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On the roots of Wiener polynomials of graphs

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ABSTRACT

The *Wiener polynomial* of a connected graph G is defined as $W(G; x) = \sum x^{d(u,v)}$, where $d(u, v)$ denotes the distance between u and v, and the sum is taken over all unordered pairs of distinct vertices of G. We examine the nature and location of the roots of Wiener polynomials of graphs, and in particular trees. We show that while the maximum modulus among all roots of Wiener polynomials of graphs of order n is $\binom{n}{2}-1$, the maximum modulus among all roots of Wiener polynomials of trees of order n grows linearly in n. We prove that the closure of the collection of real roots of Wiener polynomials of all graphs is precisely $(-\infty, 0]$, while in the case of trees, it contains $(-\infty, -1]$. Finally, we demonstrate that the imaginary parts and (positive) real parts of roots of Wiener polynomials can be arbitrarily large.

1. Introduction

Let G be a connected graph of order at least 2 and *diameter* $D(G)$. The *Wiener polynomial* of G is defined as

$$W(G; x) = \sum x^{d(u,v)},$$

where $d(u, v) = d_G(u, v)$ is the *distance* between u and v, and the sum is taken over all distinct unordered pairs of vertices u and v of G. Thus if $d_i(G)$ denotes the number of pairs of vertices distance i apart in G, for $i = 1, 2, \ldots, D(G)$, then

$$W(G; x) = \sum_{i=1}^{D(G)} d_i(G)x^i.$$

If G is clear from context, then we write d_i and D instead of $d_i(G)$ and $D(G)$, respectively. Note that we restrict our discussions to connected graphs of order at least 2 throughout, so that the Wiener polynomial is well-defined and nonzero. Adding loops or multiple edges to a connected graph has no effect on the Wiener polynomial, so we lose no generality by considering only simple graphs.

The successful study of the chromatic [13], characteristic [22], independence [20] and reliability [4] polynomials of graphs has motivated the study of various other graph polynomials. The Wiener polynomial was introduced in [17] and independently in [24], and has since been studied several times (see [12,14,29,31], for example). Unlike many other graph polynomials (such as the chromatic, reliability and independence polynomials), the Wiener polynomial can be calculated in polynomial time.

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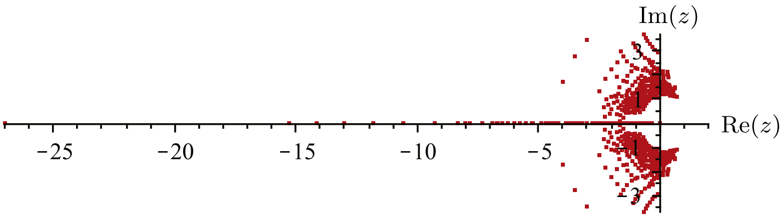

Fig. 1. The Wiener roots of all connected graphs of order 8.

Interest in the Wiener polynomial first arose out of work on the *Wiener index* of a connected graph, introduced in [30] and defined as the sum of the distances between all pairs of vertices of the graph. It can readily be seen that the Wiener index of G is obtained by evaluating the derivative of the Wiener polynomial of G at $x = 1$. The Wiener index of a molecular graph is closely correlated with certain physical properties of the substance, such as its melting and boiling point; see [15,23,27,30]. Applications of the Wiener index have also been found outside chemistry, for example in the design of architectural floor plans [21].

Wiener polynomials of trees will be of particular interest to us, so we mention that the Wiener polynomial of a tree also arises in the context of network reliability. Given a graph G in which each edge is operational with probability p, the *resilience* or *pair-connected reliability* of G is the expected number of pairs of vertices of G that can communicate [1,11]. In particular, in a tree T, the probability that any pair of vertices u and v can communicate is simply $p^{d(u,v)}$. Therefore, the resilience of T is exactly $W(T; p)$.

In this article, we focus on the study of the roots of the Wiener polynomial of a graph G, which we call the *Wiener roots* of G. The Wiener roots of all connected graphs of order 8 are shown in Fig. 1. Though the Wiener roots of some narrow families of graphs were studied in [12], little is known about the nature and location of the Wiener roots of graphs in general. Given that properties of the roots of other graph polynomials have been well-studied, it is natural to study the roots of the Wiener polynomial in greater depth.

Since $W(G; x) = x(d_1 + d_2x + \cdots + d_Dx^{D-1})$, we see that $x = 0$ is a root of every Wiener polynomial. The remaining roots are those of the polynomial $\widehat{W}(G; x) = d_1 + d_2x + \cdots + d_Dx^{D-1}$, which we will refer to as the *reduced Wiener polynomial* of G. Note that the value of d_1 is the number of edges, so that if the order of G is at least 2, then 0 is *not* a root of $\widehat{W}(G; x)$ (and hence is a simple root of the original Wiener polynomial $W(G; x)$).

The layout of the article is as follows. In Section 2, we determine that $\binom{n}{2} - 1$ is the maximum modulus among all Wiener roots of connected graphs of order n, and we describe the extremal graphs which have a root of this maximum modulus. In contrast, we then show that for trees, the rate of growth of the maximum modulus is $\Theta(n)$. Finally, we determine that $\frac{2}{n-2}$ is the minimum modulus among all nonzero Wiener roots of connected graphs of order n, and again we are able to describe the extremal graphs (which are trees). In Section 3, we prove that the closure of the collection of all real Wiener roots of connected graphs is $(-\infty, 0]$, and that for trees, the closure of all real Wiener roots still contains $(-\infty, -1]$. In Section 4, we study the real and imaginary parts of Wiener roots. We show that there are Wiener roots of trees with arbitrarily large imaginary part, and that there are Wiener roots of trees with arbitrarily large positive real part. This work culminates in a proof of the fact that the collection of complex Wiener roots of all graphs is not contained in any *half-plane* (a region in the complex plane consisting of all points on one side of a line and no points on the other side). Finally, we prove that almost all graphs have all real Wiener roots, and we find purely imaginary Wiener roots. Throughout, we compare and contrast our results with what is known about the roots of other graph polynomials.

2. Bounding the modulus of Wiener roots

Bounding the modulus of roots of various graph polynomials has been a central point of interest in the literature. For example, Sokal [25] settled an outstanding problem in proving that the modulus of a chromatic root (a root of the chromatic polynomial) of a graph of maximum degree Δ is at most a constant times Δ. This implies that the modulus of any chromatic root of a graph of order n is at most Cn for some positive constant C; the precise value of the smallest such constant is still unknown. The *independence polynomial* of a graph G is the generating function for the number of independent sets of each cardinality in G. Among all graphs of order n and fixed independence number β, the maximum modulus of an independence root is $(n/\beta)^{\beta-1} + O\left(n^{\beta-2}\right)$ [7]. For the *all-terminal reliability* polynomial, it is suspected that the collection of all roots is bounded in modulus (as no roots have been found outside of the disk $|z - 1| \leq 1.2$). Currently the best known upper bound on the modulus of the roots for all graphs of order n is linear in n, as shown in [6]. For the independence polynomial, the all-terminal-reliability polynomial, and the chromatic polynomial, the extremal graphs that have a root of maximum modulus (among all graphs of order n) are not known. In contrast, we completely determine the extremal graphs whose Wiener polynomials have a root of maximum modulus (among all Wiener polynomials of connected graphs of order n). To do so, we will make use of the classical Eneström–Kakeya Theorem [19].