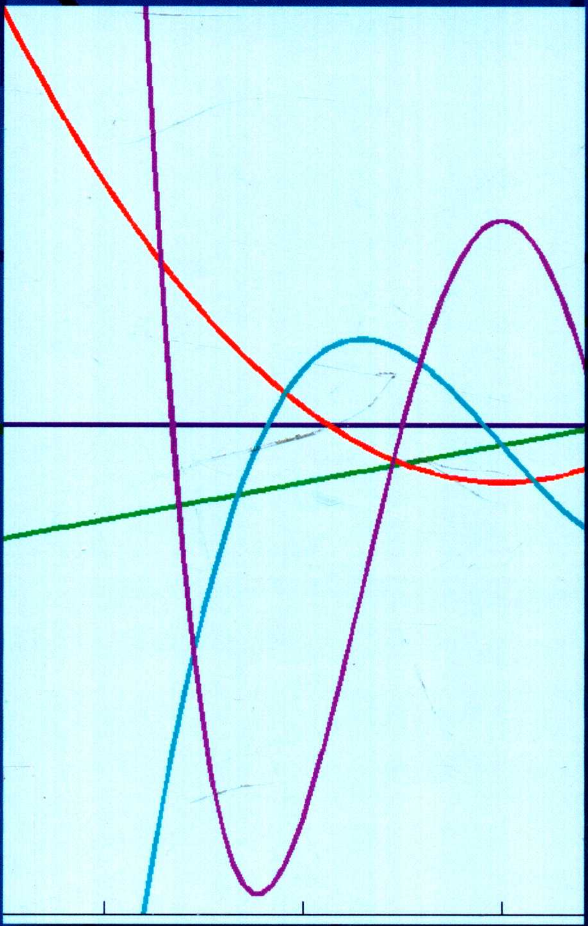
DISCRETE MATHEMATICS AND ITS APPLICATIONS

Graph Polynomials



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Preface

Graph polynomials have been developed for measuring structural information of networks using combinatorial graph invariants and for characterizing graphs. Various problems in graph theory and discrete mathematics can be treated and solved in a rather efficient manner by making use of polynomials. Various graph polynomials have been proven useful in discrete mathematics, engineering, information sciences, mathematical chemistry, and related disciplines.

In general, graph polynomials encode graph-theoretical information of the underlying graph in various ways. A particular graph polynomial may be interesting if it encodes useful graph parameters. An example is the Wiener polynomial whose coefficients are based on distances in a graph. Then for simple graph classes, the Wiener polynomial provides a simple and compact characterization of these graphs which can be analyzed quantitatively. In addition, graph polynomials and their zeros have been a valuable source for investigating various problems in discrete mathematics and related areas. It seems that graph polynomials were first introduced by J.J. Sylvester in 1878, and further studied by J. Petersen. Until now, there have been plenty of graph polynomials, such as the chromatic polynomial, characteristic polynomial, matching polynomial, Tutte polynomial, Whitney (rank) polynomial, Jones polynomial, Hosoya polynomial, Wiener polynomial, distance polynomial, edge-difference polynomial, independence polynomial, adjacency polynomial, flow polynomial, knot polynomial, topological transition polynomial, interlace polynomial, permanental polynomial, homomorphism polynomial, and so on. While studying these polynomials, it is crucial to study their particular properties such as location of zeros, interpretation of zeros, and so forth.

The main goal of this book is to present how graph polynomials characterize graph parameters efficiently, by emphasizing theoretical and practical problems. In the past few decades, many graph polynomials have been studied and plenty of theoretical and practical approaches have been developed. The topics addressed in this book cover a broad range of concepts and methods in terms of graph polynomials. The topics range from analyzing mathematical properties of graph polynomials to applying the polynomials in several application areas. By covering this broad range of topics, the book aims to fill a gap in contemporary literature in disciplines such as applied mathematics, information sciences, and mathematical chemistry.

Many colleagues, whether consciously or unconsciously, have provided us with input, help, and support before and during the preparation of this book. In particular, we thank Abbe Mowshowitz, Frank Emmert-Streib, Zengqiang Chen, Bo Hu, Shailesh Tripathi, Martin Trinks, and Guihai Yu, and we apologize to all whose names have been inadvertently omitted. Also, we thank our editors, Sunil Nair and Alexander Edwards from CRC Press/Taylor & Francis Group, who have always been available and helpful. Last but not least, Yongtang Shi, Matthias Dehmer, and Xueliang Li thank the National Natural Science Foundation of China and Nankai University for their support. Matthias Dehmer thanks the Austrian Science Funds (project no. P26142) for supporting this work. Matthias Dehmer also thanks his sister, Marion Dehmer-Sehn, who passed away in 2012, for all her mental support.

To date, no book dedicated exclusively to graph polynomials has been published. Therefore, we hope this book will broaden the scope of the scientists who deal with topics related to graph polynomials rooted in graph theory, discrete mathematics, algebra, chemical graph theory, applied mathematics, computer science, information sciences, and related disciplines. Finally, we hope this book conveys the enthusiasm and joy we have for this field and inspires fellow researchers in their own practical or theoretical work.

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Contents

Chapter 1

The Interlace Polynomial

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1.1 Introduction

The interlace polynomial of a graph arises in a number of settings both theoretical (e.g., isotropic systems) and applied (e.g., DNA sequencing by hybridization). We begin with the most straightforward, that of a recursive method for counting Eulerian circuits in two-in, two-out digraphs arising from an application in DNA sequencing. The interlace polynomial of a simple graph is obtained by generalizing the recursion used to solve this counting problem. We then discuss a closed form for the polynomial in terms of its adjacency matrix, the structure of which suggests definitions for analogous polynomials as well as a two-variable generalization. Another context in which the interlace polynomial arises is in isotropic systems, where it appears as a specialization of the Tutte–Martin polynomials, a connection we follow by way of the Martin polynomials of 4-regular graphs. Finally, we review generalizations of the polynomial to square matrices and delta-matroids.

In the context of counting Eulerian circuits in two-in, two-out digraphs, the interlace polynomial arose through Arratia et al.'s work on DNA sequencing [2]. In DNA sequencing by hybridization, the goal is to reconstruct a string of DNA knowing only information about its shorter substrings. The problem is to determine, from knowledge about the shorter substrings, whether a unique reconstruction exists.

More precisely, if $A = a_1a_2 \cdots a_m$ is a sequence consisting of m base pairs, the l-spectrum of A is the multiset containing all l-tuples consisting of l consecutive base pairs in A. Given the knowledge of the l-spectrum, the goal is to determine the number $k_l(m)$ of sequences of base pairs of length m having that l-spectrum.

In [2], the authors associate with a given l-spectrum its *de Bruijn graph*: a two-in two-out digraph D such that the Eulerian circuits of D are in bijection with sequences of base pairs having that l-spectrum. The problem, then, is to count the number of Eulerian circuits of D. This approach led to the discovery of a recursive formula for computing the number of Eulerian circuits of D based on an associated interlace graph. In [3], Arratia et al. generalized this recursion to define the interlace polynomial of an arbitrary simple graph.

The Eulerian circuits and cycle decompositions of 4-regular graphs have been an area of significant interest among graph theorists for many years, and approaches using graph polynomials have frequently proved fruitful [36,35,33,29]. The Martin polynomial [36,35], in particular, is closely related to the interlace polynomial as it counts, for any k, the number of k-component circuit partitions of a 4-regular graph.

This connection can be made explicit and, indeed, generalized. In a series of papers in the 1980s–1990s, Bouchet introduced the notion of an isotropic system to unify aspects of the study of 4-regular graphs and binary matroids [8,12,14], including a generalization of the Martin polynomials to this area [14]. Shortly after the discovery of the interlace polynomial, it was noticed that the interlace polynomial can be found as a specialization of the (restricted) Tutte–Martin polynomial of an isotropic system [13,1].

A connection between the interlace polynomial and the Tutte polynomial can be found by way of the Martin polynomial. However, this connection only captures the Tutte polynomial $t(G; x, y)$ for plane graphs when $x = y$, and so does not provide any strong link between the interlace polynomial and the many specializations of the Tutte polynomial, such as the chromatic polynomial. In recent work, Traldi has introduced a matroid associated with a graph, called its *isotropic matroid*, such that the interlace polynomial(s) of the graph can be recovered from parameterized Tutte polynomial(s) of its isotropic matroid [44].

Many generalizations of the interlace polynomial have been obtained. In [4], Arratia et al. defined a two-variable interlace polynomial of which the single-variable polynomial is a specialization. In doing so, they discovered, concurrently with Aigner and van der Holst [1], a closed form for the single-variable interlace polynomial in terms of its adjacency matrix. This closed form has a natural extension to arbitrary square matrices, and using a delta-matroid associated with the adjacency matrix of a graph, Brijder and Hoogeboom obtained a generalization of the interlace polynomial to delta-matroids [22]. In each case, the recursive definition of the interlace polynomial has also been generalized.

1.2 The Interlace Polynomial of a Graph

We begin by defining the interlace polynomial recursively by way of counting Eulerian circuits in two-in, two-out digraphs, and then discuss a closed form, an analogous polynomial, and a two-variable generalization. We conclude with selected evaluations of the interlace polynomial.

1.2.1 Preliminary definitions

We first establish some standard definitions and notation to be used throughout the chapter. Formally speaking, a *graph* G is a triple $(V(G), E(G), \phi)$ where $V(G)$ is a finite set of *vertices*, $E(G)$ is a finite set of *edges*, and ϕ is a function from $E(G)$ to $\{\{a, b\} : a, b \in V(G)\}$. Let $e \in E(G)$. If $\phi(e) = \{a\}$ is a singleton set, then e is said to be a *loop* and a is called a *looped vertex*. If $\phi(e) = \{a, b\}$, then we say e is an edge *between* a and b, a and b are *adjacent*, a and b are the *endpoints* of e, and both a and b are *incident* to e. In general, we will suppress the function ϕ, define an edge by its endpoints, and define the graph G by the pair $(V(G), E(G))$. The *degree* of a vertex is the number of edges to which it is incident, counting loops twice. A graph is said to be *k-regular* if every vertex has degree k. If a and b are vertices with more than one edge between them, then we say there is a *multiple edge* between a and b. A graph is *simple* if it contains no loops or multiple edges. A *walk* in G is an alternating sequence of vertices and edges $v_1e_1v_2e_2\cdots v_ke_kv_{k+1}$ such that e_i is incident to v_i and v_{i+1} for each i. A walk is *closed* if its first and last vertices are the same. A closed walk repeating no edges is a *circuit*. A circuit in which no vertices are repeated is called a *cycle*. A *path* is a walk beginning and ending at distinct vertices and containing no repeated vertices. A graph is *connected* if for any vertices a and b there is a path from a to b. A *component* of a graph is a maximal connected subgraph. We denote by $k(G)$ the number of components of G. For $T \subseteq V(G)$ the *subgraph induced by T*, denoted $G[T]$, is the graph (T, E') where E' is the set of edges in $E(G)$ with both endpoints in T. If $v \in V(G)$, define $G \setminus v$ to be the subgraph of G induced by $V(G) \setminus \{v\}$.

The *adjacency matrix* of a graph G, denoted $A(G)$, is the $|V(G)| \times |V(G)|$ matrix over $GF(2)$ with rows and columns indexed by $V(G)$ defined by setting $A(G)_{ab} = 1$ if a and b are adjacent and 0 otherwise. For $T \subseteq V(G)$, define the *rank* $r(G[T])$ to be the matrix rank $r(A(G[T]))$, and the *nullity* $n(G[T])$ to be the matrix nullity $n(A(G[T]))$. By convention, $n(G[\emptyset]) = 0$. Note that for a graph G, the nullity and rank of G are sometimes defined by $n(G) = |E(G)| - |V(G)| + k(G)$ and $r(G) = |V(G)| - k(G)$.

A *digraph*, informally speaking, is a graph where each edge is given a direction, that is, the function ϕ has codomain $V(G) \times V(G)$. If a directed edge e goes from a to b, then a is called the *tail* of e and b is called the *head* of e. The indegree of a vertex in a digraph is the number of edges for which the vertex is the head, the outdegree the number for which it is the tail. A *two-in, two-out digraph* is a 4-regular digraph such that each vertex has both indegree and outdegree equal to 2. A walk $v_1e_1v_2e_2\cdots v_ke_kv_{k+1}$ in a digraph is *directed* or *consistently oriented* if e_i is directed from v_i to v_{i+1} for each i.

A *planar graph* is a graph that can be embedded in the plane (i.e., drawn in the plane by associating vertices to points and edges to curves between their endpoints, such that no two edges intersect other than at a shared endpoint). A *plane graph* is a planar embedding of a (planar) graph.

For sets A and B, the *symmetric difference* of A and B is $A\Delta B = (A \cup B) \setminus (A \cap B)$.

We can now begin defining the interlace polynomial by way of counting Eulerian circuits in two-in, two-out digraphs.

Definition 1.2.1 (interlace graph) Let G be a two-in, two-out digraph. A *Eulerian circuit* of G is a closed, directed walk of G containing each edge exactly once. Given a Eulerian circuit C of G, we say that vertices a and b are *interlaced* if the cycle visits them in the order $\ldots a \ldots b \ldots a \ldots b \ldots$ and *noninterlaced* otherwise. The *interlace graph* or *circle graph* of C, denoted $H(C)$, is the graph whose vertices are the vertices of G with an edge between two vertices if they are interlaced in C (see Figure 1.1b and c).

Interlace graphs have been extensively studied [11,9,15,26,41,40] and were characterized by Bouchet in [9,15]. A particular focus of the area, due to a Gauss problem, has been characterizations of the interlace graphs arising from Eulerian cycles in plane 4-regular graphs [26,41,40].

There is a natural operation defined on Eulerian circuits of two-in, two-out digraphs in terms of this interlace relation.

Definition 1.2.2 At each vertex of a two-in, two-out digraph G, there are two possible (orientation consistent) pairings of in-edges and out-edges. For a pair of vertices a and b

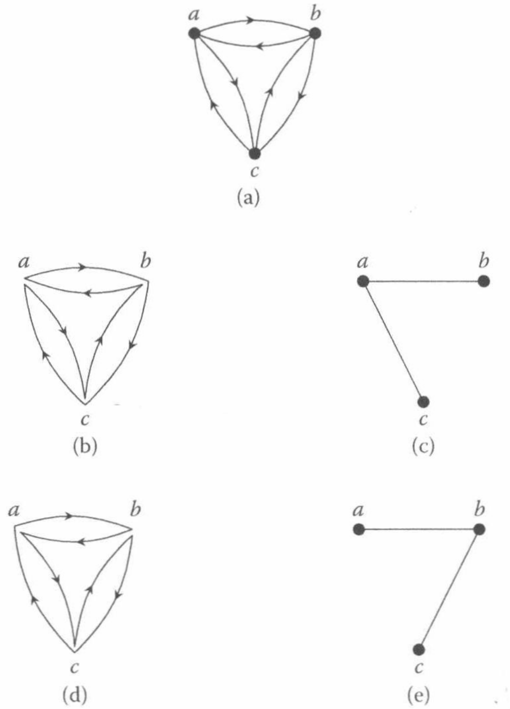

FIGURE 1.1: Transpositions of Eulerian circuits and the interlace graph: (a) a two-in, two-out digraph G; (b) a Eulerian cycle C in G; (c) the interlace graph $H(C)$; (d) the Eulerian circuit C^{ab}; (e) the interlace graph $H(C^{ab})$.

interlaced in a Eulerian circuit C of G, define the transposition C^{ab} to be the Eulerian circuit obtained by switching the pairing of edges at a and b (see Figure 1.1b and d).

The Eulerian circuits of G form a single orbit under the action of transposition, the proof of which can be found in [3] but was known previously in more general form in [39,47]. Observation of the effect on the interlace relation by performing the above operation to a Eulerian circuit leads to a corresponding definition for interlace graphs, presented here for graphs in general.

Definition 1.2.3 Let G be any graph. Let $v \in V(G)$. For any pair of vertices $a, b \in V(G)$, partition the remaining vertices of G into the following sets: (1) vertices adjacent to a and not b, (2) vertices adjacent to b and not a, (3) vertices adjacent to both a and b, and (4) vertices adjacent to neither a nor b. Define the pivot G^{ab} to be the graph obtained by inserting all possible edges between the first three of these sets, and deleting those that were already present in G (see Figure 1.2). Denote by G_{ab} the graph G with the labels of the vertices a and b swapped.

Although the above definition of pivot is attributable to Arratia et al. [2], the idea of the pivot appeared in the earlier work of Kotzig [34] on local complementations and the graph $(G^{ab})_{ab}$ is defined by Bouchet in [12] as the *complementation of G along the edge ab.* The precise connection to both is as follows:

Definition 1.2.4 Let G be a graph. For $v \in V(G)$, define the *open neighborhood* of v to be $N(v) = \{w \in V(G) \setminus \{v\} : w \text{ is adjacent to } v\}$. Note that $v \notin N(v)$ even if v is a looped vertex. We define the *local complement* $G * v$ to be the graph obtained from G

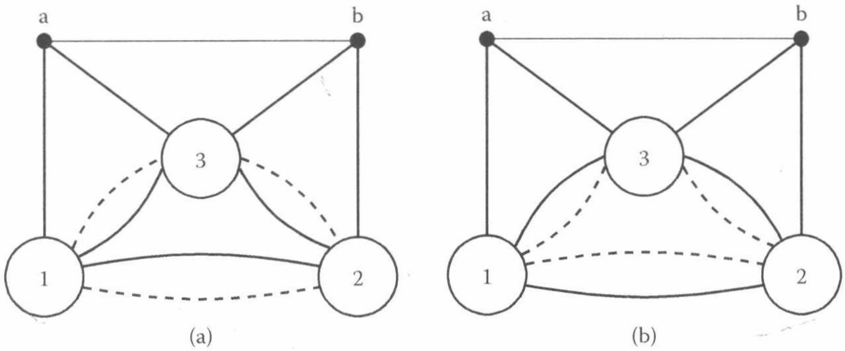

FIGURE 1.2: (a) A graph G with edge ab and vertices partitioned as in Definition 1.2.3 (the parts of G unaffected by pivoting are not shown). Dashed lines represent the edges not present in the graph. (b) Pivot G^{ab} is obtained by toggling edges/nonedges among the sets of vertices labeled $1, 2$, and 3.

by interchanging edges and nonedges in $N(v)$. By convention, we read graph operations left-to-right; therefore, $G * v * w * v = ((G * v) * w) * v$.

Theorem 1.2.1 [18,12] *Let G be a graph. If ab is an edge in G with neither a nor b a looped vertex, then* $(G^{ab})_{ab} = G * a * b * a$.

In the case of interlace graphs, the pivot operation captures the behavior of a transposition of a Eulerian circuit in the following sense.

Theorem 1.2.2 [3] *For a Eulerian circuit C of a two-in, two-out digraph G, we have* $(H(C))^{ab} = (H(C^{ab}))_{ab}$.

We can now define the interlace polynomial of a graph. Arratia et al. proved in [3] that the recurrence below does not depend on the order in which the edges are chosen; that is, the polynomial is well defined.

Definition 1.2.5 (The interlace polynomial [3]) Let G be a simple graph. The *interlace polynomial of G*, denoted $q_N(G;x)$, is defined by

$$q_N(G;x) = \begin{cases} q_N(G \setminus a;x) + q_N(G^{ab} \setminus b;x), & ab \in E(G) \\ x^n, & G \cong E_n \end{cases},$$

where E_n is the graph on n vertices with no edges.

Note that while the recurrence above is presented in its original form, in generalizations of the interlace polynomial, the label-switching operation G_{ab} (see Definition 1.2.3) occurs as part of the generalized pivot operation. In the case of the recurrence above, this can be obtained, using local complementation in place of the pivot operation (see Theorem 1.2.1). Under that convention, the recurrence above becomes $q_N(G;x) = q_N(G \setminus a;x) + q_N(G * a * b * a \setminus a;x)$, which aligns with the form of the recurrence used in subsequent sections. In addition, the interlace polynomial was originally denoted by $q(G)$. We follow [4] in reserving that notation for the two-variable generalization.

Definition 1.2.5 is stated for simple graphs. It can, however, be extended to the case of looped graphs (i.e., graphs with loops, but without multiple edges). In this case, the recurrence above only holds for edges where neither endpoint has a loop, and an additional