Chung, 97], [Wilf et al., 98], [Golin et al., 04], [Wilf, 06]....

## 1.2. Examples

The eigenvalues of a graph characterize the topological structure of the graph.

Examples:

- (1) if  $\lambda_1(G) = -\lambda_n(G)$ , then  $G$  is bipartite;
- (2) if  $\lambda_2(G) = 0$ , then  $G$  is complete multi-partite;
- (3) if  $\lambda_2(G) = -1$ , then  $G$  is a complete graph;
- (4) ...

Representatives: [Cvetkovic et al., 95], [Biggs, 95], [Wilf et al., 98], [Yong, 99], [Wilf, 06] .....

## Why Eigenvalues of Graphs? (cont'd)

The technique is usually efficient in counting structures, e.g., acyclic digraphs, spanning trees, Hamiltonian cycles, independent sets, Eulerian orientations, cycle covers,  $k$ -colorings etc.. [Golin et al., 05] and its Refs., [Wilf, 06].

If a graph possesses certain properties, using its eigen-properties it is possible to derive (recurrence) formulas for counting the number of structures. Therefore, **counting structures can be algorithmic for certain graphs.**

Many graphs from applied sciences have the properties. [Stanley, 73], [Yong et al., 02], [Golin et al., 05],.....



## 1.3. The Eigenvalues in Applied Sciences

### 1.3.1. The Eigenvalues in Information Theory

In [Shannon information theory](#), the channel capacity, which characterizes the maximum amount of information that is transmitted over a channel or stored into a storage medium per bit, can be expressed in terms of the eigenvalues of its channel graph, e.g., [Wilf, 98], [Cohn, 95].

Combinatorically, the quantity is approached by counting the number of closed walks of length  $k$  in the channel graph  $G$  and then by letting the  $k$  tend to infinity.

Construction of the encoder/decoder for a given code is based on **the largest eigenvalue** of its channel graph. ([The information transmission rate](#) must be less than, but be expected to be very close to, the largest eigenvalue) [Cohn, 95], [Immink, 99].

### 1.3.2. The Eigenvalues in Coding Theory

In coding theory, the minimum *Hamming distance* of a linear code can be represented by the second largest eigenvalue of a regular graph. (the *Hamming distance* is the number of entries in which two codewords differ.)

A code with minimum Hamming distance  $d$  allows the correction of  $\lfloor d/2 \rfloor$  errors during the transmission over a noisy channel. [Spielman, 96]

Interested in regular graphs having smaller second largest eigenvalues — expanders.

### 1.3.3. The Eigenvalues in Quantum Chemistry

In **quantum chemistry**, the skeleton of a non-saturated hydrocarbon is represented by a graph. **The energy levels of the electrons in such a molecule are the eigenvalues of the graph.** The stability of molecules is closely related to the spectrum of its graph. [Cvetkovic et al., 95].

**Correspondences :**

*vertex* — *carbon atom*

*edge* — *bond*

*vertex degree* — *valency*

*adjacency matrix* — *topological matrix* — *Huckel matrix* ....

### 1.3.4. The Eigenvalues in Geographic Studies

In **geographic studies**, the eigenvalues and eigenvectors of a transportation network provide information about its connectedness. It is proven that the more highly connected in a transportation network  $G$  is, the larger is the  $\lambda_1(G)$ . [Tinkler, 72], [Roberts, 78].

Given the numbers of vertices and edges, how to design a network with a larger  $\lambda_1(G)$ ? — Interesting?

Only one paper is found, which arranges for **trees** according to the values of their largest eigenvalues [Zhang, 2002].

### 1.3.5. The Eigenvalues in Social Sciences

Social networks have been studied actively in **social sciences**, where the general feature is that the networks are viewed as static graphs whose vertices are 'individuals' and whose edges are the social interactions between these 'individuals'.

The problem here is to analyze the topology and dynamics of (given) data sets which have relationships between themselves in the network.

Interested in analyzing degree sequences and shortest connecting paths, which can be represented by the eigenvalues.

Representatives: [Roberts, 78], [Wasserman et al., 94], [Kochen, 89].

### 1.3.6. The Eigenvalues in Finite Dynamical Systems

A **finite dynamical system** is a time-discrete dynamical system on a finite state set, where the important thing is to link the structure of the system with its dynamics (e.g., Boolean networks used in computational biology) [Albert et al., 03], [Celada et al., 92], ...

The number of state transitions usually has *exponential size* in the number of model variables, so **analyzing the dynamics of the models without calculating the state transitions is important.**[Omar et al., 04]

In the case of linear systems, this can be attacked by examining the primitivity of a graph — algebraically, by checking if its largest eigenvalue is simple and strictly dominant. [Berman et al., 94]

### 1.3.7. The Eigenvalues in Epidemiology

In epidemiology, an epidemic threshold (a notion of prediction introduced recently) is a critical state beyond which infections become endemic. [Wang et al., 2003]

The epidemic threshold depends fundamentally on the structure of the graph, where the challenge is to capture the structure in as few parameters as possible. Wang et al. presented, recently, a model that can predict the epidemic threshold with the largest eigenvalue.

Again, bounding the largest eigenvalue!

### 1.3.8. The Eigenvalues in Game Theory

There are a number of papers that develop [network models for large-population game theory and economics](#). e.g., [Kearns, 05].

In those models, each player/organization is represented by a vertex of a graph, and the payoffs and transactions are restricted to obey the topology of the graph. This allows a detailed specification of its rich structure (social, organizational, political etc.) in strategic and economic systems.

We would like to repeat that [the eigenvalues of a graph specify the topological structure of it](#). [Farkas, 02]



## 1.4. The Tools for Attacking the Problems

(More applications ....)

In attacking the problems stated above, to the best of our knowledge, the main tools are combinations of the techniques from algebraic graph theory, combinatorics and advanced matrix analysis (intrinsic to random graphs).

Many of them can be modified to evaluate the number of walks of length  $k$  in their graphs – which can be represented by the eigenvalues of the graphs involved.

## 1.5. What are the Difficulties of Attacking the Problems?

- (1) Getting **better bounds of the eigenvalues** requires getting more information on their eigenspaces - not easy.
- (2) The **Sizes of graphs are usually very large**, so direct calculation of eigenvalues is usually not good.
- (3) **The dominant roots (especially, the second, the third largest)** of an integer polynomial are not easy to evaluate (For some special graphs, it is possible to derive their characteristic polynomials)

## 2. Some Recent Results on Graph Spectra

Given  $G$ , the **largest eigenvalue**  $\lambda_1(G)$  has been studied extensively in the past decades. Recently, its **second largest eigenvalue**  $\lambda_2(G)$  has also been considered by several authors.

For the **third largest eigenvalue**  $\lambda_3(G)$ , it is known that: (1)  $\lambda_3(G) = -1$  iff  $G^c$  is isomorphic to the union of a complete bipartite graph and some isolated vertices, (2) there exist no graphs such that  $-1 < \lambda_3(G) < -\frac{\sqrt{5}-1}{2} = -0.618\dots$

[Cvetkovic et al., 95], [Neumaier et al., 83], [Pertrovic, 91], [Cao, 98], etc.

...

## Some Recent Results on Graph Spectra (Cont'd)

For the **least eigenvalue**  $\lambda_n(G)$ , it is known that [Yong, 99]

$$-\frac{n}{2} \leq \lambda_n(G) \leq -\frac{1 + \sqrt{1 + 4\frac{n-3}{n-1}}}{2} = -1.618\dots$$

Motivated by the *Open Problem* by Harary et al.:

*Which graphs have distinct eigenvalues?*

There has been **research on the graphs with multiple eigenvalues**, introducing *star sets* of eigenvalues, e.g., [Pertrovic, 98].

## 2.1. What I Did Most Recently?

(I) Strengthened a known theorem on graphs with multiple eigenvalues (for regular graphs, their eigenvalues can be simple).

(II) Found two classes of graphs with multiple eigenvalues:

- graphs with negative third largest eigenvalues;
- graphs characterized by  $\lambda_{n-2}(G)$ .

## 2.2. Conventions

$K_r$  is the *clique* of order  $r$ .

$K_{i,j}$  is the complete bipartite graph with the partition numbers  $i, j$ .

Let  $a_{-n+1}, a_{-n+2}, \dots, a_{n-1}$  be a sequence of numbers. Then  $A = (a_{ij})$  is called a *Toeplitz matrix* if  $a_{ij} = a_{i-j}$  for all  $i, j = 1, 2, \dots, n$ .

## 2.3. Some Definitions

**Definition 2.1.** Let  $A = (a_{i-j})$  be a symmetric Toeplitz matrix. If  $a_{i-j} \neq 0$  for all  $0 \leq |i-j| \leq k$ , then  $A$  is a symmetric Toeplitz matrix with *width*  $k$ . A graph  $G$  with its adjacency matrix having this property is called a *Toeplitz graph* with width  $k$ .

**Definition 2.2.** ([Berman et al., 94]). An  $n \times n$  matrix  $A$  is *cogredient* to a matrix  $B$  if, for some permutation matrix  $P$ , we have  $PAP^t = B$ .

Two graphs are isomorphic *iff* their adjacency matrices are *cogredient*.

## 2.4. A General Result

**Theorem 2.1.** Let  $A$  be an  $n \times n$  real symmetric matrix. Then  $A$  has  $n$  distinct eigenvalues iff, for  $\forall P \in S = \{X | AX = XA, X \text{ is a real matrix}\}$ ,  $P$  is a real symmetric matrix.

**Corollary 2.1.** Let  $A = A(G)$  be the adjacency matrix of  $G$ . If there is a non-symmetric permutation matrix  $P$  such that  $AP = PA$ , then  $G$  has multiple eigenvalues.

Theorem 2.1 generalizes [Cvetkovic et al., Theorem 5.1]. Corollary 2.1 characterizes a graph having multiple eigenvalues. For example, if  $A$  is the adjacency matrix of a circulant graph  $C$ , and  $P$  the adjacency matrix of a *directed* Hamiltonian cycle with the same vertices, then  $AP = PA$ , so  $C$  has multiple eigenvalues. This is a known result [Biggs, 93, p.16].



## 2.5. Spectra of graphs with multiple eigenvalues

**Theorem 2.2.** If  $G$  has  $t + 1$  eigenvalues equal to  $\alpha$ :

$$\lambda_k(G) = \lambda_{k+1}(G) = \cdots = \lambda_{k+t}(G) = \alpha,$$

then (1)  $G^c$  has at least  $t$  eigenvalues equal to  $-\alpha - 1$  and

$$\lambda_{n-(k+t)+2}(G^c) = \lambda_{n-(k+t)+3}(G^c) = \lambda_{n-k+1}(G^c) = -\alpha - 1;$$

(2)  $G$  and  $G^c$  share a common eigenspace with dimension at least  $t$ .

This theorem reveals the relationships between the eigenvalues, the eigenspaces of  $G$  and of  $G^c$ . In particular, when  $\alpha = 0$  it characterizes graphs having eigenvalues equal to 0. Graphs without 0 eigenvalues are considered in [Bell, 93] etc.

## Spectra of graphs with multiple eigenvalues (cont'd)

**Corollary 2.4.** If a regular graph  $G$  with  $n$  vertices has  $t$  eigenvalues equal to  $\alpha$  and

$$\lambda_k(G) = \lambda_{k+1}(G) = \cdots = \lambda_{k+t-1}(G) = \alpha,$$

then  $G^c$  has  $t$  eigenvalues equal to  $-\alpha - 1$ , and

$$\lambda_{n-(k+t)+2}(G^c) = \lambda_{n-(k+t)+3}(G^c) = \lambda_{n-k+1}(G^c) = -\alpha - 1,$$

and  $G$  and  $G^c$  share the same eigenspace for each eigenvalue.

Combining all above, we see that a non-zero vector is an eigenvector of a regular graph  $G$  *iff* it is an eigenvector of its complement  $G^c$ . (This is known.)

## Spectra of graphs with multiple eigenvalues - Example

**Example.** Let  $G$  be a graph with  $n$  vertices. If  $G^c$  is complete  $k$ -partite, then  $G$  has  $n - k - 1$  eigenvalues equal to  $-1$ , and

$$\lambda_{k+1}(G) = \lambda_{k+2}(G) = \cdots = \lambda_{n-1}(G) = -1.$$

In fact, If  $G^c$  is complete  $k$ -partite, then [Yong, 97]

$$\lambda_2(G^c) = \lambda_3(G^c) = \cdots = \lambda_{n-k+1}(G^c) = 0.$$

Hence the assertion follows directly from Theorem 2.2.



## Spectra of graphs with $\lambda_3(G) < 0$ (cont'd)

**Theorem 3.4.** Let  $G$  be a connected graph with  $n$  vertices, and  $\lambda_3(G) < 0$ . Then

(1)  $-1$  is an eigenvalue of  $G$  except the case that  $A(G)$  is cogredient to the symmetric Toeplitz matrix with width  $\lfloor \frac{n-1}{2} \rfloor$ .

(2) Let  $V_r, V_{n-r}$  be the vertex sets of the disjoint cliques  $K_r, K_{n-r}$ , respectively. Then  $G$  has  $n - \kappa - \sigma$  eigenvalues equal to  $-1$ , where  $\kappa$  is the number of distinct degrees in  $V$  and  $\sigma = 1$  if there are 2 vertices with degree  $n - 1$  and one of which is in  $V_r$  and the other in  $V_{n-r}$ , and 0, otherwise.

## Spectra of graphs with $\lambda_3(G) < 0$ (cont'd)

**Theorem 3.5.** Let  $G$  be a connected graph with  $n$  vertices and  $\lambda_3(G) < 0$ . Let  $2r$  be the rank of  $A(G^c)$ . Then (1) if  $r < \frac{n}{2}$ , we have

$$\begin{aligned} -1 \leq \lambda_j(G) < 0, \quad j = 3, 4, \dots, r + 1, \\ \lambda_j(G) = -1, \quad j = r + 2, \dots, n - r; \end{aligned}$$

(2) if  $r = \frac{n}{2}$ , then

$$-1 \leq \lambda_j(G) < 0, \quad j = 3, 4, \dots, \frac{n}{2}; \quad \lambda_{\frac{n}{2}+1}(G) \geq -2.$$

**Corollary 3.6.** Let  $G$  be a connected graph with  $n$  vertices and  $\lambda_3(G) < 0$ . If there exists an index  $k$ ,  $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$  such that  $\lambda_k(G) = -1$ , then

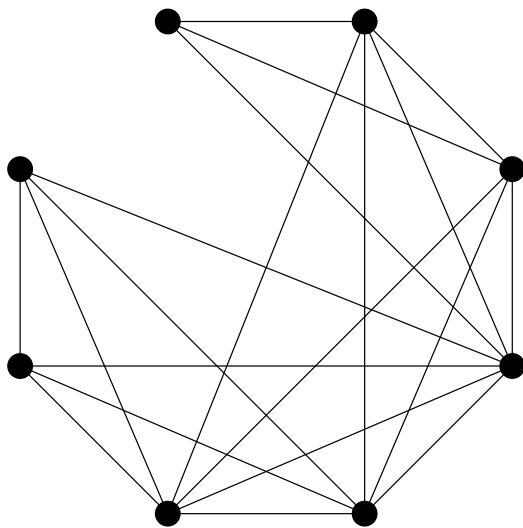
$$\lambda_j(G) = -1, \quad j = k, k + 1, \dots, n - r,$$

where  $2r$  is the rank of  $A(G^c)$  and  $r \leq k - 1$ .

## Spectra of graphs with $\lambda_3(G) < 0$ — Example

The following example indicates that the relation  $r = k - 1$  in Corollary 3.6 does not always hold. [Yong, 99].

**Example.** Let  $G$  and its adjacency matrix  $A(G)$  be given by



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

## Spectra of graphs with $\lambda_3(G) < 0$ — Example (cont'd)

By [Maple](#) we obtain that

$$\begin{aligned}\lambda_1(G) &= 5.24384, \lambda_2(G) = 1.60317, \lambda_3(G) = -0.182062, \\ \lambda_4(G) &= -1, \quad \lambda_5(G) = -1, \quad \lambda_6(G) = -1, \\ \lambda_7(G) &= -1.53035, \quad \lambda_8(G) = -2.1346.\end{aligned}$$

The rank of  $A(G^c)$  is 4, so  $r = 2$ . From the above theorem

$$\lambda_4(G) = \lambda_5(G) = \lambda_6(G) = -1.$$

Comparing this with Corollary 3.6, we see that this is the case that  $r = 2, k = 4, n = 8$ .



## Spectra of graphs with $\lambda_3(G) < 0$ (cont'd)

Two special cases:

**Corollary 3.7.** Let  $G$  be a connected graph with  $n$  vertices. Then

(1)  $\lambda_3(G) = -1$  iff  $G^c$  is the union of a complete bipartite graph and some isolated vertices.

(2)  $\lambda_3(G) = -1$  implies that  $\lambda_j(G) = -1$ ,  $j = 3, 4, \dots, n - 1$ .

This corollary generalizes the corresponding results obtained in [Cao, 95] and in [Cvetkovic et al., 95].

#### 4. Graphs characterized by $\lambda_{n-2}(G)$

A graph has multiple eigenvalues equal to  $-1$  if the third least eigenvalue of its complement is zero.

**Lemma 4.1.** Given  $G$  with at least seven vertices, we have  $\lambda_4(G) \geq -1$ . Moreover, if  $G^c$  is not 3-partite, then  $\lambda_4(G) \geq \frac{1-\sqrt{5}}{2}$ .

**Corollary 4.2.** Let  $G$  be a graph with at least seven vertices. If  $\lambda_4(G^c) < \frac{1-\sqrt{5}}{2}$ , then the chromatic number of  $G$  is 3.

## Spectra of graphs characterized by $\lambda_{n-2}(G)$ (cont'd)

**Theorem 4.3.** Let  $G$  be a graph with  $n \geq 7$  vertices. Then

(1)  $\lambda_{n-2}(G) \leq 0$ ; and  $\lambda_{n-2}(G) = 0$  implies  $\lambda_4(G^c) = -1$  and  $G$  is isomorphic to a graph with its adjacency matrix being the following form,

$$A(G) = \begin{pmatrix} 0 & A_{12} & A_{13} \\ A_{12}^t & 0 & A_{23} \\ A_{13}^t & A_{23}^t & 0 \end{pmatrix},$$

and each  $B_{ij} = \begin{pmatrix} 0 & A_{ij} \\ A_{ij}^t & 0 \end{pmatrix}$ ,  $1 \leq i, j \leq 3$ , is cogredient to

$$\begin{pmatrix} 0 & \begin{pmatrix} J_1 & J_2 & J_3 \\ J_4 & J_4 & J_6 \end{pmatrix} \\ * & 0 \end{pmatrix},$$

where  $J_i$  are either all 1's matrices of appropriate sizes or the 0 matrices, for each  $i = 1, 2, \dots, 6$ ;

(2)  $\lambda_{n-2}(G) = 0$  implies  $\lambda_{n-\lceil \frac{n}{3} \rceil + 2}(G) = \lambda_{n-\lceil \frac{n}{3} \rceil + 3}(G) = \dots = \lambda_{n-2}(G) = 0$ ;

(3)  $\lambda_{n-2}(G) = 0$  implies  $\lambda_1(G) \leq -2\lambda_n(G)$ .

## 5. Two Conjectures

There are many *open problems or conjectures*. In the following are two of them:

**Conjecture 1.** Given  $G$  of  $n$  vertices, if  $k$  is the smallest index that satisfies (1)  $k \leq \lceil \frac{n}{2} \rceil$  (2)  $\lambda_k(G^c) < \frac{1-\sqrt{5}}{2}$ , (3)  $\lambda_1(G) + (k-3)\lambda_n(G) > 0$ , then  $k-1$  is the chromatic number of  $G$ .

The Four-Color Theorem could be re-proven from here, if the conjecture would be true.

The conjecture is true for  $k = 2, 3, 4$ . If the conjecture would be true in general, then  $(-v+3)\lambda_n(G) \leq \lambda_1(G) \leq (-v+1)\lambda_n(G)$ , where  $v$  is the chromatic number.

## Two Conjectures (Cont'd)

**Conjecture 2.** Let  $A$  be an  $n \times n$   $(0, 1)$ -matrix. Then

$$|\det(A)| \leq F_n$$

where  $F_n$  is the Fibonacci number:  $F_n = F_{n-1} + F_{n-2}$ , with  $F_0 = 0$ ,  $F_1 = 1$ .

There are a number of rough bounds on  $|\det(A)|$ . The conjecture is true for many  $(0, 1)$ -matrices and the equality holds for a class of Hessenberg matrices.

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