Barabasi–Albert trees are hypoenergetic

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Abstract
We prove that graphs following the model of Barabasi–Albert tree with $n$ vertices are hypoenergetic in the large $n$ limit.

Keywords Barabasi–Albert tree · Graph energy

Mathematics Subject Classification 05C50 · 05C80

1 Introduction and statements of results

The graph energy is a graph invariant that was defined by I. Gutman [7] from his studies of mathematical chemistry.

The energy of a graph $G$, denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of the eigenvalues of the adjacency matrix $A = A(G)$, i.e.,

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

In other words, the energy of a graph is the trace or nuclear norm of its adjacency matrix.

Many results on inequalities for $\mathcal{E}(G)$ have been established and there are many examples of deterministic graphs whose energy is known. An excellent introduction to the theory of graph energy can be found in the monograph [14]. However, very few research papers have studied the properties of energy on random graphs.

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To the best of our knowledge the only papers considering the energy of a random graph are due Nikiforov [16, 17]. In these papers, Nikiforov describes precisely the asymptotic behavior, as the size of the graph goes to infinity, of the energy of two families of random graphs: Erdős–Rényi graph with fixed $p$, [16], and uniform $d$-regular graphs, [17]. Both of these results rely on the fact that the explicit limiting distributions of the adjacency matrix of these graphs are well known.

This paper contributes to the theory of graph energy in two ways. First, by the use of Ky Fan’s inequality we propose a new inequality for the energy of a tree in Theorem 3.1, which in some cases dramatically improves known inequalities such as McClelland’s, Koolen and Moulton’s and their variants. Second, we use the previous inequality and modify its proof to show that Barabasi–Albert trees are asymptotically hypoenergetic, (i.e., the energy is smaller than the number of vertices), as the size of the matrix goes to infinity. We state this second result as our main theorem.

**Theorem 1.1** With probability tending to 1, as the size tends to infinity, the energy of a typical tree chosen with the preferential model of Barabasi–Albert is smaller than the size of the tree.

Let us mention that the results of [16] show that almost all graphs on $n$ vertices have energy of order $(\frac{4}{3\pi} + o(n))n^3/2$ and, in particular, are hyperenergetic (i.e., their energy is larger than the energy of the complete graph). Theorem 1.1 contrasts with this and shows that there are plenty of trees of size $n$, with energy smaller than $n$. This should not be as surprising since trees or tree-like graphs are very rare when considering uniform random graphs. We believe that in order to compare Erdős–Rényi graphs with random trees one needs to set $p = \frac{2}{n}$, so that at least the expected number of edges coincides. We try to build some intuition in the last section of the paper.

Apart from this introduction, the paper contains four more sections. Section 2 gives the necessary preliminaries. Section 3 proves our new inequality for the energy of a tree. The main theorem of the paper is proved in Sect. 4. We present some simulations, leading to open problems and conjectures in final Sect. 5.

## 2 Preliminaries

### 2.1 Notation on graphs

We consider finite simple undirected graphs. For definitions used here we refer to Diestel [6]. A graph is called a tree if it is connected and has no cycles.

For a graph $G = (V, E)$ and a vertex, $v \in V$, the closed neighborhood of $v$ is the set $N(v) = \{v\} \cup \{w \in V | w \sim v\}$, and the degree of $v$, denoted by $d(v) = \deg(v)$ is the number of neighbors of $v$, i.e., $d(v) = |N(v)| - 1$.

A tree is called a star graph if it consists of one vertex which is joined to $n - 1$ vertices. We denote the star graph with $n$ vertices by $S_n$, which is also called the $n$-star.
A tree is called a path if it consists of \(n\) vertices, \(v_1, \ldots, v_n\), such that \(v_i \sim v_j\). We denote the path of size \(n\) by \(P_n\).

### 2.2 Inequalities for the energy of a graph

In this section we remind the reader of some inequalities for the energy of a graph.

The first inequality is the well-known McClelland’s inequality \([15]\) which says that

\[
\mathcal{E}(G) \leq \sqrt{2mn}.
\]

Two other inequalities due to Koolen and Moulton are the following. First, in \([10]\) they prove that for any graph with \(n\) vertices and \(m\) edges we have

\[
\mathcal{E}(G) \leq 2 \frac{2m}{n} + \sqrt{(n-1) \left(2m - \left(\frac{2m}{n}\right)^2\right)}.
\] (2.1)

If, moreover, one knows that \(G\) is bipartite graph, from \([11]\), one has

\[
\mathcal{E}(G) \leq 2 \frac{2m}{n} + \sqrt{(n-2) \left(2m - 2 \left(\frac{2m}{n}\right)^2\right)}.
\] (2.2)

The following theorem of Ky-Fan will be very useful, which in particular shows that the graph energy satisfies a triangle inequality.

**Theorem 2.1** Let \(A, B,\) and \(C\) be square self-adjoint matrices of order \(n\), such that \(A + B = C\). Then

\[
\sum_{i}^{n} |\lambda_i(A)| + \sum_{i}^{n} |\lambda_i(B)| \geq \sum_{i}^{n} |\lambda_i(C)|
\]

We state a version of Ky-Fan’s inequality for subgraphs.

**Theorem 2.2** (Ky-Fan’s inequality for subgraphs) Let \(G\) be a graph and \(H_1, H_2, \ldots, H_n\) be subgraphs of \(G\) whose adjacency matrices satisfy the condition \(A(G) = A(H_1) + A(H_2) + \cdots + A(H_n)\). Then

\[
\mathcal{E}(G) \leq \mathcal{E}(H_1) + \mathcal{E}(H_2) + \cdots + \mathcal{E}(H_n)
\] (2.3)

**Definition 2.3** Let \(G = (V, E)\) be a simple graph. A graph partition is a collection \(\mathcal{G} = \{G_i = (V_i, E_i)\}_{i \in I}\) of subgraphs of \(G\) with the following properties.

1. For any edge \(e \in E\), there is \(G_i \in \mathcal{G}\) such that \(e \in E_i\)
2. Any \(G_i, G_j \in \mathcal{G}\) with \(G_i \neq G_j\) do not share edges, i.e., \(E_i \cap E_j\) is empty.
Note that graph partitions satisfy the hypotheses of the Ky-Fan’s inequality. The following lemma is a direct consequence of this.

**Lemma 2.4** Let $G$ be a graph partition of $G$ then

$$
\mathcal{E}(G) \leq \sum_{H \in \mathcal{G}} \mathcal{E}(H)
$$

Finally, we would like to mention the following inequality found by Arizmendi and Juarez [3] in their study of the energy of a vertex. We give a new simple proof by the use of Ky-Fan’s theorem, Theorem 2.1.

**Lemma 2.5** (Arizmendi and Juarez [3]) For a graph $G$ with vertices of degrees $d_1, \ldots, d_n$

$$
\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_i}
$$

(2.4)

**Proof** For each vertex $i$, consider the self-adjoint matrix $A^{(i)}$ such that $A^{(i)}_{ji} = 1/2$ if $i \sim j$, $A^{(i)}_{ji} = A^{(i)}_{ij} = 0$ if $j \not\sim i$ and $A^{(i)}_{ik} = 0$ if $l, k \neq i$.

Since $2A^{(i)}$ is the adjacency matrix of a $d_i$-star graph, $\sum_{k=1}^{n} |\lambda_k(A^{(i)})| = \sqrt{d_i}$. Finally, since $A^{(i)}_{ij} + A^{(i)}_{ij} = 1$, one easily sees that $A(G) = \sum_{i=1}^{n} A^{(i)}$. We conclude by Ky-Fan’s theorem.

### 2.3 Barabasi–Albert model

Various natural, social and technological systems are thought to have a scale free degree distribution: the proportion $P(d)$ of nodes with degree $d$ is proportional to $d^{-\gamma}$, at least asymptotically, for some $\gamma$ that does not depend on the size of the network. To address this, in [2] Barabasi and Albert proposed a random graph model that grows with time and incorporates preferential attachment. That is, a new vertex attaches with higher probability to already existing vertices of higher degrees. The original construction of the model is as follows:

Starting with $m_0$ vertices, at each step we add a new vertex and $m(\leq m_0)$ edges, joining the new vertex to $m$ vertices already in the graph. These edges are randomly chosen in such a way that the probability for the new vertex to be connected to an already existing vertex $i$ is proportional to the degree of $d_i$,

$$
\Pi(d_i) = \frac{d_i}{\sum_j d_j}.
$$

We are concerned with the case where both $m_0$ and $m$ are equal to 1. Here, the graph obtained by the process in every time step is a tree. A parameter $\alpha$ is added to the model in order to consider the case of nonlinear dependency for the preferential
attachment, as seen in Krapivsky et al. [12]. In this case, the probability for a new vertex to be connected to a vertex $i$ of degree $d_i$ is now proportional to $d_i^a$. That is to say, $\Pi(d_i) = d_i^a / \sum_j d_j^a$.

### 3 A basic bound for trees

One basic problem is to find the extremal values or good bounds for the energy within some special class of graphs and to characterize graphs from this class which reach this extremal values of the energy. In this section we present an upper bound for the energy of a tree, which can be derived rather simply from the theory, specifically from Ky Fan’s inequality, but a priori not so natural. This bound turns out to be quite useful especially for trees with many vertices of degree 1, which is where the Arizmendi–Juarez bound, (2.4), seems to perform badly. This will be used in the next section when considering Barabasi–Albert trees.

**Theorem 3.1** Let $T$ be a tree with degrees $\Delta = d_1 \geq \cdots \geq d_n, n \geq 3$. Then

$$E(T) \leq \sum_{i=2}^n 2\sqrt{d_i - 1} + 2\sqrt{\Delta} \leq \sum_{i=1}^n 2\sqrt{d_i - 1} + 1 \quad (3.1)$$

**Proof** Let $v_0$ be a vertex with largest degree. We root the tree $T$ at $v_0$. For each vertex $v \neq v_0$, there is a unique path $v_0 \tilde{v}_1 \cdots \tilde{v}_k = v$ from $v_0$ to $v$. Let $a(v) = v_{k-1}$ be the last vertex in this path before arriving to $v$, which is sometimes called the parent or ancestor of $v$. Now, let $\tilde{N}(v) = v \cup N(v) \setminus \{a(v)\}$. We denote by $H(v)$, the induced subgraph of $G$, with vertex set $\tilde{N}(v)$. Notice that $H(v)$ is a star $S_{d(v)}$ so its energy is given by $2\sqrt{d(v) - 1}$. We also denote by $H(v_0)$ the subgraph induced by $v_0 \cup N(v_0)$, which is a star $S_{\Delta}$ with energy $2\sqrt{\Delta}$.

The family \( \{H(v)\}_{v \in V} \) is a graph partition of $T$. By the use of Ky-Fan’s inequality (2.3) we may deduce the first inequality.

The second inequality holds since for $\Delta \geq 2$, $\sqrt{\Delta} - \sqrt{\Delta - 1} \leq \frac{1}{2\sqrt{\Delta - 1}} \leq 1/2$. \( \square \)

**Example 3.2** A tree is called a double star $S_{p,q}$ if it is obtained by joining the centers of two stars $S_p$ and $S_q$ by an edge. The double star $S_{p,q}$ has $p + q$ vertices. Its characteristic polynomial is given by $\chi_{p,q}(x) = x^n - (p + q - 1)x^{n-2} + (p - 1)(q - 1)x^{n-4}$ and thus the 4 nonzero eigenvalues of $S_{p,q}$ are

$$\pm \frac{1}{\sqrt{2}} \sqrt{p + q - 1} \pm \sqrt{(p + q + 1)^2 - 4(pq + 1)}.$$ 

Hence, we can easily calculate the energy:
\[
\mathcal{E}(S_{p,q}) = \sqrt{2} \left( \sqrt{p + q - 1 + (p + q + 1)^2} - 4(pq + 1) \right)
+ \sqrt{p + q - 1 - (p + q + 1)^2} - 4(pq + 1) \right)
\]

In order to see the improvement in our bound, the following table compares the true values of the energy of the double star \(S_{p,q}\), for \(p = 5\) and different values of \(q\), with the bounds from McClelland Inequality, the bound from Arizmendi–Juarez (A–J, Eq. (2.4)), Koolen and Moulton Inequalities (K–M 1, Eq. (2.1) and K–M 2, Eq. (2.2)) and the above bound Eq. (3.1).

| \(p = 5\) | Energy | Thm. 3.1 | K–M 1 | K–M 2 | A–J | McClelland |
| --- | --- | --- | --- | --- | --- | --- |
| \(q = 1\) | 4.472 | 4.472 | 7.676 | 7.550 | 6. | 7.745 |
| \(q = 2\) | 6.324 | 6.472 | 9.088 | 8.961 | 8. | 9.165 |
| \(q = 3\) | 7.115 | 7.3 | 10.500 | 10.374 | 9.414 | 10.583 |
| \(q = 4\) | 7.727 | 7.936 | 11.913 | 11.787 | 10.732 | 12. |
| \(q = 5\) | 8.246 | 8.472 | 13.326 | 13.200 | 12. | 13.416 |
| \(q = 6\) | 8.705 | 8.944 | 14.739 | 14.613 | 13.236 | 14.832 |
| \(q = 7\) | 9.120 | 9.371 | 16.152 | 16.027 | 14.449 | 16.248 |
| \(q = 8\) | 9.504 | 9.763 | 17.566 | 17.441 | 15.645 | 17.663 |
| \(q = 9\) | 9.861 | 10.129 | 18.979 | 18.854 | 16.828 | 19.078 |
| \(q = 10\) | 10.198 | 10.47 | 20.393 | 20.268 | 18. | 20.493 |

**Example 3.3** Similar as for the double star we compare the different inequalities for the path of size \(n\), \(P_n\), with the energy given by,

\[
\mathcal{E}(P_{2n}) = \frac{2}{\sin(\pi/(4n + 2))} - 2, \quad \mathcal{E}(P_{2n+1}) = \frac{2 \cos(\pi/(4n + 4))}{\sin(\pi/(4n + 4))} - 2.
\]

| \(n = 2\) | Energy | Thm. 3.1 | K–M 1 | K–M 2 | A–J | McClelland |
| --- | --- | --- | --- | --- | --- | --- |
| \(n = 3\) | 2. | 2. | 2. | 2. | 2. | 2. |
| \(n = 4\) | 2.828 | 2.828 | 3.441 | 3.333 | 3.414 | 3.464 |
| \(n = 5\) | 4.472 | 4.828 | 4.854 | 5.732 | 4.828 | 4.898 |
| \(n = 6\) | 5.464 | 6.828 | 6.264 | 6.139 | 6.242 | 6.324 |
| \(n = 7\) | 6.988 | 8.828 | 7.676 | 7.550 | 7.656 | 7.745 |
| \(n = 8\) | 8.055 | 10.828 | 9.088 | 8.961 | 9.071 | 9.165 |
| \(n = 9\) | 9.517 | 12.828 | 10.500 | 10.374 | 10.485 | 10.583 |
As one can see from the above example, Theorem 3.1 performs badly, compared with the rest of the inequalities in cases where there are many vertices of degree 2 joined by an edge. In this case, compared with the bound (2.4), for each pair we get a contribution of 2 instead of $\sqrt{2}$. This observation will be useful in the next section in order to improve the bound (3.1), when proving Theorem 1.1.

4 An upper bound for BA trees

In this section we prove the main theorem, Theorem 1.1. The proof consists of modifying the partition used in the proof of Theorem 3.1 by analyzing more carefully vertices of degree 2. Before doing that, we estimate what Theorem 3.1 says about Barabasi–Albert trees.

4.1 A first bound

Let $T$ be a tree of order $n$ that follows the model of Barabasi–Albert with parameter $\alpha = 1$.

For each $d \geq 1$, we denote by $n_d$ the amount of vertices of degree $d$ in $T$. Before going into details, we notice that the total number of vertices may be calculated by

$$\sum_{d=1}^{n} n_d = n, \quad (4.1)$$

while the sum of degrees may be calculated by

$$\sum_{d=1}^{n} n_d \cdot d = 2n - 2, \quad (4.2)$$

Now, in the case of a Barabasi–Albert tree, if we denote by

$$\alpha_d = \frac{4}{(d)(d+1)(d+2)},$$

as showed by Bollobás et al. [4], for every fixed $d$, with probability tending to 1 as $n \to \infty$, we have

$$\frac{n_d}{n} = \alpha_d + o(1).$$

Let $\Delta = d_1 \geq \cdots \geq d_n$ be the degrees of the vertices in $T$. We look at the sum
Using that for any fixed \( m \in \mathbb{N} \)
\[
\sum_{d=1}^{m} \frac{4}{d(d+1)(d+2)} = 2 \sum_{d=1}^{m} \left( \frac{1}{d} + \frac{1}{d+2} - \frac{2}{d+1} \right) = 1 - \frac{2}{(m+1)(m+2)}
\]
we see that for any \( m \) fixed and large \( n \), from (4.1)
\[
\sum_{d=m+1}^{n} \frac{n_d}{n} = \frac{2}{(m+1)(m+2)} + o(1)
\]
or
\[
\sum_{d=m+1}^{n} n_d = n \frac{2}{(m+1)(m+2)} + o(n),
\]
from where, together with (4.2), by Cauchy–Schwarz we see that
\[
\sum_{d=m+1}^{n} n_d \sqrt{d} \leq \sqrt{\frac{(2n - 2)(n)}{(m+1)(m+2)}} \frac{2}{(m+1)(m+2)} + o(n) \leq n \frac{2}{m} + o(n).
\]

By using that \( \frac{n_d}{n} = \zeta_d + o(1) \) for \( 1 \leq d \leq m \), we get the relations:
\[
\frac{S}{n} = 2 \sum_{d=1}^{n} \frac{n_d}{n} \sqrt{d - 1} = 2 \sum_{d=1}^{m} \frac{4\sqrt{d - 1}}{(d)(d+1)(d+2)} + o(1) + \sum_{d=m+1}^{n} \frac{n_d}{n} \sqrt{d - 1}
\]
\[
\leq 2 \sum_{d=1}^{m} \frac{4\sqrt{d - 1}}{(d)(d+1)(d+2)} + o(1) + \frac{1}{n} \sum_{d=m+1}^{n} n_d \sqrt{d}
\]
\[
\leq 2 \sum_{d=1}^{m} \frac{4\sqrt{d - 1}}{(d)(d+1)(d+2)} + \frac{2}{m} + o(1)
\]
\[
\leq 2 \sum_{d=1}^{\infty} \frac{4\sqrt{d - 1}}{(d)(d+1)(d+2)} + \frac{2}{m} + o(1).
\]
which holds for any fixed \( m \) and large \( n \).

Since \( m \) is fixed but arbitrary, we obtain the asymptotic bound
\[
\frac{S}{n} \leq 2 \sum_{d=1}^{\infty} \frac{4\sqrt{d - 1}}{(d)(d+1)(d+2)} \approx 1.00576755.
\]
4.2 Proof of Theorem 1.1

To achieve our goal we need to look a little bit further on the degrees of the tree. So let us denote by $n_{kl}$ the proportion of edges that connect a pair of nodes of degrees $k$ and $l$ with $k \leq l$ in our graph $G$.

As we will show in Appendix, with probability tending to 1, as $n \to \infty$ we have

$$n_{2,2} = \frac{1}{45} + o(1)$$

Label the vertices of $G$ as $v_1, \ldots, v_n$ so that $v_1$ is a vertex of highest degree $\Delta$ in $G$ and partition the graph into a star $S_{\Delta+1}$ centered at $v_1$ and $n-1$ stars $S_d$ centered in each of the other vertices as in Theorem 3.1. For each vertex $v$, denote the corresponding star with center in $v$ by $H(v)$.

Let $u_1, u_2$ be adjacent vertices of degree 2 such that $H(u_1)$ is the graph induced by this pair of vertices. Let $u_0, u_3$ be the only other neighbors of $u_1$ and $u_2$, respectively. We change the partition of the graph by taking out $H(u_1), H(u_2)$ from it and replacing them with their union. As both graphs are stars with one edge and they share a vertex, its union is a star $S_3$. The energy of $S_3$ is $2\sqrt{2}$, opposed to the sum of energies of $H(u_1), H(u_2)$ which is 4, so the sum of energies of all parts after this change in the partition is reduced by $(4 - 2\sqrt{2})$. We can repeat this process for each other pair of neighbors of degree 2 as long as they are different from any previously chosen pairs $\{u_1, u_2\}$ and from previous pairs of the form $\{u_0, u_1\}$ or $\{u_2, u_3\}$.

Each time we iterate this process, at most 3 pairs of neighbors of degree 2 become unusable. Therefore, we are able to do this replacement at least $\frac{1}{3} n \cdot n_{2,2}$ times. After iterating as many times as possible, we get a partition of $G$ into graphs $K_1, \ldots, K_m$ such that:

$$\frac{\mathcal{E}(G)}{n} \leq \frac{1}{n} \sum_{j=1}^{m} \mathcal{E}(K_j)$$

$$\leq \frac{1}{n} \sum_{i=1}^{n} (\mathcal{E}(H(v_i))) - \frac{n_{2,2}}{3} (4 - 2\sqrt{2})$$

$$= \frac{1}{n} \left( \sum_{i=2}^{n} 2\sqrt{d_i - 1} + 2\sqrt{\Delta} \right) - \frac{4 - 2\sqrt{2}}{3 \cdot 45} + o(1)$$

$$\leq \frac{S}{n} + \frac{1}{n\sqrt{\Delta - 1}} - \frac{4 - 2\sqrt{2}}{3 \cdot 45} + o(1)$$

$$\leq 2 \sum_{d=1}^{\infty} \frac{4\sqrt{d - 1}}{(d)(d + 1)(d + 2)} - \frac{4 - 2\sqrt{2}}{135} + o(1)$$

$$\approx 0.997089 + o(1)$$

This proves that with probability tending to 1 as $n \to \infty$, a graph $G$ of $n$ vertices that follows the model of Barabasi–Albert is hypoenergetic.
Finally, let us notice that the above considerations actually work for any tree, resulting in the following

**Theorem 4.1** Let $T$ be a tree with degrees $\Delta = d_1 \geq \cdots \geq d_n$, $n \geq 3$. Then

$$E(T) \leq \sum_{i=2}^{n} 2\sqrt{d_i - 1} + 2\sqrt{\Delta} - \frac{e_{2,2}^2}{3}(4 - 2\sqrt{2}) \quad (4.3)$$

where $e_{2,2}$ is the number of pairs of vertices of degree 2 which are joined by an edge.
5 Conclusion, generalizations and open problems

We end with some consideration and simulations leading to new open problems. All the simulations were done in Python 3.8.3 and plot in tikzplotlib v0.9.4.

5.1 Comparing the bound from Theorem 3.1

We calculated the values of both the quotient energy/size and the bound of Theorem 3.1 for 200 random trees of size $n = 2000$ following the Barabasi–Albert model with parameter $\alpha = 1$. The results suggest that an increase or decrease in the energy results in a similar change in the bound from Theorem 3.1. We believe that this means that for generic trees $P_n$ the energy is proportional to the energy. Also, from the tables above we conjecture that there is a constant $c < 1.5$ such that for any tree $cE(T) \geq 2 \sum_i (d_i - 1)$.

5.2 Varying $\alpha$

When considering the general framework of preferential models, naturally, one is lead to ask how the energy changes when the parameter $\alpha$ varies.

Now, as the parameter $\alpha$ changes, the influence that the degree of a vertex has in the probability of its current degree to increase also changes. As $\alpha$ increases, so does this influence. Likewise, greater values of $\alpha$ intensify the distinction of the vertices of higher degrees when compared with the rest. To be explicit, as pointed out in [12], for $\alpha > 1$ there are a few vertices which are linked to almost every other vertex and for $\alpha < 1$ hubs are much smaller. In other words, when $\alpha$ is large, the preferential tree is similar to a star, while when $\alpha$ is small it is similar to a path.

Thus, recalling that among trees of constant size, the star is the one that has the lowest energy, and the path is the one with highest energy, the intuition leads to think that, as the value of $\alpha$ increases, the energy decreases toward $E(S_n) = 2\sqrt{n - 1}$. On the contrary, when $\alpha$ is small we expect the energy to increase toward $E(P_n) \sim 1.273n$. In Fig. 4 we show a simulation where we calculate the accumulated average energy of 100 realizations, of a BA random tree with $\alpha$ in $\{-5, -2, 0, 0.5, 0.7, 1, 1.2, 1.5, 1.7, 2\}$. This simulation strengthens this intuition.

It may be possible to show by our same methods that a preferential model with parameter $\alpha > 1$ is hypoenergetic. For $\alpha < 1$ the degree distribution degree distribution does not follow a power laws, but a distribution of the form

$$q(d) = \frac{s}{d^\alpha} \prod_{i=1}^{d} \frac{i^{\alpha}}{s + i^{\alpha}}$$

where $s$ is such that $\sum_{d=1}^\infty q(d) = 1$.

It would be interesting if there is a bound from below as a function of the degrees to show that for certain $\alpha$ the BA tree is not hypoenergetic.

Moreover, in Fig. 5, we preset the plot of the average ratio between energy and the size of 50 BA random trees for various values of $\alpha$ ratio. The energy appears to
be decreasing with respect to $\alpha$. The value of $\alpha$ for which graphs start to be hypoenergetic in our simulations was $\tilde{\alpha} = 0.8006376$.

Thus let us state precisely the above observations as a conjecture.

**Conjecture 5.1** Let $\{X_n\}_n > 0$ be a sequence of trees with parameter $\alpha$.

(1) *For every $\alpha$ there exists $g(\alpha)$ such that following limit exists almost surely*
\[
\lim_{n \to \infty} \frac{\mathcal{E}(X_n)}{n} = g(x).
\]

(2) For \( x < .79 \) \( g(x) > 1 \). In particular, taking \( x = 0 \), this would imply that random recursive random trees are not hypoenergetic.

(3) For \( x > .81 \), \( g(x) < 1 \).

(4) \( g(x) \) is strictly decreasing on \( x \) and continuous.

(5) \( g(x) \to 0 \) as \( x \to \infty \) and \( g(x) \to 1.273 \) as \( x \to \infty \).

We note that since the degree distribution does not determine the energy, proving the monotonicity on \( x \) needs new ideas or tools.

### 5.3 Generic trees and Erdös–Rényi

From the main result of this paper one may be lead to the conclusion that a typical tree is hypoenergetic. However, this is not true, since the preferential model of Barabasi–Albert does not choose a tree with uniform distribution, but favors trees with certain large hubs.

The correct model to choose a tree with uniform distribution is the random recursive tree, which corresponds to \( x = 0 \) and as can be seen from Fig. 4 seems to be not hypoenergetic. It is natural to compare this model with an Erdös–Rényi model with expected number of edges equal \( n - 1 \). This is done in Fig. 6. In all of the instances, the resulting graph was also not hypoenergetic, but with smaller energy than that of uniform trees. We conjecture that this is the case in general. Of course, similarly as for \( x \), one may vary \( p \) to analyze how the energy varies.

### 5.4 Conclusions

In this paper we have shown that the energy of a BA tree is hypoenergetic. This result leads to new questions and conjectures on the behavior of other models for random trees or random graphs, which differ from the usual Erdös–Rényi graphs.

**Fig. 6** Energy/size of 200 random graphs of size \( n = 3000 \) following the Erdös–Rényi model with parameter \( p = 2/n = 0.0006 \) so that the expected number of edges is that of a tree of size 3000.
Appendix 1: Number of neighbors with degree 2

Let us denote by $n_{kl}$, the proportion of edges that connect a pair of nodes of degrees $k$ and $l$ with $k \leq l$ in our graph $G$. In [13] it was proven that as $n \to \infty$ we have

$$E(n_{kl}) = \frac{4(l-1)}{k(k+1)(k+l)(k+l+1)(k+l+2)} + \frac{12(l-1)}{k(k+l-1)(k+l)(k+l+1)(k+l+2)} + o(1).$$

In particular, $E(n_{2,2}) = \frac{1}{45} + o(1)$.

In this appendix we prove that with probability tending to 1, as $n \to \infty$ we have

$$n_{2,2} = \frac{1}{45} + o(1),$$

which is required in the proof of our main theorem. More precisely, we will prove the following theorem

**Theorem A.1** Let $T_n$ be a Barabasi–Albert tree on $n$ vertices and let $n_{2,2}(n)$ the number of edges connecting two vertices of degree 2. Then

$$
\mathbb{P}( |n_{2,2}(n) - 1/45 | > \sqrt{\log n/n}) \to 0
$$

as $n$ tends to infinity.

We follow the strategy of [4] by using Azuma–Hoeffding inequality.

**Proposition A.2** (Azuma–Hoeffding inequality) Let $(X_t)_{t=0}^{n}$ be a martingale with respect to the filtration $F_t$. Assume that there are predictable processes $(A_t)$ and $(B_t)$ (i.e., $A_t, B_t \in F_{t-1}$) and a constant $0 < c < + \infty$ such that for all $t \geq 1$, almost surely

$$A_t \leq X_t - X_{t-1} \leq B_t$$

and

$$B_t - A_t \leq c.$$

Then for all $\beta > 0$

$$
\mathbb{P}( |X_t - X_0| \geq \beta ) \leq 2 \exp \left( - \frac{\beta^2}{2c^2 n} \right).
$$

To prove the claim we will build a martingale $(X_n)_{n=0}^{n}$, such that $X_n = n_{2,2}(n)$, $X_0 = E(n_{2,2}) \approx 1/45$ and $|X_t - X_{t-1}| \leq 4/n$. If this is the case then by applying the Azuma–Hoeffding inequality to $X_n$ with $c = 4/n$ and $\beta = \sqrt{\log n}$ we obtain
\(\mathbb{P}(|X_n - E(X_n)| \geq \sqrt{\log n / n}) \leq 2 \exp\left(-\frac{\log n}{32}\right) = 2n^{-32}\),

which together with the fact the \(E(X_n) \approx 1/45\), as \(n \to \infty\), give the desired result.

To construct such martingale we consider the Barabási–Albert tree \(T_t\) as embedded in the process \(\{T_t\}_{t \geq 0}\), where \(T_t\) is built from \(T_{t-1}\) by adding joining the vertex \(v_t\) to the vertex \(v_i\) with probability proportional to \(\deg(v_i)\) as described above.

Now let \(\mathcal{F}_t\) be the \(\sigma\)-algebra generated by \(\{T_1, \ldots, T_t\}\). We claim that \(X_t = E(n_{2,2}(n)|F_t)\) satisfies the above properties. The fact that it is a martingale with \(X_n = n_{2,2}(n)\) and \(X_0 = E(n_{2,2}(n))\) is clear. So the main thing to check is the \(|X_t - X_{t+1}| \leq 4\). To see this note as in [4] that whether at stage \(t\) we join \(v_t\) to \(v_i\) or \(v_j\) does not affect the degrees at later times of vertices \(v_k, k \notin \{i,j\}\).

More precisely, the joint distribution of all other degrees is the same in either case.

So we are only interested in the number of vertices \(v\) attached to \(v_i\) or \(v_j\) with degree 2, provided that \(v_i\) or \(v_j\) have degree 2. There are at most 2 such vertices for in either case and thus, choosing \(v_i\) instead of \(v_j\) changes the number of edges joining vertices of degree 2 in at most 4 and then \(n_{2,2}(n)\) changes in at most \(4/n\). Thus \(|X_t - X_{t+1}| \leq 4/n\) as desired.

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**References**

1. Albert, R., Barábasi, A.: Statistical mechanics of complex networks. Rev. Mod. Phys. 74(47), 47–97 (2002). arXiv:cond-mat/0106096
2. Albert, R., Barábasi, A.: Emergence of scaling in random networks. Science 286(5439), 509–512 (1999). arXiv:cond-mat/9910332
3. Arizmendi, O., Juarez-Romero, O.: On bounds for the energy of graphs and digraphs. In: Contributions of Mexican Mathematicians Abroad in Pure and Applied Mathematics (vol. 709, pp. 1–19). Sociedad Matemática Mexicana, American Mathematical Society (2018)
4. Bollobás, B., Riordan, O., Spencer, J., Tusnády, G.: The degree sequence of a scale-free random graph process. Random Struct. Algorithms 18, 279–290 (2001). https://doi.org/10.1002/rsa.1009
5. Brouwer, A.E., Haemers, W.H.: Spectra of Graphs. Springer Science and Business Media, Berlin (2012)
6. Diestel, R.: Graduate texts in mathematics. Graph theory, 173 (2000)
7. Gutman, I.: The Energy of a graph. Berichte der Mathematische Statistischen Sektion im Forschungszentrum Graz. 103, 1–22 (1978)
8. Gutman, I.: The energy of a graph: old and new results. In: Algebraic combinatorics and applications (pp. 196–211). Springer, Berlin (2001)
9. Gutman, I.: On graphs whose energy exceeds the number of vertices. Linear Algebra Appl. 429(11), 2670–2677 (2008)
10. Koolen, J.H., Moulton, V.: Maximal energy graphs. Adv. Appl. Math. 26, 47–52 (2001)
11. Koolen, J.H., Moulton, V.: Maximal energy bipartite graphs. Graphs Comb. 19(1), 131–135 (2003)
12. Krapivsky, P.L., Redner, S., Leyvraz, F.: Connectivity of growing random networks. Phys. Rev. Lett. 85, 4629–4632 (2000)
13. Krapivsky, P.L., Redner, S.: Organization of growing random networks. Phys. Rev. E 63(6), 066123 (2001)
14. Li, X., Shi, Y., Gutman, I.: Graph Energy. Springer Science & Business Media, Berlin (2012)
15. McClelland, B.: Properties of the latent roots of a matrix: the estimation of Sipi S-electron energies. J. Chem. Phys. 54(2), 640–643 (1971)
16. Nikiforov, V.: The energy of graphs and matrices. J. Math. Anal. Appl. 326(2), 1472–1475 (2007)
17. Nikiforov, V.: Remarks on the energy of regular graphs. Linear Algebra Appl. 508, 133–145 (2016)
18. Zhou, B., Gutman, I., de la Peña, J.A., Rada, J., Mendoza, L.: On spectral moments and energy of graphs. MATCH Commun. Math. Comput. Chem. 57, 183–191 (2007)

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