Advanced Topics in Computer Science

236603-2011

Graph Polynomials

Location: Taub 4

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Reception hours: Monday: 16:30-19:00 or by appointment (via e-mail)

LECTURE 1

Outline of Lecture 1

- Organisational matters

- Purpose of the course

- Graph invariants

- Graph polynomials:
  A tour through a bizarre landscape

Organzational matters

Course prerequisites and requirements

Lectures:

Weekly two hour lectures.

Homework:

This course requires **active participation** in the form of weakly homework by the participants, complementing material of the course.
No hand-in required.
Connect passive and active knowledge. Measure your understanding.
Control it yourself or with a partner.

Course requirements:

Either: Edit and complete notes of at least one lecture.
or: Prepare a new lecture.
or: Prepare notes for additional material.

Ideally we want to have **publishable course notes**.

Purpose of the course

We want to explore

combinatorial, algebraic and algorithmic graph theory

- Graph polynomials.
- Reducibilitry between graph polynomials.
- Linear recurrences for graph polynomials.
- Complexity theory for graph polynomials.
- Parametrized complexity of graph polynomials.

"…. the goal of theory is the mastering of examples"

H. Lüneburg

The Catalogue of Graph Polynomials

We work on a book

The Catalogue of Graph Polynomials

- You are invited to contribute!
- You can edit parts;
- You can prepare new parts;
- You can help finding new graph polynomials.

Graph invariants

and

graph polynomials

Graph isomorphims

Let $\mathcal{DG}$ be the class of finite graphs $\langle V(G), E(G)\rangle$ where $V = V(G)$ is a finite set and $E = E(G) \subseteq V^2$ is a set of (directed edges). $G \in \mathcal{DG}$ is called a directed graph. $\mathcal{G}$ be the class of finite graphs, i.e. where E is symmetric.

For $G_1, G_2 \in \mathcal{DG}$ $f : G_1 \to G_2$ is an **isomorphisms** if

(i) f is a bijection, and

(ii) For $u, v \in V(G_1)$ we have
$(u, v) \in E(G_1)$ iff $(f(u), f(v)) \in E(G_2)$.

G_1 **and** g_2 **are isomorphic**, denoted by $G_1 \simeq G_2$,
if there is an isomorphism $f : G_1 \to G_2$.

Rings $\mathcal{R}$

Let $\mathcal{R}$ a ring.

- $\mathcal{R} = \mathcal{B}_2$ the two element bolean ring.
- $\mathcal{R} = \mathbb{Z}_2$ the two element field.
- $\mathcal{R} = \mathbb{Z}$, the ring of integers.
- $\mathcal{R} = \mathbb{Z}[X]$, the polynomial ring over the integers with one indeterminate.
- $\mathcal{R} = \mathbb{Z}[X_1, \ldots, X_k]$, the polynomial ring over the integers with k indeterminates.
- $\mathcal{R} = \mathbb{R}$, the ring of real numbers.

Definition 1 *Graph invariants over a ring $\mathcal{R}$*

Let $\mathcal{R}$ a ring, $\mathcal{G}$ the class of finite graphs.
A function

$$f : \mathcal{G} \to \mathcal{R}$$

is a graph invariant if for any two isomorphic graphs G_1, G_2 we have $f(G_1) = f(G_2)$.

Example 2 *Boolean graph invariants*

Here the ring is $\mathcal{B}_2$,
or any ring $\mathcal{R}$, but the values of the invariant are either 0 or 1.

- Connectedness
- Regular, or regular of degree r.
- Any First Order expressible graph property.
- Any Second Order expressible graph property.
- Belonging to any specific class of graph closed under isomorphisms.
- There are continuum many boolean graph invariants.

Example 3 *Numeric graph invariants*

Here the ring is $\mathbb{Z}$.

- The cardinality of $V(G)$ or $E(G)$.
- The number of connected components of G, usually denoted by $k(G)$.
- The coloring number of G.
- The size of the maximal clique (independent set).
- The diameter of G.
- The radius of G.
- The minimum length of a cycle in G, if it exists, called the girth of the graph G.

Example 4 *Graph polynomials*

Here the ring is $\mathbb{Z}[X]$.

The graph polynomial $p(G, X)$ gives for each value of X a graph invariant, hence it encodes a possibly infinite family of graph invariants.

The study of graph polynomials has a long history concentrating on particular polynomials.

The **classic** and very readable book is:

- Norman Biggs
  Algebraic Graph Theory
  Cambridge University Press
  1974 (2nd edition 1993)

Example 5 *The chromatic polynomial*

- Let $\chi(G, X)$ denote the number of vertex colorings of G with X colors.
  We shall prove that $\chi(G, X)$ is a polynomial in X,
  called the **chromatic polynomial of** G.

The chromatic polynomial was first introduced by G.D. Birkhoff in 1912.

It led to a very rich theory, although it was introduced
in a (failed) attempt to prove the 4-color conjecture.

The most comprehensive monograph about the chromatic polynomial is

- F.M. Dong, K.M. Koh and K.L. Teo
  Chromatic polynomials and chromaticity of graphs
  World Scientific, 2005

What can we do with a graph polynomial?

- Study its zeros.
- Interpret its coefficients in various normal forms.
- Interpret its evaluations.
- Study graphs uniquely determined by the polynomial.
- Study graph classes having the same graph polynomial.
- Study the strength of the graph invariant.

Digression 1:

Typical theorems about the chromatic polynomial

Theorem 101 (G. Birkhoff, 1912)

$\chi(G, X)$ is indeed a polynomial in X of degree $|V(G)|$.

Proof Let $e = (a, b)$ be an edge of the graph G. $G - e$ and G/e are obtained from G by deleting, respectively contracting the edge e.
We use induction over $E(G)$.

- First we observe that for disjoint unions $G = G_1 \sqcup G_2$ we have $\chi(G, X) = \chi(G_1, X) \cdot \chi(G_2, X)$.
- For n isolated points $\bar{K}_n$ we have $\chi(\bar{K}_n, X) = X^n$.
- $\chi_{a \neq b}(G, X)$ is the number of X-colorings of G with a and b having different colors.
- $\chi_{a=b}(G, X)$ is the number of X-colorings of G with a and b having the same color.
- $\chi(G - e, X) = \chi_{a \neq b}(G - e, X) + \chi_{a=b}(G - e, X) = \chi(G, X) + \chi(G/e, X)$
- $\chi(G, X) = \chi(G - e, X) - \chi(G/e, X)$ Q.E.D.

Normal forms of $\chi(G, X)$, I

As $\chi(G, X)$ is a polynomial we can write it as

$$\chi(G, X) = \sum_{i}^{|V(G)|} b_i(G) X^i$$

For the disjoint union we noted that

Proposition 102

$$\chi(G_1 \sqcup G_2, X) = \chi(G_1, X) \cdot \chi(G_2, X).$$

Normal forms of $\chi(G, X)$, II

We define $X_{(i)} = X \cdot (X-1) \cdot \ldots \cdot (X-i+1)$.
We write

$$\chi(G, X) = \sum_{i}^{|V(G)|} c_i(G) X_{(i)}$$

We define a an operation $\circ$ on the $X_{(i)}$ by $X_{(i)} \circ X_{(j)} = X_{(i+j)}$ and extend it naturally to polynomials in $X_{(i)}$.

The join of two graphs G_1, G_2, $G_1 + G_2$,
is obtained by taking the disjoint union and
adding all the edges between $V(G_1)$ and $V(G_2)$.

Theorem 103

$$\chi(G_1 + G_2, X) = \left(\sum_{i}^{|V(G)|} c_i(G_1) X_{(i)} \circ \sum_{i}^{|V(G)|} c_i(G_2) X_{(i)} \right)$$

Trees and tree-width

- For trees T with n vertices we have $\chi(T, X) = X \cdot (X-1)^{n-1}$.
  I particular, any two trees on n vertices have
  the same chromatic polynomial.

- (R. Read, 1968)
  Conversely, for G a simple graph, if $\chi(G, X) = X \cdot (X-1)^{n-1}$, then G is a tree.

- (C. Thomassen, 1997)
  If G has tree-width $k \geq 2$ then for every real number $a > k$ we have $\chi(G, a) \neq 0$.

- (B. Courcelle, J.A. Makowsky, U. Rotics, 2000)
  For graphs G with tree-width at most k the polynomial $\chi(G, X)$ can be computed in time $O(c_1(k) \cdot n^d)$.

- (J.A. Makowsky, U. Rotics, 2005)
  For graphs G with clique-width at most k the polynomial $\chi(G, X)$ can be computed in time $O(n^{c_2(k)})$.

Planar graphs and the chromatic polynomial.

Theorem 104 (P.J. Heawood, 1890)
Every planar graph is 5-colorable.
$\chi(G, 5) \neq 0$ *for* G *planar.*

Theorem 105 (G. Birkhoff and D. Lewis, 1946)
$\chi(G, a) \neq 0$ *for* G *planar and* $a \in \mathbb{R}, a \geq 5$.

Note that this is much stronger than the 5-color theorem.

Theorem 106 (K. Appel and W. Haken, 1977)
Every planar graph is 4-colorable.
$\chi(G, 4) \neq 0$ *for* G *planar.*

Problem 107
Find an analytic proof of the 4-color theorem.

Conjecture 108 (G. Birkhoff and D. Lewis, 1946)
For G *planar, there are no real roots of* $\chi(G, a)$ *for* $4 \leq a \leq 5$.

Real roots of $\chi(G, X)$

We note that $\chi(G, 0) = 0$ always, and $\chi(G, 1) = 0$ any graph with at least one edge.

Theorem 109 (D. Woodall, 1977)
Let G be any graph.

- *There are no negative real roots of $\chi(G, X)$.*
- *There are no real roots of $\chi(G, X)$ in the open interval $(0, 1)$.*

Theorem 110 (B. Jackson, 1993)

- *There are no real roots of $\chi(G, X)$ in the semi-open interval $(1, \frac{32}{27}]$.*
- *For any $\epsilon > 0$ there is a graph G_ϵ such that $\chi(G_\epsilon, X)$ has a root in $(\frac{32}{27}, \frac{32}{27} + \epsilon)$.*

Theorem 111 (S. Thomassen, 1997)
For any real numbers a_1, a_2 with $\frac{32}{27} \leq a_1 < a_2$ there exists a graph G such that $\chi(G, X) = 0$ for some $a \in (a_1, a_2)$.

Other counting interpretations: Acyclic orientations

An **orientation** of a graph G is a function which for every edge $e = (a, b)$ selects a source value $s(e) \in \{a, b\}$

An orientation is **acyclic**, of there are no oriented cycles.

Theorem 112 (R.P. Stanley, 1993)
The number of acyclic orientations of a graph G is given by the absolute value $|\chi(G, -1)|$.

Subgraph expansions

Let G be a graph with $k(G)$ connected components.
Let $S \subset E(G)$ and denote by $\langle S \rangle$ the subgraph generated by S in G.

- The **rank** $r(G)$ is defined as $r(G) = \mid V(G) \mid - k(G)$.
- The **corank** $s(G)$ is defined as $s(G) = \mid E(G) \mid - \mid V(G) \mid + k(G)$.
- The **rank polynomial** of a graph is defined by

$$R(G; X, Y) = \sum_{S \subseteq E(G)} X^{r(\langle S \rangle)} Y^{s(\langle S \rangle)}$$

Theorem 113 (H. Whitney, 1932)

(i) $\chi(G, X) = \sum_{S \subseteq E(G)} (-1)^{|S|} X^{|V(G)| - r(\langle S \rangle)}$

(ii) $\chi(G, X) = X^{|V|} R(G, -X^{-1}, -1)$

The complexity of the chromatic polynomial, I

Let us look at the chromatic polynomial $\chi(G, X)$.

- $\chi(G, X)$ has integer coefficients,
  and for $X \geq 0$ non-negative values,
  hence evaluating it at $X = a, a \in \mathbb{N}$ is in $\sharp\mathbf{P}$.

- For $a = 0, 1, 2$ evaluating $\chi(G, X)$ is in $\mathbf{P}$.

- For integer $a \geq 3$ evaluating $\chi(G, X)$ is $\sharp\mathbf{P}$-complete.

- What about evaluating $\chi(G, X)$ for $X = b$ with
  $b \in \mathbb{Z}$, $b \leq 0$?
  $b \in \mathbb{R}$ or $b \in \mathbb{C}$?

Given evaluations of $\chi(G, X)$ at $\mid V(G) \mid +1$ many points, we can compute the coefficients of $\chi(G, X)$ efficiently.

The complexity of the chromatic polynomial, II

Theorem 114
(F. Jaeger, D. Vertigan and D. Welsh, 1990)

For any two points $a, b \in \mathbb{C}$ different from $0, 1, 2$,
there is a **polynomial time algebraic reduction**
from the evaluation of $\chi(G, a)$ to the evaluation of $\chi(G, b)$.

Hence they are all **equally difficult***.*

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There are a few problems with the exact formualtion of the theorem:

- What is the computational model behind **polynomial time algebraic reductions**?
- What is the computational model behind **equally difficult**.
- The hardness result is obtained by a reduction to $\sharp\mathbf{P}$-complete problem, but most instances are not in $\sharp\mathbf{P}$.

End of digression on typical theorems about the chromatic polynomial

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Example 6 *The characteristic polynomial*

- Let $V = [n]$ and let A_G be the (symmetric) adjacency matrix of G with $(A)_{j,i} = (A)_{i,j} = 1$ iff there is an edge between vertex i and vertex j.

- We denote by $P(G, X)$ the polynomial

$$\det(X \cdot \mathbf{1} - A)$$

  $P(G, X)$ is a graph invariant and a polynomial in X, called the **characteristic polynomial of** G.

- The set of roots of $P(G, X)$ (with multiplicities) are the eigenvalues of A_G, and are called the **spectrum of the graph** G.

The characteristic polynomial and the spectrum of a graph was first studied in the 1950ties

T.H. Wei 1952, L.M. Lihtenbaum 1956,
L. Collatz and U. Sinogowitz 1957,
H. Sachs 1964, H.J. Hoffman 1969

The characteristic polynomial: Literature

The characteristic polynomial and spectra of graphs have a very rich literature with important applications in chemistry under the name **Hückel theory**.

- N. Biggs, Algebraic Graph Theory,
  Cambridge University Press, 1994 (2nd edition)

- D.M. Cvetković, M. Doob and H. Sachs
  Spectra of Graphs
  Johann Ambrosius Barth, 1995 (3rd edition)

- D.M. Cvetković, P. Rowlinson and S. Simić
  Eigenspaces of Graphs
  Encyclopedia of Mathematics, vol. 66
  Cambridge University Press, 1997

- N. Trinajstić
  Chemical Graph Theory
  CRC Press, 1992 (2nd edition)

Digression 2:

Typical theorems about the characteristic polynomial

Coefficients of $P(G, X)$

We write

$$P(G, X) = \sum_{i=0}^{|V(G)|} c_i(G) \cdot X^{n-i}$$

Proposition 201

(i) $c_0 = 1$

(ii) $c_1 = 0$

(iii) $-c_2 = \mid E(G) \mid$ *is the number of edges of* G.

(iv) $-c_3$ *is twice the number of triangles of* G.

Eigenvalues of G, I

As in linear algebra, the zeros of $P(G, X)$ are called **eigenvalues of the matrix** A_G, or **eigenvalues of the graph** G,

Proposition 202

(i) *All the eigenvalues of G are real.*

(ii) *If G is connected, the largest eigenvalue of G has multiplicity* 1.

(iii) *If G is connected and of diameter at least d, the G has at least $d+1$ distinct zeros.*

(iv) *The complete graph is the only connected graph with exactly two distinct eigenvalues, $P(K_n, X) = (X+1)^{n-1}(X-n+1)$.*

(v) *Let $\Lambda(G)$ be the largest eigenvalue of G.*
G is bipartite iff $-\Lambda(G)$ is also an eigenvalue of G.

Eigenvalues of G, II

Proposition 203
Let G be a regular graph of degree r. Then

(i) *r is an eigenvalue of G*

(ii) *If G is connected, then the multiplicity of r is* 1.

(iii) *For any eigenvalue λ of G we have $\mid \lambda \mid \leq r$.*

(iv) *The multiplicity of the eigenvalue r is the number of connected components of G.*

Eigenvalues of G, III

$\lambda(G)$ denotes the smallest eigenvalue of G.
$\lambda_2(G)$ denotes the second largest eigenvalue of G.
$\Lambda(G)$ denotes the largest eigenvalue of G.

Proposition 204

(i) If H is an induced subgraph of G, then $\lambda(H) \leq \lambda(G)$.

*(ii) If H is an induced subgraph of G, then $\Lambda(H) \leq \Lambda(G)$.
If H is a proper induced subgraph, then $\Lambda(H) < \Lambda(G)$.*

(iii) For no graph G is $\lambda(G) \in (-1, 0)$.

*(iv) Let G have at least two vertices.
$\lambda(G) = -1$ iff G is a complete graph.*

(v) For no graph G is $\lambda(G) \in (-\sqrt{2}, -1)$.

(vi) (J. Smith, 1970) $\lambda_2(G) \leq 0$ iff G is a complete multipartite graph.

End of digression on typical theorems about the characteristic polynomial