

## Note on cospectral graphs with simple eigenvalues

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Dedicated to Professor H. Sachs on the occasion of his 75 birthday

### 1 Introduction

Let  $G = (V, E)$  be a graph with vertex set  $V = V(G) = \{1, 2, \dots, n\}$ , edge set  $E = E(G) \subset V \times V$ , adjacency matrix  $A = A(G) = (a_{ij})$  and  $I$  denotes the  $n \times n$  unit matrix. The characteristic polynomial  $f_A(x) = \det(xI - A)$  and the eigenvalues of  $A$  ( i.e., the roots of the equation  $f_A(x) = 0$  ) are called the characteristic polynomial of  $G$ , denoted by  $f_G(x)$  and the eigenvalues of  $G$ , respectively. For eigenvalue  $x_k, k = 1, 2, \dots, \nu$  denote  $\mu_k = \mu(x_k)$  the multiplicity of  $x_k$  ( $\mu_1 + \mu_2 + \dots + \mu_\nu = n$ ). Two non-isomorphic graphs  $G_1, G_2$  are called isospectral ( cospectral ) iff  $f_{G_1}(x) = f_{G_2}(x)$ .

Let  $G = G(n)$  denote the set of all non-isomorphic graphs with  $n$  vertices and let  $S = S(n) \subset G$  denote a Set of all Isospectral Non-isomorphic Graphs ( briefly: a SING<sup>1</sup> ). For graph  $G \in G(n)$  let  $\pi = \pi(G)$  be a property function;  $\pi(G) = \gamma$  and  $\pi(G) = \sigma$  means that  $G$  is connected or that  $G$  has simple eigenvalues, respectively. In this paper we give briefly an algorithm to calculate all SING's for  $n = 3, 4, \dots, 10$ .

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<sup>1</sup>In analogy to the acronym PING in [1].

## 2 Calculation of non-isomorphic graphs

For a given number  $n$  of vertices, a set of  $2^{\binom{n}{2}}$  different graphs can be determined. By removing all isomorphic graphs from this set one gets  $G(n)$ . It can serve as a base for different theoretical researches on graphs.

$$G(2) = \{ \circ \circ, \bullet \bullet \} \quad G(3) = \{ \circ \circ, \bullet \circ, \circ \bullet, \bullet \bullet \}$$

Starting with the set  $G(2)$ , we generate step by step the following sets. The main part of the algorithm, shown in Fig. 1, is the isomorphism test. Table 1 can be calculated by using Polya's counting theory which is described in [2]. We determine the characteristic polynomial for all graphs and store the sets up to  $n = 10$  for further observations.

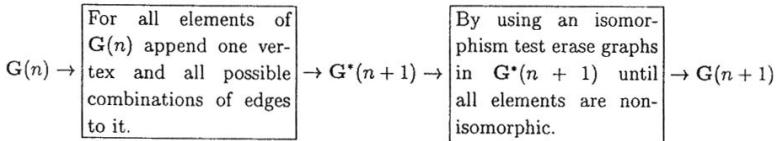


Figure 1: The two main steps of the algorithm are given. The temporary set  $G^*(n + 1)$  consists of  $2^n \cdot |G(n)|$  elements.

Table 2 shows the number of SING's for up to 10 vertices. Each set of numbers in one line gives the counted SING's with different number of graphs. Furthermore, the property of graphs in a SING are included.

n	3	4	5	6	7	8	9	10
v	4	11	34	156	1044	12346	274668	12005168

Table 1: The table shows the number of non-isomorphic graphs for  $n$  from 3 to 10.

n	$\pi(G)$	SING =2	3	4	5	6	7	8	9	10
5	no	1								
6	no	5								
	$\gamma$	2								
	no	52	2							
7	$\gamma$	30	1							
	$\sigma$	26								
	$\gamma, \sigma$	23								
	no	771	52	6						
8	$\gamma$	617	27	4						
	$\sigma$	438	19	4						
	$\gamma, \sigma$	405	17	4						
	no	21025	2015	551	95	37	1	2	0	2
9	$\gamma$	19410	1728	470	79	32	1	2	0	2
	$\sigma$	16640	1540	424	79	30	1	2	0	2
	$\gamma, \sigma$	16046	1445	403	72	28	1	2	0	2
	no	1003384	110807	36749	5667	4693	948	870	125	142
10	$\gamma$	966851	103873	34645	5018	4385	844	810	115	129
	$\sigma$	825956	83150	29119	3930	3672	684	671	94	96
	$\gamma, \sigma$	811204	80964	28394	3768	3576	668	655	92	94
n	$\pi(G)$	11	12	13	14	15	16	21		
	no	72	28	9	13	10	4	2		
10	$\gamma$	69	26	9	10	9	4	2		
	$\sigma$	57	20	7	9	8	3	1		
	$\gamma, \sigma$	57	20	7	9	8	3	1		

Table 2: Number of SING's with different properties.

### 3 Distribution for a graph invariant

The graph invariant  $X_G$  of a graph  $G$  is defined as

$$X_G = \sum_{k=1}^n |x_k|$$

with eigenvalues  $x_k$ . This formula is, e.g., for the skeleton  $S = G(B)$  of an benzenoid hydrocarbon  $B$  a correct definition for the so called Hückel energy  $E_G = E_B$  of  $B$ . Therefore, Gutman and Polansky [3, 4] have introduced the notion "energy  $E_G$  of graph  $G$ " for every

graph  $G$ . We calculate the graph invariant  $X_G$  for all non-isomorphic graphs  $G$  with up to 10 vertices. The distribution of this value is given in Fig. 2.

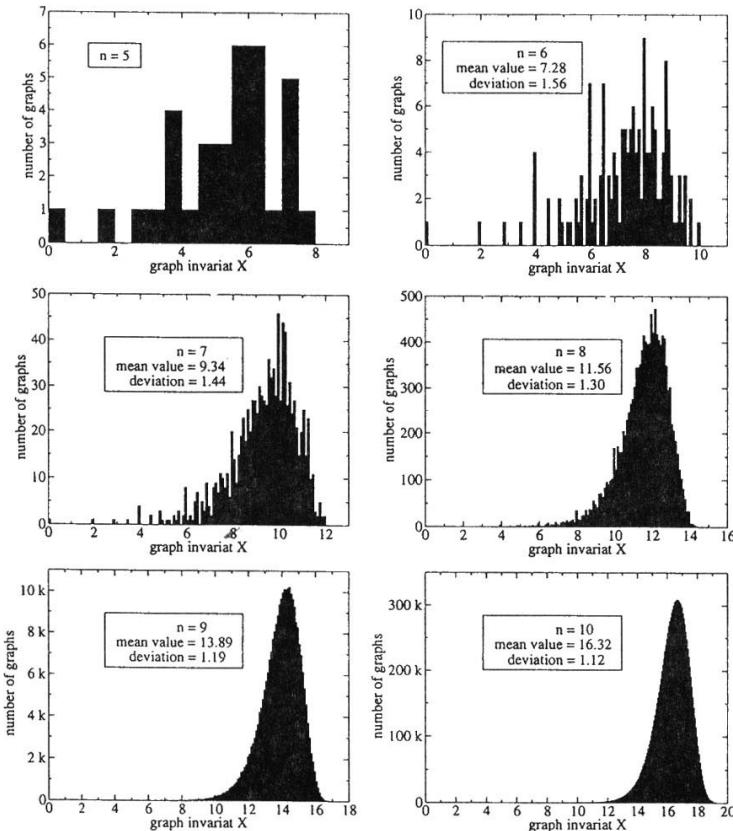


Figure 2:

Remark: If you write a short e-mail to [ortlepp@gmx.de](mailto:ortlepp@gmx.de), I will send you a copy of the programs for all calculations in this article.

0|00|000|1100|11100|101010|1101110|11101010|01110111  
 0|00|000|1100|11100|111010|1100110|10111010|01110111  
 0|00|000|1100|11100|100110|1110100|11011110|01110111  
 0|00|000|1100|11100|100110|1110100|10111011|01110111  
 0|00|000|1100|11100|101100|0011101|10101111|11011110  
 0|00|000|1100|11100|100110|1101110|00111110|10110111  
 0|00|100|0100|10100|111100|1010110|11101110|011110111  
 0|00|000|1100|11100|101100|0101101|10101111|11011110  
 0|00|000|1100|10110|011010|1110110|00111110|011111110  
 0|00|100|0100|11100|110100|1010110|01111011|100111111  
 0|00|100|0100|11100|101100|1110010|11101110|011110111  
 0|00|100|0100|11100|110100|1110110|11100110|011110111  
 0|00|100|0100|11100|110100|1111001|11001110|101111011  
 0|00|000|1100|10110|011010|1011100|11100110|110111111  
 0|00|000|1100|11100|001110|1011010|11101010|011111111  
 0|00|000|1100|10110|011010|1101100|11010110|011111111  
 0|00|100|0100|11100|101100|011110|11101010|011111111  
 0|00|100|0100|10100|111100|0111100|01111101|110111111  
 0|00|000|1100|10110|011010|1011100|01110011|110111111  
 0|00|000|1100|11100|101100|0101101|11101010|011111111

$$f(x) = x^{10} - 25x^8 - 38x^7 + 96x^6 + 182x^5 - 103x^4 - 240x^3 + 23x^2 + 72x - 16$$

$$\{x_1, \dots, x_{10}\} = \{-2.689, -2.200, -1.764, -1.227, -1, 0.265, 0.423, 1.282, 1.648, 5.263\}$$

Figure 3: For  $n = 10$  vertices, we find one SING  $S_1 = S_1(10)$  with 21 elements and simple eigenvalues. All elements of  $S_1$  are represented by their adjacency matrices. Every row is the upper right part of the adjacency matrix of the respective element of  $S_1$ . The characteristic polynomial  $f(x)$  and its roots are also given.

## References

- [1] Cvetkovic', D.M. und Doob M. und Sachs H. : *Spectra of Graphs Theory and Applications*, Johann Ambrosius Barth Verlag, Heidelberg Leipzig 1995, p. 24 and p. 156ff
- [2] Colbourn, C.J. and Dinitz, J.H. : *The CRC Handbook of Combinatorial Design*, CRC Press, Boca Raton New York London Tokyo 1996, p. 645
- [3] Gutman, I. : *The energy of a graph*, BER.MATH.-STAT.SEKT. FORSCHUNGSZENTRUM GRAZ 103 1978 p. 1-22.
- [4] Gutman, I. and Polansky, O.E. : *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin 1986, p. 137ff