HYPERENERGETIC GRAPHS AND CYCLOMATIC NUMBER

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Abstract. Let \( G \) be a graph with \( n \) vertices and \( m \) edges. Then its cyclomatic number is \( c = m - n + 1 \). If \( \lambda_1, \lambda_2, \ldots, \lambda_n \) are the eigenvalues of \( G \), then its energy is \( E(G) = \sum_{i=1}^{n} |\lambda_i| \). The graph \( G \) is said to be hyperenergetic if \( E(G) > E(K_n) = 2n - 2 \). It is known [Nikiforov, J. Math. Anal. Appl. 327 (2007) 735-738] that almost all graphs are hyperenergetic. We now show that for any \( c < \infty \), there is only a finite number of hyperenergetic graphs with cyclomatic number \( c \). In particular, there are no hyperenergetic graphs with \( c \leq 8 \).

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1. Introduction

Let \( G \) be a simple graph with \( n \) vertices and \( m \) edges. Then the cyclomatic number of \( G \) is \( c = m - n + 1 \). Throughout this paper, without loss of generality, we assume that \( G \) is connected. If so, then a graph with \( c = 0 \) is called a tree. Graphs with \( c = 1, 2, 3, 4, \ldots \) are said to be unicyclic, bicyclic, tricyclic, tetracyclic, \ldots, respectively.
Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the graph $G$ [3, 5]. Then the energy of $G$ is defined as

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|.$$ 

Details on the mathematical theory of graph energy can be found in the recent reviews [7, 10, 20]; for the chemical background and applications of $E$ see [8, 12].

Earlier empirical studies (especially those restricted to molecular graphs) showed that the energy can be approximated by [13, 14, 15, 21] or bounded by [2, 21] expressions in which the only variables are $n$ and $m$, and in which $E$ is a monotonically increasing function of $m$. This observation lead to the conjecture that the complete graph $K_n$, possessing the greatest possible number of edges, has maximum energy. The conjecture was found to be false [2]. In [2] it was shown that for $n \leq 7$ the $n$-vertex graph with maximal energy is $K_n$. However, for $n \geq 8$ there exist graphs with energy exceeding $2n - 2$. Graphs whose energy exceeds the energy of the complete graph, i.e., $n$-vertex graphs for which $E(G) > E(K_n) = 2n - 2$, were named hyperenergetic graphs [6].

The first systematic construction of hyperenergetic graphs was discovered by Walikar et al. [27]. After that, hyperenergeticity was verified for numerous classes of graphs [1, 11, 16, 19, 23, 24, 25]. Some other graphs were shown to be not hyperenergetic [9, 26]. Researches along these lines were much slowed down after Nikiforov discovered that almost all graphs are hyperenergetic [22]. In fact, Nikiforov proved a much stronger result:

**Theorem 1.** [22] For almost all graphs

$$\left(\frac{1}{4} + o(1)\right) n^{3/2} < E(G) < \left(\frac{1}{2} + o(1)\right) n^{3/2}.$$ 

2. Hyperenergetic graphs with fixed cyclomatic number

Bearing in mind Theorem 1, it is somewhat surprising that the number of hyperenergetic graphs with any fixed value $c$ of the cyclomatic number is limited. Namely, we have:

**Theorem 2.** For any value of $c$, $0 \leq c < \infty$, the number of hyperenergetic graphs with cyclomatic number $c$ is finite.
In fact, there is an even stronger restriction:

**Theorem 3.** No graph with cyclomatic number $c$ and more than $c$ vertices is hyperenergetic.

**Proof.** The energy of any graph $G$ with $n$ vertices and $m$ edges is bounded from above by [17, 18]

$$E(G) \leq \frac{2m}{n} + \sqrt{(n - 1) \left[ 2m - \left( \frac{2m}{m} \right)^2 \right]}.$$ 

Therefore, if

$$\frac{2m}{n} + \sqrt{(n - 1) \left[ 2m - \left( \frac{2m}{m} \right)^2 \right]} \leq 2n - 2 \quad (1)$$

then the respective graph cannot be hyperenergetic.

Inequality (1) can be transformed into

$$2m^2 - m(n - 1)(n + 4) - 2n(n - 1)^2 \geq 0$$

whose solutions are $m \geq n(n - 1)/2$ and $m \leq 2(n - 1)$. It cannot be $m > n(n - 1)/2$, since an $n$-vertex graph has at most $n(n - 1)/2$ edges. Therefore, the graphically feasible solutions of (1) are $m = n(n - 1)/2$ and $m \leq 2(n - 1)$. The solution $m = n(n - 1)/2$ is not interesting, since then $G \cong K_n$. Thus $m \leq 2(n - 1)$ i.e., $m < 2n - 1$ is a sufficient condition for non-hyperenergeticity of the graph $G$. Now,

$$m < 2n - 1 \iff m - n + 1 < n \iff n > c$$

which implies Theorem 3, which in turn implies Theorem 2. \qed

3. Applications to graphs with small cyclomatic number

**Lemma 4.** A graph with cyclomatic number $c$ has at least $\left\lfloor \frac{3 + \sqrt{1 + 8c}}{2} \right\rfloor$ vertices.
Proof. The cyclomatic number of the complete graph is \( c(K_n) = (n - 1)(n - 2)/2 \), from which

\[
n(K_n) = \frac{3 + \sqrt{1 + 8c(K_n)}}{2}.
\]

Lemma 4 follows now from the fact that if \( c(K_n) < c(K_{n+1}) \), then the graph with cyclomatic number \( c \) must have at least \( n(K_{n+1}) \) vertices.

According to Lemma 4, a graph with cyclomatic number 0, 1, 2, 3, 4, 5, and 6 must have at least 1, 3, 4, 4, 5, 5, and 5 vertices, respectively. This implies:

**Theorem 5.** (a) There are no hyperenergetic trees.
(b) There are no hyperenergetic unicyclic graphs.
(c) There are no hyperenergetic bicyclic graphs.
(d) There are no hyperenergetic tricyclic graphs.
(e) There are no hyperenergetic tetracyclic graphs.
(f) There are no hyperenergetic pentacyclic graphs.
(g) There are no hyperenergetic hexacyclic graphs.

Proof. According to Theorem 3, in order that a tree, unicyclic, bicyclic, tricyclic, and tetracyclic graph be hyperenergetic, these must have less than 1, 2, 3, 4, and 5 vertices, respectively. By Lemma 4, this is impossible. This proves (a), (b), (c), (d), and (e).

By Theorem 3, in order that a pentacyclic graph be hyperenergetic, it must have less than 6 vertices. By Lemma 4, a pentacyclic graph must have at least 5 vertices. Therefore, we need to examine pentacyclic graphs with 5 vertices, i.e., graphs with \( n = 5 \) and \( m = 9 \). The only such graph is \( K_5 - e \), obtained by deleting an edge from \( K_5 \). Since \( E(K_5 - e) = 7.2915 \ldots < 2 \cdot 5 - 2 \), this graph is not hyperenergetic. This proves (f).

By Theorem 3, in order that a hexacyclic graph be hyperenergetic, it must have less than 7 vertices. By Lemma 4, a hexacyclic graph must have at least 5 vertices. Therefore, we need to examine hexacyclic graphs with 5 and 6 vertices. The only hexacyclic graph with 5 vertices is \( K_5 \), which by definition is not hyperenergetic. We therefore have to examine the hexacyclic graphs with 6 vertices, i.e., graphs with \( n = 6 \) and \( m = 11 \). From the available tables of six-vertex graphs \([4]\) we get that there exist exactly nine such graphs. These are depicted in Fig. 1, together with the calculated energies. None of these graphs has energy greater than 10, implying that none of these are hyperenergetic. This proves (f). \( \square \)
Hyperenergetic graphs and cyclomatic number

By an analogous way of reasoning, but assisted by use of computers, we could extend Theorem 5 also to the cases $c = 7$ and $c = 8$. If $c = 7$ then all heptacyclic graphs with 6 and 7 vertices need to be constructed and their energies calculated. If $c = 8$ then all octacyclic graphs with 6, 7, and 8 vertices need to be constructed and their energies calculated. After this has been done we found that none is hyperenergetic. This leads to:

**Proposition 6.** (h) *There are no hyperenergetic heptacyclic graphs.*

(i) *There are no hyperenergetic octacyclic graphs.*

For greater values of $c$, the considerations become so complicated that, without a massive use of computers, are not feasible. Anyway, at some point we must reach a value of $c$ for which there exist $c$-cyclic hyperenergetic graphs. This value of the cyclomatic number is less than or equal to 11, as seen from the example shown in Fig. 2.
In the work [2], by means of a computer–aided combinatorial optimization method (called “variable neighborhood search”), it was found that for $n \leq 7$ there are no hyperenergetic graphs, and that there exist hyperenergetic graphs with $n = 8$. If we would accept this finding as mathematically correct, then both Theorem 5 and part (h) of Proposition 6 would follow immediately. In addition, in order to verify part (i) of Proposition 6, it would be sufficient to check only the octacyclic graphs with 8 vertices.

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Hyperenergetic graphs and cyclomatic number


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