Chemistry and Related Mathematics

Selections from

A Mathematical Bibliography of
Signed and Gain Graphs and Allied Areas
Sixth Edition, Revision b

1999 September 4

(Working copy as of this date.)

Compiled by
Thomas Zaslavsky

Department of Mathematical Sciences
Binghamton University
Binghamton, New York, U.S.A. 13902-6000

E-mail: `zaslav@math.binghamton.edu`

Subject Classification Codes

A Adjacency matrix, eigenvalues.
Alg Algorithms.
Aut Automorphisms, symmetries, group actions.
B Balance (mathematical), cobalance.
Chem Applications to chemistry (partial coverage).
Cl Clusterability.
Col Vertex coloring.
E Enumeration of types of signed graphs, etc.
Exp Expository.
Fr Frustration (imbalance); esp. frustration index (line index of imbalance).
Gen Generalization.
I Incidence matrix, Kirchhoff matrix.
K Signed complete graphs.
N Numerical and algebraic invariants of signed graphs, etc.
P All-negative or antibalanced signed graphs; parity-biased graphs.
Phys Applications in physics (partial coverage).
Ref Many references.
SG Signed graphs: mathematical properties.
Str Structure theory.
Sw Switching of signs or gains.
VS Vertex-signed graphs ("marked graphs"); signed vertices and edges.
WD Weighted digraphs.
WG Weighted graphs.

K. Balasubramanian

1988a Computer generation of characteristic polynomials of edge-weighted graphs, heterographs, and directed graphs. *J. Computational Chem.* 9 (1988), 204–211.

Here a "signed graph" means, in effect, an acyclically oriented graph D along with the antisymmetric adjacency matrix $A_{\pm}(D) = A(+D \cup -D^*)$, D^* being the converse digraph. [That is, $A_{\pm}(D) = A(D) - A(D)^{\mathrm{t}}$. The "signed graphs" are just acyclic digraphs with an antisymmetric adjacency matrix and, correspondingly, what we may call the 'antisymmetric characteristic polynomial'.] Proposes an algorithm for the polynomial. Observes in some examples a relationship between the characteristic polynomial of Γ and the antisymmetric characteristic polynomial of an acyclic orientation.
(**SD, wg: A: N: Alg, Chem**)

1991a Comments on the characteristic polynomial of a graph. *J. of Computational Chem.* 12 (1991), 248–253. MR 92b:92057.

Argues (heuristically) that a certain algorithm is superior to another, in particular for the antisymmetric polynomial defined in (1988a).
(**SD: A: N: Alg**)

1992a Characteristic polynomials of fullerene cages. *Chemical Physics Letters* 198 (1992), 577–586.

Computed for graphs of six different cages of three different orders, in both ordinary and "signed" (see (1988a)) versions. Observes a property of the "signed graph" polynomials [which is due to antisymmetry, as explained by P.W. Fowler (Comment on "Characteristic polynomials of fullerene cages". *Chemical Physics Letters* 203 (1993), 611–612)]. (**SD: A: N: Chem**)

1994a Are there signed cospectral graphs? *J. of Chemical Information and Computer Sciences* 34 (1994), 1103–1104.

The "signed graphs" are as in (1988a). Simplified contents: It is shown by example that the antisymmetric characteristic polynomials of two nonisomorphic acyclic orientations of a graph (see (1988a)) may be equal or unequal. [Much smaller examples are provided by P.W. Fowler (Comment on "Characteristic polynomials of fullerene cages". *Chemical Physics Letters* 203 (1993), 611–612).] [*Question.* Are there examples for which the underlying (di)graphs are nonisomorphic?] [For cospectrality of other kinds of signed graphs, see Acharya, Gill, and Patwardhan (1984a) (signed K_n's).]
(**SD: A: N**)

Chung-Chien Chang and Cheng-Ching Yu

1990a On-line fault diagnosis using the signed directed graph. *Industrial and Engineering Chem. Res.* 29 (1990), 1290–1299.

Modifies the method of Iri, Aoki, O'Shima, and Matsuyama (1979a) of constructing the diagnostic signed digraph, e.g. by considering transient and steady-state situations. (**SD: Appl, Ref**)

A.C. Day, R.B. Mallion, and M.J. Rigby

1983a On the use of Riemannian surfaces in the graph-theoretical representation of

Möbius systems. In: R.B. King, ed., *Chemical Applications of Topology and Graph Theory* (Proc. Sympos., Athens, Ga., 1983), pp. 272–284. Stud. Physical Theoret. Chem., 28. Elsevier, Amsterdam, 1983. MR 85h:05039.

A clumsy but intriguing way of representing some signed (or more generally, $\mathbb{Z}_n$-weighted) graphs: via 2-page (or, n-page) looseleaf book embedding (all vertices are on the spine and each edge is in a single page), with an edge in page k weighted by the "sheet parity index" $\alpha_k = (-1)^k$ (or, $e^{2\pi ik/n}$). (Described in the [unnecessary] terminology of an n-sheeted Riemann surface.) [A $\mathbb{Z}_n$-weighted) graph has such a representation iff the subgraph of edges with each weight is outerplanar.]

A variation to get switching classes of signed polygons: replace α_k by the "connectivity parity index" $\alpha_k^{\sigma_k}$ where σ_k = number of edges in page k. [The variation is valid only for polygons.] [*Questions* vaguely suggested by these procedures: Which signed graphs can be switched so that the edges of each sign form an outerplanar graph? Also, the same for gain graphs. And there are many similar questions: for instance, the same ones with "outerplanar" replaced by "planar."]

(**SG: sw, A, T, Chem: Exp, Ref**)(**WG: A, T: Exp, Ref**)

Ante Graovac, Ivan Gutman, and Nenad Trinajstić

1977a *Topological Approach to the Chemistry of Conjugated Molecules.* Lecture Notes in Chemistry, 4. Springer-Verlag, Berlin-Heidelberg-New York, 1977. Zbl. 385.05032.

§2.7. "Extension of graph-theoretical considerations to Mobius systems."

(**SG: A, Chem**)

A. Graovac and N. Trinajstić

1975a Mobius molecules and graphs. *Croatica Chemica Acta (Zagreb)* 47 (1975), 95–104.

1976a Graphical description of Möbius molecules. *J. Molecular Structure* 30 (1976), 416–420.

The "Möbius graph" (i.e., signed graph of a suitably twisted ring hydrocarbon) is introduced with examples of the adjacency matrix and characteristic polynomial. (**Chem: SG: A**)

Ivan Gutman

See also D.M. Cvetković, A. Graovac and S.-L. Lee.

1978a Electronic properties of Möbius systems. *Z. Naturforsch.* 33a (1978), 214–216. MR 58 #8800. (**SG: A, Chem**)

1988a Topological analysis of eigenvalues of the adjacency matrices in graph theory: A difficulty with the concept of internal connectivity. *Chemical Physics Letters* 148 (1988), 93–94.

Points out an ambiguity in the definitions of Lee, Lucchese, and Chu (1987a) in the case of multiple eigenvalues. [See Lee and Gutman (1989a) for the repair.] (**VS, SGw**)

Ivan Gutman, Shyi-Long Lee, Yeung-Long Luo, and Yeong-Nan Yeh

1994a Net signs of molecular graphs: dependence of molecular structure. *Internat. J. Quantum Chemistry* 49 (1994), 87–95.

How to compute the balanced signing of Γ that corresponds to eigenvalue λ_i (see Lee, Lucchese, and Chu (1987a)), without computing the eigenvector X_i. Theorem: If v_r, v_s are adjacent, then $X_{ir}X_{is} = \sum_P f(P;\lambda_i)$,

where $f(P;\lambda) := \varphi(G - V(P);\lambda)/\varphi'(G;\lambda)$, $\varphi(G;\lambda)$ is the characteristic polynomial, and the sum is over all paths connecting v_r and v_s. Hence $\sigma_i(v_r v_s) = \operatorname{sgn}(X_{ir} X_{is})$ is determined. [An interesting theorem. *Questions.* Does it generalize if one replaces Γ by a signed graph, this being the balanced (all-positive) case? In such a generalization. if any, how will σ enter in—by restricting the sum to positive paths, perhaps? What about graphs with real gains, or weights?] **(VS, SGw)**

Ivan Gutman, Shyi-Long Lee, Jeng-Horng Sheu, and Chiuping Li

1995a Predicting the nodal properties of molecular orbitals by means of signed graphs. *Bull. Inst. Chem., Academica Sinica* No. 42 (1995), 25–31.

Points out some difficulties with the method of Lee and Li (1994a). **(VS, SGw, Chem)**

Ivan Gutman, Shyi-Long Lee, and Yeong-Nan Yeh

1992a Net signs and eigenvalues of molecular graphs: some analogies. *Chemical Physics Letters* 191 (1992), 87–91.

A connected graph Γ has n eigenvalues and n corresponding balanced signings (see Lee, Lucchese, and Chu (1987a)). Let $S_1 \geq S_2 \geq \cdots \geq S_n$ be the net signs of these signings and $m = |E|$. The net signs satisfy analogs of properties of eigenvalues. (A) If $\Delta \subset \Gamma$, then $S_1(\Delta) < S_1$. (B) $S_1 = m \geq S_2 + 2$. (C, D) For bipartite Γ, $S_n = -m$. Otherwise, $S_n \geq -m+2$. From (B, C, D) we have $|S_i| \leq m-2$ for all $i \neq 1$ and, if Γ is bipartite, $i \neq n$. (E, F) If Γ is bipartite, then $S_i = -S_{n+1-i}$ and at least $a-b$ net signs equal 0, where $a \geq b$ are the numbers of vertices in the two color classes. The analogy is imperfect, since $S_1 + S_2 + \cdots + S_n \geq 0$, while equality holds for eigenvalues. [*Questions.* Some of these conclusions require Γ to be bipartite. Does that mean that they will generalize to an arbitrary balanced signed graph Σ in place of the bipartite Γ, the eigenvectors being those of Σ? Will the other results generalize with Γ replaced by any signed graph? How about real gains, or weights?] **(VS, SGw)**

Masao Iri, Katsuaki Aoki, Eiji O'Shima, and Hisayoshi Matsuyama

1976a [A graphical approach to the problem of locating the system failure.] (In Japanese.) [???] 76 (135) (1976), 63–68. **(SD, VS: Appl)**

1979a An algorithm for diagnosis of system failures in the chemical process. *Computers and Chem. Eng.* 3 (1979), 489–493 (1981).

The process is modelled by a signed digraph with some nodes v marked by $\mu(v) \in \{+,-,0\}$. (Marks $+,-$ indicate a failure in the process.) Object: to locate the node which is origin of the failure. An oversimplified description of the algorithm: μ is extended arbitrarily to V. Arc (u,v) is discarded if $0 \neq \mu(u)\mu(v) \neq \sigma(u,v)$. If the resulting digraph has a unique initial strongly connected component S, the nodes in it are possible origins. Otherwise, this extension provides no information. (I have overlooked: special marks on "controlled" nodes; speedup by stepwise extension and testing of μ.) [This article and/or (1976a) seems to be the origin of a whole literature. See e.g. Chang and Yu (1990a), Kramer and Palowitch (1987a).] **(SD, VS: Appl, Alg)**

Shyi-Long Lee

See also I. Gutman.

1989a Comment on 'Topological analysis of the eigenvalues of the adjacency matrices in graph theory: A difficulty with the concept of internal connectivity'. *J. Chinese Chemical Soc.* 36 (1989), 63–65.

Response to Gutman (1988a). Proposes weighted net sign: divide by number of nonzero vertex signs. The goal is to have the ordering of net signs correlate more closely with that of eigenvalues. (**VS, SGw, Chem**)

1989b Net sign analysis of eigenvectors and eigenvalues of the adjacency matrices in graph theory. *Bull. Inst. Chem., Academica Sinica* No. 36 (1989), 93–104.

Expounds principally Lee, Lucchese, and Chu (1987a) and Lee and Gutman (1989a). Examples include all connected, simple graphs of order ≤ 4 and some aromatics. (**VS, SGw, Exp, Chem**)

1992a Topological analysis of five-vertex clusters of group IVa elements. *Theoretica Chimica Acta* 81 (1992), 185–199.

See Lee, Lucchese, and Chu (1987a). More examples; again, eigenvalue and net-sign orderings are compared. (**VS, SGw, Chem**)

Shyi-Long Lee and Ivan Gutman

1989a Topological analysis of the eigenvectors of the adjacency matrices in graph theory: Degenerate case. *Chemical Physics Letters* 157 (1989), 229–232.

Supplements Lee, Lucchese, and Chu (1987a) to answer an objection by Gutman (1988a), by treating vertex signs corresponding to multidimensional eigenspaces. (**VS, SGw, Chem**)

Shyi-Long Lee and Chiuping Li

1994a Chemical signed graph theory. *Internat. J. Quantum Chem.* 49 (1994), 639–648.

Varies Lee, Lucchese, and Chu (1987a) by taking net signs of all balanced signings, instead of only those obtained from eigenvectors, for small paths, polygons, and polygons with short tails. The distribution of net sign, over all signings of each graph, is more or less binomial. (**VS, SGw, Chem**)

1994b On generating molecular orbital graphs: the first step in signed graph theory. *Bull. Inst. Chem., Academica Sinica* No. 41 (1994), 69–75.

Abbreviated presentation of (1994a). (**VS, SGw: Exp**)

Shyi-Long Lee and Feng-Yin Li

1990a Net sign approach in graph spectral theory. *J. Molecular Structure (Theochem)* 207 (1990), 301–317.

Similar topics to S.-L. Lee (1989a, 1989b). Several examples of order 6. (**VS, SGw, Exp, Chem**)

1990b Net sign analysis of five-vertex chemical graphs. *Bull. Inst. Chem., Academica Sinica* No. 37 (1990), 83–97.

See Lee, Lucchese, and Chu (1987a). Treats all connected, simple graphs of order 5. (**VS, SGw, Chem**)

Shyi-Long Lee, Feng-Yin Li, and Friday Lin

1991a Topological analysis of eigenvalues of particle [*sic*] in one- and two-dimensional simple quantal systems: Net sign approach. *Internat. J. Quantum Chem.* 39 (1991), 59–70.

See Lee, Lucchese, and Chu (1987a). §II: Net signs calculated for paths.

§§III, IV: Planar graphs with two different types of potential, yielding complicated results. (**VS, SG, Chem**)

Shyi-Long Lee, Robert R. Lucchese, and San Yan Chu

1987a Topological analysis of eigenvectors of the adjacency matrices in graph theory: The concept of internal connectivity. *Chemical Physics Letters* 137 (1987), 279–284. MR 88i:05130. Zbl. none.

Introduces the net sign of a (balanced) signed graph. A graph has vertices signed according to the signs of an eigenvector X_i of the adjacency matrix, $\mu(v_r) = \operatorname{sgn}(X_{ir})$, and $\sigma(v_r v_s) = \mu(v_r)\mu(v_s)$ [hence Σ is balanced]. Note that a vertex can have 'sign' 0. Net sign of a [hydrocarbon] chemical graph is applied to prediction of properties of molecular orbitals.

(**VS, SGw, Chem**)

Shyi-Long Lee, Yeung-Long Luo, and Yeong-Nan Yeh

1991a Topological analysis of some special graphs. III. Regular polyhedra. *J. Cluster Sci.* 2 (1991), 105–116.

See Lee, Lucchese, and Chu (1987a). Net signs for the Platonic polyhedra (Table I). (**VS, SGw, Chem**)

Shyi-Long Lee and Yeong-Nan Yeh

1990a Topological analysis of some special classes of graphs. Hypercubes. *Chemical Physics Letters* 171 (1990), 385–388.

Follows up Lee, Lucchese, and Chu (1987a) and Lee and Gutman (1989a), calculating net signs of eigenspatially signed hypercube graphs of dimensions up to 6 by means of a general graph-product formula. (**VS, SGw, Chem**)

1993a Topological analysis of some special classes of graphs. II. Steps, ladders, cylinders. *J. Math. Chem.* 14 (1993), 231–241. MR 95f:05079.

See Lee, Lucchese, and Chu (1987a). Net signs and eigenvalues are compared.

(**VS, SGw, Chem**)

Nenad Trinajstić

See also A. Graovac.

1983a *Chemical Graph Theory.* 2 vols. CRC Press, Boca Raton, Florida, 1983. MR 86g:92044.

Vol. I: Ch. 3, §VI: " Möbius graphs." Ch. 5, §VI: "Extension of Sachs formula to Möbius systems." §VII: "The characteristic polynomial of a Möbius cycle." Ch. 6, §VIII: "Eigenvalues of Möbius annulenes."

(**SG: Chem, A: Exp**)

1992a *Chemical Graph Theory, Second Ed.* CRC Press, Boca Raton, Florida, 1992. MR 93g:92034.

Ch. 3, §V.B: "Möbius graphs." Ch. 4, §I: "The adjacency matrix": see pp. 42–43. Ch. 5: "The characteristic polynomial of a graph", §II.B: "The extension of the Sachs formula to Möbius systems"; §III.D: "Möbius cycles". Ch. 6, §VIII: "Eigenvalues of Möbius annulenes" (i.e., unbalanced polygons); §IX: "A classification scheme for moncyclic systems" (i.e., characteristic polynomials of polygons). (**SG: A, Chem**)

Ch. 7: "Topological resonance energy," §V.C: "Möbius annulenes"; §V.G: "Aromaticity in the lowest excited state of annulenes". (**Chem**)