



The expression in monadic second-order logic of some graph polynomials

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Some general objectives :

Logical descriptions of graph polynomials

Application to their computations

Systematic construction of recursive definitions

Building a *Theory of Graph Polynomials* with methods from Term Rewriting Systems and Logic, rather than accumulating anecdotal results.

(A project initiated by J. Makowsky; see the dissertation of I. Averbouch, 2011, Technion, Haïfa).

Many graph polynomials (chromatic, interlace, matching, etc.) have been defined. Some questions about them are :

- particular values, or combinatorial interpretation

of their coefficients, or of their roots,

- equivalent definitions, explicit or recursive,
- relationships with other polynomials

I will consider :

- (1) Logical definitions and algorithmic applications
- (2) Equivalences of definitions by bijective proofs
- (3) Remarks on recursive definitions by elimination.

0. Introduction: Different types of polynomials.

The chromatic polynomial: The function

 $P_{chrom}(G)(x) :=$ the number of proper x-colorings of G

is a polynomial function because it satisfies :

 $P_{chrom}(G)(x) = P_{chrom}(G - e)(x) - P_{chrom}(G / e)(x)$

 $P_{chrom}(\bullet)(x) = x$

G - e: edge deletion; G / e: edge contraction.

of acyclic orientations of $G := (-1)^n P_{chrom}(G)(-1)$

Explicit expression : $P_{chrom}(G) = \sum_{A \subseteq E} (-1)^{|A|} x^{k(A)}$

E: edges, k(A) = # of connected components of G[A]=(V,A).

The recursive definition gives proofs of these facts, but no *explanations*.

The values matter; its coefficients also have combinatorial meanings.

Generating functions

The Matching polynomial:

$$M(G)(x) := \sum_{k} match_{k} \cdot x^{k}$$

match_k is the number of k-matchings of G (= 0 if 2k > n).

The Vertex Cover polynomial :

$$VC(G)(x) := \sum_{k} vcover_{k} \cdot x^{k}$$

 $vcover_k$ is the number of vertex covers of G of size k

The coefficients matter more than the values.

The chromatic polynomial, having negative coefficients, is not of this type

1. Multivariate (enumerating) polynomials

Idea: - variables are indexed by vertices or edges: x_e , x_v

- these variables may take meaningful values: probabilities, weights, etc.

If A = $\{e1, ..., ep\} \subseteq E$, then :

$$x_{A} := x_{e1}...x_{ep}$$
 with $x_{\emptyset} := 1$.

If S is a set of subsets of E, then, the polynomial

$$\operatorname{Enum}_{x}(S) := \sum_{A \in S} x_{A}$$

describes **S** (with $\text{Enum}_{x}(\emptyset) = 0$).

Remark: Enum_x(S)[$x_e \leftarrow 1$; all e] = |S|.

Polynomials defined as generating functions "come from" multivariate enumerating polynomials:

 $M(G) := Enum_x(set of matchings of G)$ with variables indexed by edges. Clearly,

 $M(G) = M(G)[x_e \leftarrow x]$

A "mixed" example (Sokal, "Potts model" in physics).

 $Z(G)(u; x_e, e \in E) = \sum_{A \subseteq E} x_{A, u}^{k(A)}$

Multivariate polynomials can be defined with Logic

A general and basic form (enumerating polynomials of sets of triples of sets):

 $\sum_{\psi(A,B,C)} x_{A} y_{B} z_{C}$

where $\psi(A,B,C)$ is a condition on sets of vertices and/or edges expressed in a logical language: first-order or monadic second-order logic. Example of monadic second-order property:

for $G = (V_G \cup E_G, \underline{<}, in_G)$

with $in_G(e,v)$ if and only if v is an edge of e.

For $A \subseteq E_G$, G[A] is not connected iff G satisfies:

 $\begin{array}{l} \exists \ X, \ set \ of \ vertices \ (\exists x \in X \land \exists y \in V_G \text{-} X \land \\ \forall e \in A \ (\forall u, v \ (in(e, u) \land in(e, v) \land u \in X \ \Rightarrow v \in X) \) \end{array}$

Example of Z(G) (using \leq)

$$Z(G)(u; x_e, e \in E) = \sum_{\psi(A,B)} x_{A, u}|_{B}$$

 $\psi(A,B)$ means :

A is a set of edges, B is the set of minimal vertices of the connected components of G[A]. Hence k(A) = |B| The linear order associates a unique B with each A. Z(G) is order-invariant.

 $Z(G) = (\sum_{\psi(A,B)} x_{A, u_B})[u_v \leftarrow u; all vertices v]$

Evaluations and computations

Evaluation: for given values of the variables

Computation : the polynomial, or part of it, typically its monomials of degree at most given d.

Usually difficult:

 $P_{chrom}(G)(3) > 0$ if and only if G is 3-colorable (NP-complete).

VC(G) has a non-null coefficient for x^k if and only if G has a vertex cover of size k (NP-complete).

Theorem : Monadic second-order polynomials can be computed in linear time for input graphs of bounded treewidth or clique-width.

"linear" = O(size of input + size of output).

This result covers the following ones (non-multivariate) :

1) Tutte polynomial for graphs of bounded tree-width (Noble, Andrzejak, 1998)

2) Interlace polynomial for distance-hereditary graphs (of clique-width 3) (Ellis-Monagham, Sarmiento, 2006) and graphs of bounded tree-width (Bläser, Hoffman 2010)

Ideas behind that:

(1) graphs of bounded tree-width or clique-width are built with disjoint union \oplus and certain *quantifier-free unary operations* (edge complement, relabelling of vertices, addition of new edges specified by vertex labels, ...)





(2) Sat(G, φ, X₁,...,X_n) := the set of n-tuples of sets in G that satisfy φ is computable inductively on any term representing G. Main facts:

(2.1) Splitting Theorem : One can construct formulas ψ_i , θ_i , i = 1,...,p, of no larger quantifier-height than ϕ such that for all disjoint G and H :

Sat(G \oplus H, ϕ , X₁,...,X_n) is the disjoint union of the sets

Sat(G, ψ_i , X₁,...,X_n) \diamond Sat(H, θ_i , X₁,...,X_n), i = 1,...,p,

where \diamond combines "partial answers" as follows :

 $\underline{A} \Diamond \underline{B} = \{ (A_1 \cup B_1, \dots, A_n \cup B_n) / (A_1, \dots, A_n) \in \underline{A} , (B_1, \dots, B_n) \in \underline{B} \}$

(2.2) Backwards Translation Lemma : If f is a quantifier-free mapping, every φ has a backwards translation $f^{\#}(\varphi)$ relative to f such that for all G:

$$Sat(f(G), \phi, X_1,...,X_n) = Sat(G, f^{\#}(\phi), X_1,...,X_n)$$

where $f^{\#}(\phi)$ has no larger quantifier-height than ϕ .

For the edge complement, replace in φ edg(x,y) by \neg edg(x,y)

In (2.2) : $f^{\#}(\phi)$ has no larger quantifier-height than ϕ because *f* is quantifier-free.

Application to polynomials

Take the case n=1. Then $\underline{A} \diamond \underline{B} = \{ A_1 \cup B_1 / A_1 \in \underline{A} , B_1 \in \underline{B} \}$

Let $P_{\phi}(G)(x) := Enum_x(Sat(G, \phi, X_1)).$

 $\operatorname{Enum}_{x}(\underline{A} \diamond \underline{B}) = \operatorname{Enum}_{x}(\underline{A}) \cdot \operatorname{Enum}_{x}(\underline{B})$

if <u>A</u> and <u>B</u> are over disjoint sets.

 $Enum_x(\underline{A} \cup \underline{B}) = Enum_x(\underline{A}) + Enum_x(\underline{B})$ if <u>A</u> and <u>B</u> are disjoint

The Splitting Theorem gives :

 $P_{\phi}(G \bigoplus H)(x) = \Sigma_i P_{\psi i}(G)(x) \cdot P_{\theta i}(H)(x)$

The polynomials $P_{\psi i}$ and $P_{\theta i}$ must splitted similarly.

For the unary operations, the *Backwards Translation Lemma* gives :

 $P_{\phi}(f(G))(x) = P_{f \#(\phi)}(G)(x)$

For elementary graphs B, $P_{\phi}(B)$ is computed from the definitions.

We get the simultaneous computation in "linear" (sic!) time of finitely many polynomials, for the given φ and the generated auxiliary formulas.

Substitutions:

 $P_{\phi}(G \bigoplus H)(x) = \Sigma_i P_{\psi i}(G)(x) \cdot P_{\theta i}(H)(x)$

gives :

 $\mathsf{P}_{\varphi}(\mathsf{G} \bigoplus \mathsf{H})(\mathsf{x}) [\ldots] = \Sigma_i \ \mathsf{P}_{\psi i}(\mathsf{G})(\mathsf{x}) [\ldots]. \ \mathsf{P}_{\theta i}(\mathsf{H})(\mathsf{x}) [\ldots]$

where [...] is a substitution of integer or real values, or of variables or terms to the variables.

The same inductive computation applies for the evaluation or the computation of other polynomials obtained by substitutions.

3. Equivalent definitions of the Tutte polynomial:

A bijective proof at the multivariate level.

The Tutte polynomial (also for matroids).

 $T(G)(x,y) = x \cdot T(G / e)(x,y)$ if e is a "bridge"

(if deleted, yields one more c.c.)

 $T(G)(x,y) = y \cdot T(G - e)(x,y)$ if e is a loop, and otherwise

T(G)(x,y) = T(G - e)(x,y) + T(G / e)(x,y)

 $\mathsf{T}(\bullet)(x,y)=1$

Well-defined (same value independently of the order of elimination of edges).

Meanings :

T(G)(1,1) = # of spanning trees, T(G)(2,1) = # of forests \subseteq G, T(G)(2,0) = # of acyclic orientations,

probability of connectedness if one deletes edges with probability p.

 $P_{chrom}(G)(x) = (-1)^{n - k(G)} x^{k(G)} T(1 - x, 0)$

Other expressions (for G connected) :

(1)
$$T(G)(x,y) = \sum_{A \subseteq E} (x-1)^{k(A)-k(E)} (y-1)^{|A|+k(A)-|V|}$$
.

k(A) - k(E) = r(E) - r(A); |A| + k(A) - |V| = |A| - r(A) (matroid rank)

 $= R(G) [x \leftarrow x - 1; y \leftarrow y - 1] (R(G) the "rank" polynomial)$

Its "spanning tree expansion":

(2)
$$T(G, \leq)(x, y) = \sum_{i, j} t_{i, j} \cdot x^{i} y^{j}$$

where $t_{i,j}$ is the number of spanning trees that have i *internally* active edges and j externally active ones; these notions are relative to the linear order \leq , but $T(G, \leq)$ is order-invariant.

A bijective proof that $T(G, \leq) = T(G)$.

(Usual proofs, cf. Bollobas, show that the 2 definitions satisfy the recursive definition; they explain nothing.)

Lemma 1:(1) If $B \subseteq E$, $x_B[x_e \leftarrow x_e+1; all e] = Enum_x(P(B))$

(2) For $S \subseteq P(E)$:

Enum_x(S)[$x_e \leftarrow x_e$ -1; all e] has positive coefficients

if and only if S = P(B) for some $B \subseteq E$. In this case, it is equal to $x_B = \text{Enum}_x(\{B\})$

Example: $S = \{ \emptyset, \{a\}, \{b\}, \{a,b\} \}$

Enum_x(S)[$x_e \leftarrow x_e - 1$]= 1+ $x_a - 1 + x_b - 1 + (x_a - 1) \cdot (x_b - 1) = x_{\{a,b\}}$

The bijective proof that:

$$T(G) := \sum_{A \subseteq E} (x - 1)^{k(A) - k(E)} (y - 1)^{|A| + k(A) - |V|}$$

= R(G)[x \leftarrow x - 1; y \leftarrow y - 1] ("rank polynomial")
= T(G, \leftarrow) := \sum_{i, j} t_{i, j} . x^{i} y^{j}
We have T(G, \leftarrow) = T(G, \leftarrow)[x_e \leftarrow x ; y_e \leftarrow y] where

 $\mathbf{T}(\mathbf{G}, \leq) := \sum_{\mathbf{B} \text{ spanning tree } \mathbf{X}_{\mathbf{IA}(\mathbf{B})} \mathbf{Y}_{\mathbf{EA}(\mathbf{B})}$

Hence (Lemma 1) : $T(G, \leq)[x_e \leftarrow x_e+1 ; y_e \leftarrow y_e+1]$

 $= \sum_{\mathbf{B} \text{ spanning tree}} \sum_{\mathbf{C} \subseteq \mathbf{IA}(\mathbf{B}), \mathbf{D} \subseteq \mathbf{EA}(\mathbf{B})} \mathbf{X}_{\mathbf{C}} \mathbf{Y}_{\mathbf{D}}$

Lemma 2 : For every set of edges A, there is a unique spanning tree B of G such that $A - B \subseteq EA(B)$ and $B - A \subseteq IA(B)$.

Let B(A) := B, C(A) := B - A, D(A) := A - B. |C(A)| = r(E) - r(A) = k(A) - k(E)|D(A)| = |A| - r(A) = |A| + k(A) - |V|.

We have a bijection : $A \leftarrow \rightarrow (B(A), C(A), D(A)).$ $T(G, \leq)[x_e \leftarrow x_e+1 ; y_e \leftarrow y_e+1]$

$$= \sum_{\mathbf{B} \text{ sp.tree}} \sum_{\mathbf{C} \subseteq \mathbf{IA}(\mathbf{B}), \mathbf{D} \subseteq \mathbf{EA}(\mathbf{B})} x_{\mathbf{C}} y$$



 $= \sum_{\mathsf{A}\subseteq\mathsf{E}} \sum x_{\mathsf{C}(\mathsf{A})} y_{\mathsf{D}(\mathsf{A})}.$

$$\mathbf{T}(\mathbf{G}, \leq) [\mathbf{x}_{e} \leftarrow \mathbf{x}_{e} + 1 ; \mathbf{y}_{e} \leftarrow \mathbf{y}_{e} + 1] = \sum_{\mathsf{A} \subseteq \mathsf{E}} \sum x_{\mathsf{C}(\mathsf{A})} y_{\mathsf{D}(\mathsf{A})}.$$

By applying the substitution [$x_e \leftarrow x$; $y_e \leftarrow y$], we get

$$T(G, \leq)[x \leftarrow x+1 ; y \leftarrow y+1] = \sum_{A \subseteq E} \sum x^{|C(A)|} y^{|D(A)|} = R(G).$$

Hence, $T(G, \leq) = R(G)[x \leftarrow x-1 ; y \leftarrow y-1].$

Conclusion : Now we know the property that yields the equality : $T(G, \leq) = R(G)[x \leftarrow x - 1; y \leftarrow y - 1]$

and (with Lemma 1(2)), we understand why the coefficients of $R(G)[x \leftarrow x -1; y \leftarrow y -1]$ are not negative.

Remarks :

(1) There is a monadic second-order formula $\theta(A,C,D)$ expressing in (G,\leq) that C=C(A) and D=D(A). Hence, R(G) is an *MS*-definable polynomial.

(2) There is a monadic second-order formula $\psi(B,J,K)$ expressing in (G, \leq) that B is a spanning tree, J = IA(B) and K= EA(B). Hence, T(G, \leq) is an *MS-definable polynomial*:

$$T(G, \leq) = (\sum_{\psi(B, J, K)} x_J y_K z_B) [x_e \leftarrow x ; y_e \leftarrow y ; z \leftarrow 1]$$

This fact shows the existence of a polynomial algorithm for computing it on graphs of bounded tree-width.

3. Recursive definitions of polynomials

Two types:

- Induction of the structure of graphs of bounded treewidth or clique-width : yields polynomial algorithms.
- Elimination of edges or vertices (cf. chromatic polynomial) :

Useful to prove properties, but proofs are not informative (as can be bijective proofs, cf. Tutte polynomial)

No efficient algorithms ; not always well-defined

Do not help to understand the "meaning" of the considered polynomial.

But give some criteria to classify and compare graph polynomials.

Examples illustrating these points.

The following definitions are all "multiplicative":

 $P(\emptyset) = 1$, $P(G \oplus H) = P(G).P(H)$ (\oplus : disjoint union)

(1) The most general "chromatic" polynomial:

$$U_{chrom}(x,y,z) = z \cdot U_{chrom}(G - e) + y \cdot U_{chrom}(G / e)$$
$$U_{chrom}(\bullet)(x,y,z) = x$$

Fact 1 : $U_{chrom}(G)$ is well-defined (same result for every order of elimination of edges) because edge deletions and contractions commute:

G-e-f = G-f-e, G/e/f = G/e/f,G-e/f = G/f-e. Fact 2 : Every polynomial of "chromatic type" is obtained from $U_{chrom}(G)$ by a substitution to x,y,z

Fact 3 : We get the explicit expression of $U_{chrom}(G)$:

$$U_{chrom}(G)(x,y,z) = \sum_{A \subseteq E} x^{k(A)} y^{|A|} z^{|E-A|}.$$

Hence :

 $U_{chrom}(G)(x,y,z) = z^{|E|} U_{chrom}(G)(x,y/z,1)$

Two variables suffice (in $U_{chrom}(G)(x,y,1)$) to get the full expressive power.

(2) Other families of polynomials based on edge elimination :

"Universal Matching polynomial":

 $U_{match}(G) = \alpha \cdot U_{match}(G - e) + \beta \cdot U_{match}(G \lor e)$ $U_{match}(\bullet) = \gamma$ where $G \downarrow e$ is the induced subgraph G[V- the ends of e]. Origin: the "matching polynomial" : $\alpha = \gamma = 1$, $\beta = x$. $M(G)(x) = \sum_{k} m(G,k) x^{k}$, m(G,k) = # of k-matchings. **Fact** : U_{match} is well-defined if and only if $(\alpha - 1)\beta = 0$.

"Universal edge elimination polynomial":

 $\begin{array}{l} U_{edgelim}(G) = \\ \alpha . U_{edgelim}(G - e) + \beta . U_{edgelim}(G \checkmark e) + \delta . U_{edgelim}(G/e) \\ U_{edgelim}(\bullet) = \gamma \\ \hline Fact 1 : well-defined if and only if (\alpha - 1) \beta = 0. \\ which gives two types : \\ \alpha . U_{chrom}(G - e) + \delta . U_{chrom}(G/e) \\ U_{vcover}(G - e) + \beta . U_{vcover}(G \checkmark e) + \delta . U_{vcover}(G/e) \end{array}$

Fact 2 : For $\alpha = \delta = 1$, $\beta = x$, $\gamma = x+1$, we get

 $VC(G) = \sum_{k} vc(G,k) x^{k}$ (vc(G,k) = # of vertex covers of size k)

Conclusions

1. Computation and evaluation are difficult in general.

2. Almost all graph polynomials are MS definable (using substitutions in "basic MS polynomials"), hence have "efficient" algorithms for graphs of bounded *-width. But more direct algorithms are interesting (Bläser,Hoffmann, STACS 2008).

3. Bijective proofs at the multivariate level help to understand matters: see above for Tutte's (and Gioan's work). 4. Explicit definitions are more informative than "vertex/edge eliminating recursive definitions". Are there general tools for obtaining such recursive definitions from explicit ones, and/or *vice versa*?

Which "elimination rules" are appropriate for which polynomials?

Relationships with well-quasi orders (minors, vertex minors) ?

5. Some definitions look arbitrary: p.ex., the (x-1) factors in the interlace polynomial (but not in Tutte's as seen above). A classification should uniformize the numerous definitions.