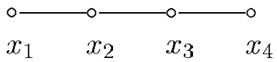
MAXIMAL ENERGY GRAPHS TEND TO HAVE A SMALL NUMBER OF DISTINCT EIGENVALUES

Dragoš Cvetković

Faculty of Electrical Engineering, University of Belgrade, P.O.Box 35–54,
11120 Belgrade, Serbia

e-mail: ecvetkod@etf.bg.ac.yu



adjacency matrix $A = \begin{Vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{Vmatrix}$.

characteristic polynomial and spectrum

$$P_G(\lambda) = \begin{vmatrix} \lambda & -1 & 0 & 0 \\ -1 & \lambda & -1 & 0 \\ 0 & -1 & \lambda & -1 \\ 0 & 0 & -1 & \lambda \end{vmatrix} = \lambda^4 - 3\lambda^2 - 1\,.$$

$$S_p(G) = \left[\, \frac{1+\sqrt{5}}{2},\ \frac{-1+\sqrt{5}}{2},\ \frac{1-\sqrt{5}}{2},\ \frac{-1-\sqrt{5}}{2} \,\right].$$

Let G be a simple undirected graph on n vertices with $m > 0$ edges. Let $x_1, x_2, \ldots, x_n$ be the eigenvalues of G. Let $I = \{1, 2, \ldots, n\}$.

The following relations are well-known:

$$\sum_{i \in I} x_i = 0, \qquad \sum_{i \in I} x_i^2 = 2m.$$

The energy $E(G)$ of G is defined by

$$E(G) = \sum_{i \in I} |x_i|.$$

The energy of a graph was defined by I. Gutman in

Gutman I., The energy of a graph, Berichte Math. Stat. Sekt. Forschungszentrum Graz, 103(1978), 1–22.

This invariant has attracted much attention from researchers in the last few years.

Cvetković D., Gutman I., *The computer system "Graph", A useful tool in chemical graph theory*, J. Comput. Chem., **7**(1986), No. 5, 640-644.

G. Caporossi, P. Hansen, *Variable Neighborhood Search for Extremal Graphs I*, Discrete Math., 212(2000), 29–44.

Caporossi G., Cvetković D., Gutman I., Hansen P., *Variable neighborhood search for extremal graphs*, 2. *Finding graphs with extremal energy*, J. Chem. Inform. Comp. Sci., **39**(1999),984-996.

Vertices	Graph6	Edges	Energy	Distinct Eigenvalues	Spectrum
7	F`~~w	17	12	4	$5, 1, -1^4, -2$
8	G`lv~{	21	14.325	7	$5.427,\ 1.118,\ 0.618,\ -1^2,\ -1.618,\ -1.679,\ -1.865$
9	HEutZhj	21	17.060	6	$4.702,\ 1.414^2,\ 1,\ -1.414^2,\ -1.702,\ -2^2$
10	I~qkzXZLw	30	20	3	$6, 1^4, -2^5$
11	JJ^em]uj[v_	36	22.918	5	$6.585,\ 1.874,\ 1^3,\ -1.459,\ -2^5$
12	K~z\c\qRXVa~	42	26	5	$7,\ 2^2,\ 1^2,\ -1,\ -2^6$

Table 1: Maximal energy graphs

It is known that for $n \leq 7$, the graphs with maximal energy are the complete graphs K_n, $n = 1, 2, \ldots, 7$. Maximal values of energy for graphs with n vertices have been determined heuristically by the system AutoGraphiX (AGX) for $n \leq 12$ and checked with Brendan McKay's Nauty program.

It is proved in

Koolen J., Moulton V., *Maximal energy graphs*, Advances Appl. Math., 26(2001), 47–52.

that for a graph G on n vertices the following inequality holds:

$$E(G) \leq \frac{n}{2}(1+\sqrt{n}),$$

with equality if and only if G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+\sqrt{n})/4, (n+\sqrt{n})/4)$. Such strongly regular graphs exist for $n = 4\tau^2$ for $\tau = 2^m$, $m = 1, 2, \ldots$.

¿From the theory of strongly regular graphs, one can deduce that a graph with such parameters has distinct eigenvalues $\tau(2\tau+1), \pm\tau$.

The smallest such graph, the Clebsch graph, has 16 vertices and the spectrum $10, 2^5, -2^{10}$.

The conjecture that, for any $\epsilon > 0$, for almost all n, there exists a graph G on n vertices such that

$$E(G) \geq (1-\epsilon)\frac{n}{2}(1+\sqrt{n})$$

has been confirmed in a slightly improved form in

Nikiforov V., *Graphs and matrices with maximal energy*, J. Math. Anal. Appl., 327(2007), 735–738.

Define

$$I = I_+ \cup I_-, \text{ where}$$

$$I_+ = \{i | i \in I, x_i \geq 0\} \quad \text{and} \quad I_- = \{i | i \in I, x_i < 0\}.$$

Then the energy can be represented in the following form:

$$E = \sum_{i \in I_+} x_i - \sum_{i \in I_-} x_i.$$

Extremal values of the function E satisfying the constraints

$$\sum_{i \in I} x_i = 0, \qquad \sum_{i \in I} x_i^2 = 2m$$

can be found by an auxiliary function involving these constraints :

$$F = \sum_{i \in I_+} x_i - \sum_{i \in I_-} x_i + \alpha \sum_{i \in I} x_i + \beta \left(\sum_{i \in I} x_i^2 - 2m \right),$$

where α, β are Lagrange multipliers.

By equating the partial derivatives of function F with 0 we get

$$\frac{\partial F}{\partial x_j} = \pm 1 + \alpha + 2\beta x_j = 0, \quad j \in I$$

The first term in the sum is equal to $+1$ if $j \in I_+$ and is equal to -1 if $j \in I_-$. Hence we obtain

$$x_j = \frac{-\alpha \mp 1}{2\beta}, \quad j \in I.$$

This means that a graph with extremal energy should have only two distinct eigenvalues.

Assume that an extremal graph has some fixed and given eigenvalues $\mathcal{K}$, consisting of x_i, $i \in K$. Let $J = I \setminus K$, so that the eigenvalues x_i, $i \in J$, are considered unknown. Index sets J and K are further partitioned, as I was partitioned, intosubsets corresponding to non-negative and negative eigenvalues:

$$J = J_+ \cup J_- \quad \text{and} \quad K = K_+ \cup K_-.$$

Now we have

$$E = \sum_{i \in J_+} x_i - \sum_{i \in J_-} x_i + \sum_{i \in K_+} x_i - \sum_{i \in K_-} x_i;$$

and

$$\sum_{i \in J} x_i + \sum_{i \in K} x_i = 0 \quad \text{and} \quad \sum_{i \in J} x_i^2 + \sum_{i \in K} x_i^2 = 2m.$$

Let

$$C_+ = \sum_{i \in K_+} x_i,\ C_- = \sum_{i \in K_-} x_i,\ C = \sum_{i \in K} x_i, \text{ and } D = \sum_{i \in K} x_i^2.$$

We can write

$$F = \sum_{i \in J_+} x_i - \sum_{i \in J_-} x_i + C_+ - C_- + \alpha \left(\sum_{i \in J} x_i + C \right) + \beta \left(\sum_{i \in J} x_i^2 + D - 2m \right).$$

Using partial derivatives for any $j \in J$, we get

$$\frac{\partial F}{\partial x_j} = \pm 1 + \alpha + 2\beta x_j = 0 \to x_j = \frac{-\alpha \mp 1}{2\beta}.$$

Assuming that both sets J_+ and J_- are non-empty, this means that unknown eigenvalues should have only two values in a graph with extremal energy.

Denote the two values obtained by x, y and the corresponding multiplicities by p, q.

The set J contains $|J| = n - |K| = k$ elements. Suppose that an extremal solution contains eigenvalues x, y with multiplicities p, q respectively. The following system of equations must be satisfied, where p, q, and k are positive integers and x, y, C, and D are real numbers:

$$p + q = k, \quad px + qy = -C, \quad px^2 + qy^2 = 2m - D.$$

In this notation, the energy is $E = p|x| + q|y| + C_+ - C_-$.

Our examples are computed using a small Mathematica program.

Given the number of vertices, the number of edges, and a list of known eigenvalues that define $\mathcal{K}$, the program prints all 4-tuples (p, q, x, y) satisfying the above system of equations . For each solution, the program also prints the corresponding energy E and $\frac{1}{6}\sum_{i \in I} x_i^3$.

Let $n = 16$, $m = 80$, and $\mathcal{K} = \{10\}$. This implies that $|K| = 1$, $|J| = 15$, $C = 10$, and $D = 100$. Our program gives the following results.

p	q	x	y	E	$\frac{1}{6}\left(\Sigma_{i=1}^{n} x_i^3\right)$
1	14	−7.7220	−0.1627	20.0000	89.9136
1	14	6.3887	−1.1706	32.7773	206.3830
2	13	−5.4741	0.0729	21.8963	111.9900
2	13	4.1407	−1.4063	36.5629	184.3060
3	12	−4.4379	0.2761	26.6274	123.0070
3	12	3.1046	−1.6095	38.6274	173.2900
4	11	−3.7936	0.4704	30.3489	130.4600
4	11	2.4603	−1.8037	39.6822	165.8360
5	10	−3.3333	0.6667	33.3333	136.2960
5	10	2.0000	−2.0000	40.0000	160.0000
6	9	−2.9761	0.8729	35.7128	141.3050
6	9	1.6427	−2.2063	39.7128	154.9910
7	8	−2.6825	1.0972	37.5547	145.9080
7	8	1.3491	−2.4305	38.8880	150.3880

The value $p = 5$ corresponds to maximal energy $E = 40$ and we get the Clebsch graph with the spectrum $10, 2^5, -2^{10}$.

Consider now $n = 10$

$m = 30$ edges

A maximal energy graph in $\mathcal{G}$ cannot be complete. Therefore it must have at least three distinct eigenvalues. Restrict our search further to connected graphs with largest eigenvalue 6 (which is simple). Then $\mathcal{K} = \{6\}$. (The complement of the Petersen graph is in $\mathcal{G}$.) Now we have $|K| = 1$, $|J| = 9$, $C = 6$, and $D = 36$. Our program gives the following solutions.

p	q	x	y	E	$\frac{1}{6}\left(\sum_{i=1}^{n} x_i^3\right)$
1	8	-4.8830	-0.1396	12.0000	16.5911
1	8	3.5497	-1.1937	19.0994	41.1866
2	7	-3.4555	0.1302	13.8221	22.2487
2	7	2.1222	-1.4635	20.4888	35.5290
3	6	-2.7749	0.3874	16.6491	25.3752
3	6	1.4415	-1.7208	20.6491	32.4025
4	5	-2.3333	0.6667	18.6667	27.7778
4	5	1.0000	-2.0000	20.0000	30.0000

For $p = 4$, we find that $L(K_5)$, the line graph of the complete graph K_5, has distinct eigenvalues 6, 1, -2 with multiplicities 1, 4, 5 respectively. The graph $L(K_5)$ is known to have maximal energy among all 10 vertex graphs .

$m = 9$ edges

graphs having a simple eigenvalue $\mathcal{K} = \{3\}$. Thus $|K| = 1$, $|J| = 9$, $C = 3$, and $D = 9$.

p	q	x	y	E	$\frac{1}{6}(\Sigma_{i=1}^{n} x_i^3)$
1	8	−3.0000	0.0000	6.0000	0.0000
1	8	2.3333	−0.6667	10.6667	6.2222
2	7	−2.0972	0.1706	8.3887	1.4313
2	7	1.4305	−0.8373	11.7220	4.7910
3	6	−1.6667	0.3333	10.0000	2.2222
3	6	1.0000	−1.0000	12.0000	4.0000
4	5	−1.3874	0.5099	11.0994	2.8300
4	5	0.7208	−1.1766	11.7661	3.3922

For $p = 1$ we get the star $K_{1,9}$ (stars are minimal energy graphs among the trees) and for $p = 3$, we get that the graph $K_4 \cup 3K_2$ has maximal energy .

Partially confirmed tendency of eigenvalues of high multiplicity (i.e., small number of distinct eigenvalues) in maximal energy graphs. However, in some cases a large number of distinct eigenvalues occur. Among trees paths have maximal energy.

Examples with a high number of distinct eigenvalues show that, in these cases, several sets of eigenvalues produced by our procedure by specifying families of eigenvalues $\mathcal{K}$ do not actually correspond to graphs.

Let $\pi_1, \pi_2, \ldots, \pi_n$ be (distinct) eigenvalues of a path P_n on n vertices. Let $\mathcal{K}_i = \{\pi_1, \pi_2, \ldots, \pi_i\}, i = 1, 2, \ldots, n-2$. By applying our procedure in turn with these sets we come to P_n only after $n-2$ iterations.

Conclusion

Looking for extremal graphs using tools from calculus.

Graphs with extremal energy “should” have a small number of distinct eigenvalues.

Discrete nature of the problem often prevents the expected “nice” solutions.

Results by J.H. Koolen and V. Moulton and by V. Nikiforov give a solution of the maximal energy problem in an asymptotic sense.

A small number of distinct eigenvalues in extremal graphs appears rarely (complete graphs for $n \leq 7$ and strongly regular graphs for $n = 10$ and $n = 4\tau^2$). Our results for $n = 8, 9, 10, 11, 12$ show that, at least for moderate values of n, the structure of maximal graphs could vary unexpectedly. Having in mind the fact that paths are maximal energy trees, such effects also appear in some form for large values of n.

The idea for this work arose during the workshop *"Spectra of families of matrices described by graphs, digraphs, and sign patterns"* which was held at American Institute of Mathematics in Palo Alto, California, U.S.A. on October 23–27, 2006.

J. Grout, Department of Mathematics, Brigham Young University,
Provo, UT 84602, USA e-mail: grout@math.byu.edu

Cvetkovic D., Grout J., *Maximal energy graphs should have a small number of distinct eigenvalues*, Bull. Acad. Serbe Sci. Arts, Cl. Sci. Math. Natur., Sci. Math., to appear.