Relationship Between the Hosoya Polynomial and the Hyper-Wiener Index

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Abstract—The Hosoya polynomial of a graph, \( H(G, z) \), has the property that its first derivative, evaluated at \( z = 1 \), equals the Wiener index, i.e., \( W(G) = H'(G, 1) \). In this paper, an equation is presented that gives the hyper-Wiener index, \( WW(G) \), in terms of the first and second derivatives of \( H(G, z) \). Also defined here is a hyper-Hosoya polynomial, \( HH(G, r) \), which has the property \( WW(G) = HH'(G, 1) \), analogous to \( W(G) = H'(G, 1) \). Uses of higher derivatives of \( HH(G, z) \) are proposed, analogous to published uses of higher derivatives of \( H(G, z) \). © 2002 Elsevier Science Ltd.

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1. INTRODUCTION

The adjacency matrix \( A \) of an undirected graph on \( n \) vertices is a \((0, 1)\) \( n \times n \) matrix with entries \( a_{i,j} = 1 \) if an edge joins vertices \( i \) and \( j \), zero otherwise. The distance matrix \( D \) has entries \( d_{i,j} \) equal to the number of edges in the shortest path connecting vertices \( i \) and \( j \). It is possible to calculate \( D \) from \( A \) without further reference to the graph, and several methods for performing this calculation have appeared [1]. Each distance occurs twice in \( D \), since the distance from \( i \) to \( j \) is necessarily the same as that from \( j \) to \( i \). Over a half century ago, Wiener introduced [2] the index \( W(G) \) that now bears his name and is defined as \( W(G) = (1/2) \sum d_{i,j} \), the sum of all distances in the graph. Many authors write \( W(G) = \sum d_{i,j} \) and specify the summation as only over \( i > j \), and the remainder of the present paper uses that convention. Many publications have shown correlations of \( W(G) \) with various physicochemical and biological parameters, and references to these studies were recently collected [3]. Much later, Randić introduced [4] an extension of the Wiener index for trees, and this has come to be known as the hyper-Wiener index, \( WW(G) \). Klein et al. [5] generalized this extension to cyclic structures as \( WW(G) = (1/2) \sum d_{i,j} ^{2} + (1/2) \sum d_{i,j} \), \((i > j)\). Like \( W(G) \), \( WW(G) \) has seen widespread use in correlations; references may be found in [3] and also in [6]. Diudea [7,8] has treated both \( W(G) \) and \( WW(G) \) in a common matrix framework.

In 1988, Hosoya [9] introduced what he termed the Wiener polynomial of a graph:

\[ H(G, x) = \sum_{k=1}^{l} d(G, k)x^k, \]
where \(d(G, k)\) is the number of pairs of vertices in the graph \(G\) that are distance \(k\) apart, and \(l\) is the maximum value of \(k\). Some authors call this polynomial the Wiener-Hosoya polynomial [3, p. 423; 10], or simply the Hosoya polynomial [11]. Some results for specific types of graphs have been published [12–15], and Sagan et al. [16] produced a treatment apparently independent of Hosoya’s. Perhaps the most interesting property of \(H(G, x)\) is that its first derivative, evaluated at \(x = 1\), equals the Wiener index: \(W(G) = H'(G, 1)\) [11]. This is so because

\[
H'(G, x) = \sum_{k=1}^{l} k \times d(G, k) x^{k-1}.
\]

The summation now starts at \(k = 1\), and, evaluated at \(x = 1\), equals the sum of each distance in the graph multiplied by the number of occurrences of that distance, the definition of \(W(G)\). Higher derivatives of \(H(G, x)\) have also been used as descriptors [10,17].

2. RESULTS

Using the expression from [5], \(WW(G) = (1/2) \sum d_{i,j}^2 + (1/2) \sum d_{i,j}\), one also finds a relationship between \(WW(G)\) and \(H(G, x)\), namely, \(WW(G) = H'(G, 1) + (1/2)H''(G, 1)\), where \(H''(G, 1)\) is the second derivative of the Hosoya polynomial, evaluated at \(x = 1\). The derivation is as follows.

The second part of the expression, \((1/2) \sum d_{i,j}\), is simply half of \(W(G)\), and therefore, equal to \((1/2)H'(G, 1)\). To get \(\sum d_{i,j}^2\), it is necessary to multiply the distance counts, i.e., the coefficients of \(H(G, x)\), by their respective distances twice. Taking the first derivative accomplishes the first multiplication, but reduces the exponents by one. Therefore, the desired operation for the second multiplication is to restore the exponents, then take the derivative of the result, \(d(H'(G,x))\). Using the standard form \(d(uv) = u dv + v du\), \(d(H'(G,x)) = (\frac{d}{dx})H'(G,x) + xH''(G,x)\). Adding half of this value to the second part of the expression, then evaluating the entire expression at \(x = 1\), gives

\[
WW(G) = H'(G, 1) + \frac{1}{2}H'(G, 1) + \frac{1}{2}(1 \times H''(G, 1)) = H'(G, 1) + \frac{1}{2}H''(G, 1).
\]

\(H'(G, 1) = W(G)\), but higher derivatives of the Hosoya polynomial have been used as descriptors as well [10,17]. Therefore, one defines a hyper-Hosoya polynomial, \(HH(G, x)\), which has the property that its first derivative, evaluated at \(x = 1\), equals the hyper-Wiener index, i.e., \(WW(G) = HH'(G, 1)\). This polynomial may be had by simply integrating the expression for \(WW(G)\):

\[
HH(G, x) = \int \left( H'(G, x) + \frac{1}{2}xH''(G, x) \right) dx.
\]

The first part, \(\int (H'(G, x)) dx\), is simply \(H(G, x)\). The second part may be conveniently evaluated using the standard form \(\int u \frac{dv}{dx} dx = uv - \int v \frac{du}{dx} dx\) and substituting \(u = x\) and \(v = H'(G, x) \Rightarrow \frac{dv}{dx} = H''(G, x)\). Carrying out the manipulations gives

\[
HH(G, x) = \frac{1}{2} (H(G, x) + xH'(G, x)) + c,
\]

where \(c\) is the constant of integration. By both Hosoya’s [9] and Sagan’s [16] original definition of \(H(G, x)\), the constant term was zero (summation over \(1 \leq k \leq l\)), but some later authors [3, p. 78; 11] specify it as the number of vertices in the graph (summation over \(0 \leq k \leq l\)). The latter seems more consistent with Hosoya’s expressions for \(H'\) and \(H''\) in [9]. By choosing for \(HH(G, x)\) half the number of vertices in the graph, \(HH(G, x)\) may be conveniently expressed as

\[
HH(G, x) = \sum_{k=0}^{l} \frac{k + 1}{2} d(G, k) x^k.
\]

where \(k\), \(l\), and \(d(G, k)\) are defined as for \(H(G, x)\). The value of the constant term will, of course, not affect any of the derivatives.
3. CONCLUSIONS

The Hosoya polynomial, $H(G, z)$, which has long been known to be related to the Wiener index, $W(G)$, by $W(G) = H'(G, 1)$, is shown to be related to the hyper-Wiener index, $WW(G)$, by $WW(G) = H'(G, 1) + (1/2)H''(G, 1)$. A hyper-Hosoya polynomial, $HH(G, x)$, is defined which has the property $WW(G) = HH'(G, 1)$, analogous to $W(G) = H'(G, x)$.

REFERENCES