Graduate Seminar in Theoretical Computer Science 238900
Graph Polynomials

Location: Taub 4

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Reception hours: Monday: 14:30-16:00

Outline of Lecture 1

- Organisational matters
- Purpose of the seminar
- Graph invariants
- Graph polynomials:
  A tour through a bizarre landscape

Course prerequisites and requirements

Seminar lectures:

Weekly two hour seminar lectures by the participants.

Homework:

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

Seminar requirements:

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

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

Purpose of the seminar

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

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 polynomial time.

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

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 $\mid \chi(G, -1) \mid$.

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) $-c_2 = | E(G) |$ *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 $|\lambda| \leq r$.

(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

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Example 7 *The acyclic or matching defect polynomial, I*

We denote by $m_k(G)$ the number of k-matchings of a graph G, with $m_0(G) = 1$ by convention.

- The polynomial

$$m(G, X) = \sum_{k}^{\frac{n}{2}} (-1)^k m_k(G) X^{n-2k}$$

  is called the **acyclic polynomial of** G and also the **reference polynomial** or **matching defect polynomial**.

The acyclic or matching defect polynomial, II

The acyclic polynomial has important applications in Chemistry (Hückel theory again) and and Molecular Physics of Ferromagnetisms. It was first studied in the 1970 (Heilman and Lieb, Kunz)

- L. Lovász and M.D. Plummer
  Matching Theory
  Annals of Discrete mathematics, vol. 29
  North-Holland 1986

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

- P.J. Garratt
  Aromaticity
  John Wiley and Sons, 19xx

Example 8 *The matching (generating) polynomial*

- The polynomial

$$g(G, X) = \sum_{k}^{n} m_k(G) X^k$$

is called the **matching polynomial of** G or the **matching generating polynomial of** G.

- It is easy to verify the identity

$$m(G, X) = X^n g(G, (-X^{-2}))$$

Example 9 *Multi-variate graph polynomials*

Inspired by H. Whitney's work (1932) W.T. Tutte (1947, 1954) investigated generalizations of the chromatic polynomial to a polynomial in two variables, which he called the **dichromatic polynomial**, but now is called the **Tutte polynomial**, $T(G, X, Y)$.

The Tutte polynomial and its many generalizations became prominent, due to its many combinatorial interpretations in fields outside graph theory:

- Knot theory (via the Jones polynomial and its relatives)
- Statistical mechanics
- Quantum theory and quantum computing
- Chemistry

Example 10 *The Tutte polynomial*

Let $G = (V, E)$ be a graph,
and for $A \subseteq E$, let $G_A = (V, A)$ be a spanning subgraph.

The rank $r(G; A)$ is defined as $\mid V(G) \mid - k(G_A)$.

The **Tutte polynomial of** G is defined as

$$T(G; X, Y) = \sum_{A \subseteq E} (X - 1)^{r(G;E) - r(G;A)} \cdot (Y - 1)^{|A| - r(G;A)}$$

This looks confusing and innocent at the same time.

The fascination with the Tutte polynomial

The Tutte polynomial is like
a **magician's hat** with
rabbits, birds and other surprises coming out.

Easy manipulations produce various combinatorial counting functions. We have, at first glance surprisingly, the following

- $T(G, 1, 1)$ counts the number of spanning trees of G.
- $T(G, 2, 1)$ counts the number of forests of G.
- $T(G, 2, 0)$ counts the number of acyclic orientations of G.
- The chromatic polynomial is given by
$$\chi(G, X) = (-1)^{r(G;E)} X^{k(G)} T(G; 1 - X, 0)$$
- The reliability polynomial and the flow polynomial can also be derived with similar formulas.

Definition 11 *Complete graph invariants*

A graph invariant f is **graph-complete** if for any two graphs G_1, G_2 with $f(G_1) = f(G_2)$ we have also $G_1 \simeq G_2$.

The following is a graph-complete graph invariant.

- Let $X_{i,j}$ and Y be indeterminates.
  For a graph $\langle V, E \rangle$ with $V = [n]$ we put

$$Compl(G, Y, \bar{X}) = Y^{|V|} \cdot \left(\sum_{\sigma \in \mathfrak{S}_n} \prod_{(i,j) \in E} X_{\sigma(i),\sigma(j)} \right)$$

  Here $\mathfrak{S}_n$ is the permutation group of $[n]$.

Challenge: Find a polynomial in a constant finite number of indeterminates which is a graph-complete graph invariant.

An "unnatural" graph-complete invariant

Let $g : \mathcal{G} \rightarrow \mathbb{N}$ be a Gödel numbering for labeled graphs of the form $G = \langle [n], E, <_{nat} \rangle$.

We define a graph polynomial using g:

$$\Gamma(G, X) = \sum_{H \simeq G} X^{g(H)}$$

Clearly this is a graph invariant.

But it is "obviously unnatural" !

Can we make precise

what a **natural** graph polynomial should be?

Comparing graph invariants

In the literature we often find statements or questions of the form

- The Tutte polynomial is generalization of the chromatic polynomial.
- The Tutte polynomial does not determine the matching polynomial.
- Is there a natural most general graph polynomial?

We attempt to make this precise

Definition 12 *Induced graph invariants*

Let $\mathcal{H} \subseteq \mathcal{G}$ be a class of graphs closed under isomorphisms.
Let F be a set of graph invariants in a ring $\mathcal{R}$,
and let g be one more graph invariant.

We say that F **induces** g **on** $\mathcal{H}$,
or g **is a consequence of** F,
if for any two graphs $G_1, G_2 \in \mathcal{H}$ such that $f(G_1) = f(G_2)$ for all $f \in F$
we also have $g(G_1) = g(G_2)$.

We denote by $Ind_{\mathcal{R}}^{\mathcal{H}}(F)$ the set of graph invariants in $\mathcal{R}$ induced by F on $\mathcal{H}$.

We write also $F \models_{\mathcal{R}}^{\mathcal{H}} g$ for $g \in Ind_{\mathcal{R}}^{\mathcal{H}}(F)$.

How do we see if $F \models_{\mathcal{R}}^{\mathcal{H}} g$?

Example 13

Algebraically derived invariants

Let f, g be two graph invariants in $\mathcal{R}$.
Then the following are derived invariants of $F = \{f, g\}$:

- $f + g, f - g, f \times g$
- The formal derivative f'.
- Let $\phi : \mathcal{R}^2 \rightarrow \mathcal{R}$ be a function.
  Then $\phi(f, g)$ is induced by F.

Examples 14

Invariants induced by the characteristic polynomial

The characteristic polynomial $P(G, X)$ induces

- The number of vertices $\mid V \mid$.
- The number of edges $\mid E \mid$.
- The number of triangles of G.

We also have $P(K_{1,4}, X) = P(C_4 \sqcup E_1, X)$
but $K_{1,4}$ has no 2-matchings, whereas C_4 does.
Hence the $P(G, X)$ does not induce the number of connected components $k(G)$ nor $m(G, X)$.

Example 15

Invariants induced by the acyclic polynomial.

The acyclic polynomial $m(G, X)$ induces

- The number of vertices $\mid V \mid$.
- The number of edges $\mid E \mid$.
- The number of perfect matchings.
- the matching generating polynomial.

On the otherside $m(E_n, X) = 1$ for all $n \in \mathbb{N}$,
whereas $P(E_n, X) = X^n$.
Hence the $m(G, X)$ does not induce the characteristic polynomial $P(G, X)$.

Example 16

Invariants induced by the chromatic polynomial

The following are induced by $\chi(G, X) = \sum_{i=1}^{n} (-1)^{n-i} h_i X^i$:

- The cardinality of $V(G) = n$ is the degree of $\chi(G, X)$.
- The cardinality of $E(G) = m = h_{n-1}$.
- The chromatic number $\chi(G)$ is the smallest integer a such that $\chi(G, a) > 0$.
- The number of connected components $k(G)$ is the multiplicity of zeros $X = 0$.
- The number of blocks $b(G)$ is the multiplicity of zeros $X = 1$.
- The girth $g = g(G)$ is given by the fact that for $0 \leq i \leq g - 2$ we have $h_{n-i} = \binom{E(G)}{i}$.

Example 17

The acyclic polynomial and the characteristic polynomial.

Theorem 18 (I. Gutman, 1977)

$P(G, X) = m(G, X)$ *iff* G *is a forest.*

For $\mathcal{H} = \mathcal{F}$ *the forests we have*

$$P(G, X) = m(G, X)$$

i.e., the acyclic (matching defect) polynomial and the characteristic polynomial coincide,
and we have

$$P(G, X) \models^{\mathcal{F}} m(G, X) \text{ and } m(G, X) \models^{\mathcal{F}} P(G, X).$$

and

$$P(G, X) \models^{\mathcal{F}} g(G, X) \text{ and } g(G, X) \models^{\mathcal{F}} P(G, X).$$

In general, none induces the other.

I. Gutman, The acyclic polynomial of a graph, Publ. Inst. Math. (Beograd) (N.S.) 22 (36) (1977), pp. 63-69.

Example 19

The acyclic polynomial and the chromatic polynomial.

Definition 20
The complement graph of the simple graph $G = (V, E)$
is the graph $\bar{G} = (V, V^2 - D(V) - E)$.

For a graph polynomial $g = g(G, \bar{X})$ *the* **adjoint polynomial** $\hat{g}(G, \bar{X})$ *of* g *is defined by* $\hat{g}(G, \bar{X}) = g(\bar{G}, \bar{X})$.

Theorem 21 (E.J. Farrell and E.G. Whitehead Jr. 1992)
For $\mathcal{H} = \mathcal{TF}$, *the triangle free graphs, we have*

$$\hat{\chi}(G, X) \models^{\mathcal{TF}} m(G, X) \text{ and } m(G, X) \models^{\mathcal{TF}} \hat{\chi}(G, X).$$

i.e., the acyclic (matching defect) polynomial
and the adjoint chromatic polynomial mutually induce each other.

Note that $\chi(P_4) = \chi(K_{1,3})$, $P_4 \simeq \bar{P}_4$, *but* $m(P_4) \neq m(K_{1,3})$. *On the other hand,* $m(E_n) = 1$ *for each* $n \in \mathbb{N}$, *and* $\chi(E_n) = X^n$.
Hence, in general, none induces the other.

Example 22

The chromatic polynomial and Tutte polynomial

(i) The chromatic polynomial $\chi(G, X)$ is not induced by the Tutte polynomial $T(G, X, Y)$.

(ii) On connected graphs $\mathcal{C}$ we have $T(G, X, Y) \models^{\mathcal{C}} \chi(G, X)$ for

(iii) Tutte polynomial $T(G, X, Y)$ is not induced by the the chromatic polynomial $\chi(G, X)$.

Proof:

(i) Let E_n be the graph with n vertices and no edges. We have $T(E_n, X, Y) = 1$ but $\chi(E_n, X) = X^n$.

(ii) (After W.T. Tutte, 1954) $\chi(G, X) = (-1)^{|V|-k(G)} X^{k(G)} T(G, 1-X, 0)$.

(iii) (After M. Noy, 2003) Let W_n be the wheel with n spokes. It is known that $T(G, X, Y) = T(W_n, X, Y)$ implies that $G \simeq W_n$ for all n.

But there is a $G \not\simeq W_5$ with $\chi(G, X, Y) = \chi(W_5, X, Y)$.

Example 23

The Tutte polynomial and the matching (generating) polynomial

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- The matching polynomial is not induced by the Tutte polynomial, even on connected planar graphs.
- The Tutte polynomial is not induced by the matching polynomial, even on connected planar graphs.

Proof:

(i) For trees with n vertices t_n we have $T(t_n, X, Y) = X^{n-1}$. But it is easy to see that $K_{1,n-1}$ and P_n are both trees with n vertices and their matching polynomials differ, as $K_{1,n-1}$ has no 2-matching but P_n has for $n \geq 3$.

(ii) On the other hand $C_3 \sqcup_e C_5$ and $C_4 \sqcup_e C_4$ have the same matching polynomials (check by hand) but have different Tutte polynomials, as the Tutte polynomials counts cliques of given size.

What do we learn?
What do we ask?

- Polynomial graph invariants are still a mystery.

- Can we analyze the consequence relation for polynomial invariants?

- Can we identify “good invariants”?

- What are appropriate complexity classes for graph invariants?

Outline of Lecture 2

- Computability over a ring (BSS)
- Weighted graphs and meta-finite structures
- Reducibilities
- Non-computability of induced invariants

Choosing a model of computation

We want to develop a computability and complexity theory for graph invariants.

Options are:

- Turing computability

  Coding the graphs is OK, but how can we accomodate arbitrary rings?

- Valiant's non-uniform algebraic circuits

  Here a graph invariant would be given by a non-uniform family of circuits over the adjacency matrix.

- The model of computation popularized (not invented) by Blum, Shub and Smale, BSS.

  Here a graph invariant would be given by a BSS-program over the adjacency matrix.

We will work in the BSS model.

The BSS model of computation, I

The BSS model of computation uses

- arbitrary fixed rings $\mathcal{R}$
- and is based on register machines

It has a long history going back to the 1960ties but without a developed complexity theory.

It was popularized again in the 1980ties by L. Blum, M. Shub and S. Smale, with the explicit purpose to develop a useful complexity theory.

The BSS model of computation, II

- J.V. Tucker and J.I. Zucker
  Computable functions and semicomputable sets on many-sorted algebras in: Handbook of Logic in Computer science, vol. 5 (2000) S. Abramsky, D. Gabbay and T. Maibaum, eds.
- L. Blum, F. Cucker, M. Shub and S. Smale
  Complexity and Real Computation
  Springer 1998
- E. Graedel and Y. Gurevich
  Metafinite Model Theory
  Information and Computation, 140 (1998), pp. 26-81

The BSS model of computation, III

Registers

- Number registers $n_i, i \in \mathbb{N}$
- Values assigned to number registers:
  Natural numbers in **unit cost**.
- Ring element registers $r_i, i \in \mathbb{N}$.
- Values assigned to ring registers:
  Elements of the ring $\mathcal{R} = \mathbb{R}[\bar{X}]$
  with **unit cost for elements of** $\mathbb{R}$ and
  representation cost for polynomials.

  Cost of monomial $M = \prod_i x_i^{j(i)}$: $cost(M) = \sum_i j(i)$:
  Cost of sum of monomials M_m: $cost(\sum_m M_m) = \sum_m cost(M_m)$.

The BSS model of computation, IV

Basic instructions with labels $a, b, c \in \mathbb{N}$.

- a : `stop`

- $a : n_i := n$ for $n \in \mathbb{N}$
  $a : i_i := r$ for $r \in \mathcal{R}$

- $a : n_i := n_j \pm 1$ direct adress
  $a : n_i := r_{[n_j]} \pm 1$ indirect address

- $a : r_i := r_j \circ r_k$ direct adress
  $a : r_i := r_{[n_j]} \circ r_{[n_k]}$ indirect address
  where $\circ$ is $+, -$ or $\times$.

- a : `if` $n_i = 0$ `do` b `else` c
  a : `if` $r_i = 0$ `do` b `else` c

The BSS model of computation, V

Programs are sequences of labeled instructions.

Program semantics is explained as usual.

The cost of an instruction is defined as

- the maximum of the cost of the inputs for addition and subtraction
- the sum of the cost of the inputs for multiplication

Remark:

- We can select special registers as **input registers** and **output registers**.
- We could also omit the labels of the instructions and have structured programs with **composition** of programs, **tests** and **while loops**

The BSS model of computation, VI

Computation with and without parameters

Proposition 1
For every set $X \subseteq \mathbb{N}$ there is a real number $a_X \in \mathbb{R}$ and a program $\Pi_X(-, a_X)$ such that for every $b \in \mathbb{R}$ the program stops on input b iff $b \in X$.

Proof: Let a_X encode the charactersitic function of X, i.e. the ith digit of a_X is 1 iff $i \in X$. Q.E.D.

Proposition 2
For programs with parameters and functions $f : \mathbb{Z}^m \to \mathbb{Z}$ the function f is Turing computable iff f is BSS computable.

Proof: $\mathbb{Z}$ is a subring of $\mathbb{R}$. Q.E.D.

The BSS model of computation, VII

Time-bounded computations

Proposition 3
*The set $\mathbb{N} \subseteq \mathbb{R}$ is computable in BSS over $\mathbb{R}$,
but there is no function f which bounds the computation
in the size of the input (in our cost model).*

Proof: Every $a \in \mathbb{R}$ has size 1, but the computation may be arbitrarily long.
Q.E.D.

Definition 4
Time-bounded computations *are computations for which there is a function f which bounds the computation in the size of the input (in our cost model).*

The BSS model of computation, VIII

Complexity classes

- $TIME(f(n)$-computations
- Polynomial time $\mathbf{P}_{\mathcal{R}}$
- Non-deterministic classes via guessing.

  Polynomial search space in $\mathbb{R}$ is infinite.
  It is not obvious that $\mathbf{NP}_{\mathbb{R}}$ is computable !!!
- Counting classes are not abvious at all

Weighted graphs

We want to look at graphs in a way that we can compute graph invariants in the BSS model over $\mathbb{R}[\bar{X}]$.

Definition 5
A **edge weighted graph** G *is given by*

$$\langle V, v_{vertex}, w_{edge} \rangle$$

where V *is a finite set of vertices and*

$$v_{vertex} : V \to \mathbb{R}[\bar{X}]$$

and

$$w_{edge} : V^2 \to \mathbb{R}[\bar{X}]$$

are weight functions.

In case $v_{vertex}(v_1) = 1$ *and* $w_{edge}(v_1, v_2) = w_{edge}(v_2, v_2) \in \{0, 1\}$ *for all pairs of vertices,* w_{edge} *is another way of representing the adjacency matrix of a graph* $G = \langle V, E \rangle$*.*

To compute with weighted graphs we store the values of v_{vertex} and w_{edge} in $n + n^2$ ring registers.

Meta-finite structures

Meta-finite structures were introduced by E. Graedel and Y. Gurevich in attempt to extend the relational model of databases such as to acomodate agregate functions.

Definition 6
A **meta-finite structure** $\mathfrak{A}$ **over** $\mathcal{R}$ *is given by a finite set* A *and a finite family* $w_i^{\rho(i)}$ *of weight functions*

$$w_i^{\rho(i)} : A^{\rho(i)} \to \mathcal{R}$$

where $\mathcal{R}$ *is any fixed ring.*

Besides modeling databases, Graedel and Gurevich develop and study

- Logical formalisms
- Descriptive complexity
- Pebble games
- 0-1 laws

Definition 7

Isomorphic meta-finite structures

Let $\mathfrak{A} = \langle A, a_i^{\rho(i)} \rangle$ and $\mathfrak{B} = \langle B, b_i^{\rho(i)} \rangle$ be two meta-finite structures with corresponding weight functions.

An isomorphisms $f : A \to B$ is a function such that

- f is a bijection.
- For every $\bar{a} \in A^{\rho(i)}$ we have that
$$b_i^{\rho(i)}(f(\bar{a})) = a_i^{\rho(i)}(\bar{a})$$

If the weight functions are characteristic functions of relations, this corresponds to the classical notion of isomorphism of finite structures.

Definition 8 *Computable graph invariants*

Let $\mathcal{R}$ a ring.

- A **computable graph invariant over** $\mathcal{R}$ is graph invariant f given by BSS-program $\Pi(f)$ taking square matrices M as input such that for every permutation matrix P we have $f(PMP^t) = f(M)$.

- f is **P-time computable** if $\Pi(f)$ is P-time computable in the BSS unit cost model $\mathbf{P}_{\mathcal{R}}$.

- Similarly we define **EXP-time computable** graph invariants.

All examples we have shown are EXP-time computable.

The following are P-time computable:
The number of vertices, of edges, of connected components, of blocks, the characteristic polynomial.

The following are unlikely to be P-time computable:

The matching polynomials, the chromatic polynomial, the Tutte polynomial.

Computable boolean graph invariants

The following are $\mathbf{P}_{\mathcal{R}}$ computable for any ring $\mathcal{R}$:

- Any First Order definable graph property.
  Forbidden and required subgraphs or induced subgraphs.
- Connectivity.
- Any Fixed Point definable graph property.
- Planarity, Eulerian graphs

Induced boolean graph invariants and the logical consequence relation, I

Definition 9
Given boolean invariants ϕ, ψ,

(i) ϕ *is logically valid if for every graph* G *we have* $\phi(G) = 1$.

(ii) ψ *is a* **logical consequence** *of* ϕ *if for every graph* G, $\phi(G) = 1$ *implies that* $\psi(G) = 1$.

(iii) *We write* $\phi \models_{boolean} \psi$ *for logical consequence, and* $\phi \models^{\mathcal{H}}_{boolean} \psi$, *for its restriction to a graph property* $\mathcal{H}$.

(iv) *We write* $\phi \equiv^{\mathcal{H}}_{boolean} \psi$ *for* $\phi \models^{\mathcal{H}}_{boolean} \psi$, *and* $\psi \models^{\mathcal{H}}_{boolean} \phi$,

(v) $True(G)$ *is the boolean graph invariant which constant* $= 1$.

(vi) *For arbitrary rings* $\mathcal{R}$ *we also write* $\phi \equiv^{\mathcal{H}}_{\mathcal{R}} \psi$ *for* $\phi \models^{\mathcal{H}}_{\mathcal{R}} \psi$, *and* $\psi \models^{\mathcal{H}}_{\mathcal{R}} \phi$.

Induced boolean graph invariants and the logical consequence relation, II

Proposition 10
Let G be any graph, $\mathcal{H}$ any graph property, and $\mathcal{R}$ any ring.

(i) $\phi \models_{boolean} \psi$ *iff* $(\phi \rightarrow \psi)$ *is logically valid.*

(ii) If $\phi \equiv_{boolean} \psi$ *then also* $\phi \equiv_{\mathcal{R}} \psi$.

(iii) A boolean graph invariant is ϕ *is logically valid iff* $True \models_{\mathcal{R}} \phi$ *and* $\phi(G) = 1$.

(iv) If the relation $\models_{\mathcal{R}}^{\mathcal{H}}$ *is computable, so is the relation* $\models_{boolean}^{\mathcal{H}}$.

Representation of graph invariants.

A graph invariant is a program in the BSS model.

- We can code command lines in $\mathbb{Z}$.
- We can code the use of parameters as additional input registers.
- We can also write a universal program in BSS, which takes a coded program as its input and runs it.

The decision problem

Given a finite set of computable graph invariants F
and an invariant f in a ring $\mathcal{R}$ is $F \models_{\mathcal{R}} f$ decidable?

Theorem 11
In the BSS model of computation

$$F \not\models_{\mathcal{R}} f$$

is semi-computable, but not computable,
even if restricted to boolean P-time computable invariants.

Proof: To find counterexamples for $F \not\models_{\mathcal{R}} f$ we just go over all graphs.

To show undecidability, we reduce the problem to the undecidability of the first order theory of finite graphs in the Turing model.

I.A. Lavrov, 1963, for finite graphs;

D. Ja. Kesel'man, 1974, for graphs of bounded degree, or bipartite planar graphs

Complexity of graph invariants.

There are scattered results on the complexity of graph (and knot) polynomials.

- They all use the Turing model of computation which requires that the coefficients are finitely presentable.
- Usually one shows that either a graph polynomial is P-time computable or it is $\sharp\mathbf{P}$-hard.
- In the $\sharp\mathbf{P}$-hard cases it cannot be said the the graph polynomial is in $\sharp\mathbf{P}$, as the value is not a (non-negative) integer.

  But even if $f(G, X)$ with $X = a$ gives a non-negative integer value, it is not clear that it $f(G, a) \in \sharp\mathbf{P}$.

We want to develop
a complexity theory for graph polynomials
in the BSS model.

Definition 12 *Three kinds of reducibilities*

Let F be a finite set of computable graph invariants and let f be a graph invariant.

- f **is P-time computable from** F if there is a P-time program $\Pi(F)$ which computes f from F.
- f **is circuit computable from** F if there is an algebraic circuit $\Gamma(F)$ which computes f from F.
- If $F = \{g\}$ is a singleton we say that f **is P-time reducible to** g, respectively f **is circuit reducible to** g.
- f **is a substitution instance of** g if $g = g(G, X_1, \ldots, X_m)$ and if $f = f(G, Y_1, \ldots, Y_n)$ and
$$f(G, Y_1, \ldots, Y_n) = g(G, s_1(\bar{X}, \ldots, s_n(\bar{X}))$$
- f **and** g **are P-equivalent (circuit equivalent)** if both f is P-reducible (circuit reducible) to g and vice versa.

Proposition 13 *Basics on reducibilities, I*

(i) If f is a substitution instance of g,
then f is circuit computable from g.

(ii) If f is a circuit computable from F,
then f is P-time computable from F.

(iii) If f is a circuit computable from F,
then f is induced by F.

Proposition 14 *Basics on reducibilities, II*

(i) The chromatic polynomial $\chi(G, X)$ is circuit computable from $X^{k(G)}$ and $T(G, X, Y)$, hence it is P-reducible to the Tutte polynomial $T(G, X, Y)$.

However, it is NOT induced by the Tutte polynomial.

(ii) The matching polynomial $g(G, X)$ and the acyclic polynomial $m(G, X)$ are P-equivalent.

Actually, in both directions circuit reductions suffice.

Proof:

(i) (W.T. Tutte, 1954) We have

$$\chi(G, X) = (-1)^{|V|-k(G)} X^{k(G)} T(G, 1 - X, 0).$$

(ii) E.J. Farrell, 1980) We use the identity

$$m(G, X) = X^n g(G, (-X^{-2}))$$

Definition 15 *Weakly graph-complete graph invariants*

A graph invariant (polynomial) is weakly graph-complete if it is P-equivalent to some graph-complete invariant.

Examples:

- We have seen that

$$Compl(G, \bar{X}, Y) = Y^{|V|} \cdot \left(\sum_{\sigma \in \mathfrak{S}_n} \prod_{(\sigma(i),\sigma(j) \in E} X_{\sigma(i),\sigma(j)} \right)$$

  is graph-complete.

- As $Y^{|V|}$ is P-computable from G,

$$f_2(G, \bar{X}, Y) = \sum_{\sigma \in \mathfrak{S}_n} \prod_{(\sigma(i),\sigma(j) \in E} X_{\sigma(i),\sigma(j)}$$

  is weakly graph-complete.

Definition 16 *Induced invariants vs. P-time computable invariants*

For F a set of graph invariants we denote by $PCL(F)$ the closure of F under P-computability.

A set of graph invariants F is P-closed if $F = PCL(F)$.

A graph invariant f is complete for a P-closed $F = PCL(F)$ if $PCL(f) = PCL(f)$.

- The set of P-computable graph invariants is P-closed.
- Every P-computable graph invariant is complete for P-time.
- Clearly, f is complete for $PCL(\{f\})$.

Our test problems

Here are a few challenging test problems.

- Are there naturally defined complexity classes of graph invariants which have complete problems?
- What are complete problems?
  With respect to what kind of reducibilities?
- How can we single out specially interesting graph polynomials?

Seminar talks: Graph polynomials

- The characteristic and the matching polynomial
  Speaker: Ilya Averbouch
- The density function of monotone and hereditary graph properties.
  Speaker: Arie Matsliach
- The Tutte polynomial
  Speaker: J.A. Makowsky and Yaniv Altschuler
- SOL-definable polynomials
  Speaker: J.A. Makowsky
- Graph polynomials and Chemistry
  Speaker: Bella Dubrov