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A local Invariant for Trees: Counting Schrödinger Operators

Roland Bacher*

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*Abstract*¹: We define local invariants for trees and illustrate them by counting invertible Schrödinger operator for trees over finite fields.

1 Introduction

A *Schrödinger operator* on a simple (no multiple edges or loops) unoriented graph G is a matrix which coincides with the adjacency matrix of G outside the diagonal and is arbitrary on the diagonal. (It would in fact be more accurate to call such matrices opposites of Schrödinger operators.)

We consider the counting-function $q \mapsto S(T)(q)$ enumerating invertible Schrödinger operators for a finite tree T over the finite field \mathbb{F}_q with q elements. We show that $S(T)$ is, up to a sign depending on the parity of the number of vertices in T , a monic palindromic polynomial whose roots have seemingly interesting properties. We describe a general framework for similar invariants of trees and plane trees.

2 Local construction of trees

We denote by \mathcal{T} the set of all finite trees and by \mathcal{R} the set of all finite rooted trees. (Rooted) trees will always be finite in the sequel.

Every element of \mathcal{R} can be constructed (generally not uniquely) by applying a finite number of times the following operations:

- (V) Creating a trivial rooted tree consisting of a unique root-vertex.
- (E) Extending a rooted tree by gluing (an ordinary vertex of) an edge to the root-vertex and by marking the new leaf of this extended tree as the root.

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(*M*) Merging two rooted trees by gluing their root-vertices into the root-vertex of the resulting tree.

V has no argument, E operates on elements of \mathcal{R} , the map M operates commutatively and associatively on pairs of elements in \mathcal{R} and admits V as a two-sided identity.

Finally, the “forget” operator

(*F*) Forgetting the root-structure by turning the root of a rooted tree into an ordinary vertex,

yields a surjection from \mathcal{R} onto \mathcal{T} . We have the identity

$$F(M(A, E(B))) = F(M(E(A), B)) \quad (1)$$

(for all A, B in \mathcal{R}) encoding the fact that an ordinary tree with n vertices can be rooted at n different vertices.

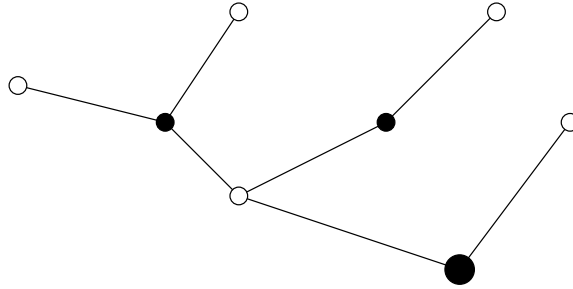


Figure 1: An example of a rooted tree.

Figure 1 shows the rooted tree encoded (for example) by

$$M\{E(M\{E(M\{E(V), E(V)\}), E(E(V))\}), E(V)\}$$

with curly brackets enclosing arguments of M . The root-vertex is shown as a large black dot. The bipartite colouring of vertices can be neglected at this stage.

2.1 Local invariants of (rooted) trees

A *local invariant of rooted trees* with values in a set \mathbb{E} is a map $i : \mathcal{R} \rightarrow \mathbb{E}$ which can be computed by replacing the construction operators V, E, M by v, e, m where $v \in \mathbb{E}$, $e : \mathbb{E} \rightarrow \mathbb{E}$ and $m : \mathbb{E} \times \mathbb{E} \rightarrow \mathbb{E}$ with m a commutative and associative binary map.

A *local invariant of trees* is a map $f \circ i$ from \mathcal{T} to a set of values \mathbb{F} where i is a local invariant of rooted trees given by $v, e, m : \mathbb{E}^* \rightarrow \mathbb{E}$ as above and where $f : \mathbb{E} \rightarrow \mathbb{F}$ is a map such that the identity

$$f(m(A, e(B))) = f(m(e(A), B))$$

corresponding to (1) holds for all A, B in \mathbb{E} .

A trivial example with $\mathbb{E} = \mathbb{F} = \mathbb{N}$ is given by $c = 0$, $e(x) = x + 1$, $m(x, y) = x + y$ and $f(x) = x$. It counts the number of edges (given by $n - 1$ for a tree with n vertices) of a tree. Replacing f with $f_1(x) = x + 1$ we count vertices instead of edges.

Remark 2.1 *The definition of local invariants for (rooted) trees is tautological: Every map $A : \mathcal{T} \rightarrow \mathbb{F}$ is a local invariant by taking $\mathbb{E} = \mathcal{R}$ and $v = V, e = E, m = M, f = A \circ F$. We are of course interested in local invariants where the maps v, e, m and f are simple, eg. given by algebraic operations over some set \mathbb{E} with a rich algebraic structure.*

2.2 First examples

2.2.1 Enumerating independent sets

A subset \mathcal{I} of vertices in a graph G is *independent* if \mathcal{I} contains no pair of adjacent (and distinct) elements. The polynomial $\sum_j \alpha_j x^j$ encoding the number α_j of independent sets with j vertices in a finite tree can be computed as a local invariant using

$$\begin{aligned} v &= (1, x), \\ e(a, b) &= (a + b, xa), \\ m((a, b), (\alpha, \beta)) &= (a\alpha, \frac{1}{x}b\beta), \\ f(a, b) &= a + b. \end{aligned}$$

We leave the easy details to the reader. (Hint: The first coefficient a of (a, b) counts independent sets without the root of rooted trees, the second coefficient b counts independent sets containing the root-vertex.)

For the tree underlying Figure 1 we get

$$1 + 8x + 21x^2 + 22x^3 + 8x^4 + x^5 .$$

2.2.2 Enumerating matchings

A *matching* of a graph is a set of disjoint edges. The polynomial $\sum_j \alpha_j x^j$ with α_j counting matchings involving j edges can be computed as the local invariant

$$\begin{aligned} v &= (1, 0), \\ e(a, b) &= (a + b, xa), \\ m((a, b), (\alpha, \beta)) &= (a\alpha, a\beta + b\alpha), \\ f(a, b) &= a + b. \end{aligned}$$

We leave the easy details to the reader. (Hint: The first coefficient a of (a, b) counts matchings of a rooted tree not involving the root, the second coefficient b counts matchings involving the root.)

For the tree underlying Figure 1 we get

$$1 + 7x + 13x^2 + 7x^3 .$$

2.2.3 The characteristic polynomial of the adjacency matrix

We write $(a, b) \in \mathbb{Z}[x]$ if the characteristic polynomial of a rooted tree is given by $-ax + b$ with ax corresponding to the contribution of the diagonal entry associated to the root. The characteristic polynomial $\det(A - x \text{Id})$ (where A is an adjacency matrix) is then a local invariant defined by

$$\begin{aligned} v &= (1, 0), \\ e(a, b) &= (-xa + b, -a), \\ m((a, b), (\alpha, \beta)) &= (a\alpha, a\beta + b\alpha), \\ f(a, b) &= -xa + b. \end{aligned}$$

For the tree underlying Figure 1 we get

$$x^8 - 7x^6 + 13x^4 - 7x^2 .$$

Similarly,

$$\begin{aligned} v &= (1, 0, 0), \\ e(a, b, c) &= -(x + c + 1)a + b, -a, 1), \\ m((a, b, c), (\alpha, \beta, \gamma)) &= (a\alpha, a\beta + b\alpha, c + \gamma), \\ f(a, b, c) &= -(x + c)a + b \end{aligned}$$

computes the characteristic polynomial of the combinatorial Laplacian of a tree.

For the tree underlying Figure 1 we get

$$x^8 + 14x^7 + 76x^6 + 204x^5 + 286x^4 + 204x^3 + 67x^2 + 8x .$$

3 The main example: counting Schrödinger operators

We consider the local invariant $S : \mathcal{T} \rightarrow \mathbb{Z}[q]$ of trees defined by

$$\begin{aligned} v &= (0, 1), \\ e(a, b) &= (b, qa + (q - 1)b), \\ m((a, b), (\alpha, \beta)) &= (a\beta + b\alpha, b\beta), \\ f(a, b) &= qa + (q - 1)b. \end{aligned}$$

The constant v is obviously an identity for m which is commutative and associative. Identity (1) amounts to the fact that

$$\begin{aligned}
& f(m((a, b), e(\alpha, \beta))) \\
&= f(m((a, b), (\beta, q\alpha + (q-1)\beta))) \\
&= f(qa\alpha + qa\beta - a\beta + b\beta, qb\alpha + qb\beta - b\beta) \\
&= q^2(a+b)(\alpha+\beta) - q(a\beta + b\alpha) + b\beta
\end{aligned}$$

is symmetric in its arguments (a, b) and (α, β) .

For the tree underlying Figure 1 we get

$$(q-1)^2(q^2 - q + 1)(q^4 + 2q^3 + q^2 + 2q + 1).$$

Remark 3.1 *As a mnemotechnical device, the formula for m corresponds to the addition $\frac{a}{b} + \frac{\alpha}{\beta} = \frac{a\beta + b\alpha}{b\beta}$ with forbidden simplification and the formula for e is, up to simplification by b , given by the homography $\frac{a}{b} \mapsto \begin{pmatrix} 0 & 1 \\ q & q-1 \end{pmatrix} \frac{a}{b} = \frac{1}{q\frac{a}{b} + q - 1}$.*

In the sequel we denote similarly by $S(R) = (a, b) \in \mathbb{Z}[q]^2$ the pair of polynomials associated to a rooted tree R .

Theorem 3.2 *$S(T)$ counts the number of invertible Schrödinger operators for T over the finite field \mathbb{F}_q .*

Proposition 3.3 (i) *$S(T)$ is monic and palindromic up to a sign (ie. $S(T)(q) = (-q)^n S(T)(1/q)$ where n is the number of vertices of T).*

(ii) *The polynomial $S(T)$ of a tree with n vertices is of the form $q^n - q^{n-1} + O(q^{n-2})$.*

Assertion (ii) of Proposition 3.3 implies that $S(T)$ has always roots with a strictly positive real part. These roots should be on the complex unit circle, according to Conjecture 3.5.

Assertion (ii) of Proposition 3.3 tells us that the number of invertible Schrödinger operators on a tree can be correctly estimated naively assuming that the determinant is a non-constant affine function of a fixed diagonal coefficient.

3.1 The value of S for a few families

3.1.1 Lines (path-graphs, Dynkin-graphs of type A)

We denote by R_n the rooted tree given by n vertices forming a path of length n with the root at a leaf. Writing $S_r(R_n) = (a_n, b_n)$, we have

$$a_n = \frac{q^{n-1} - (-1)^{n-1}}{q+1} \text{ and } b_n = \frac{q^n - (-1)^n}{q+1}$$

by an easy induction using the identity $(a_{n+1}, b_{n+1}) = e(a_n, b_n) = (b_n, qa_n + (q-1)b_n)$. This yields

$$S(T_n) = \frac{q^{n+1} - (-1)^{n-1}}{q+1}$$

for the tree T_n underlying R_n .

3.1.2 Stars

We denote by R_n the rooted graph consisting of a central root adjacent to $n-1$ leaves. Writing again $S_r(R_n) = (a_n, b_n)$ we have

$$a_n = (n-1)(q-1)^{n-2} \text{ and } b_n = (q-1)^{n-1}$$

as can be checked using

$$\begin{aligned} (a_{n+1}, b_{n+1}) &= m((a_n, b_n), e(v)) = m((a_n, b_n), (1, q-1)) \\ &= ((q-1)a_n + b_n, (q-1)b_n) . \end{aligned}$$

We have thus

$$S(T_n) = f(a_n, b_n) = (q^2 + (n-3)q + 1)(q-1)^{n-1}$$

for the non-rooted star T_n underlying R_n .

3.2 Multiple roots of $S(T)$

A vertex of degree k of a tree T can be considered as the result of gluing k rooted trees along their roots where all rooted trees are rooted at a leaf. This construction is linked to some multiple roots of $S(T)$ as follows: Given a leaf-rooted tree R , let v_1, \dots, v_n be all vertices of T involving R (ie. at least one of the rooted trees leading to v_i is isomorphic to R). Given such a vertex v_i , we denote by $r_i + 1 \geq 1$ the multiplicity of the tree R at v_i . Let $S_r(R) = (a, b) \in \mathbb{Z}[q]^2$ be the corresponding local invariant of the rooted tree R . We have then the following result:

Proposition 3.4 *The polynomial $S(T)$ is (at least) divisible by b^r where $r = r_1 + \dots + r_k$.*

Proof Gluing $k_i + 1$ copies of R together along their root gives a rooted tree with invariant $((k_i + 1)ab^{k_i}, b^{k_i+1})$. Linearity and bilinearity of the formulae for e, f and m imply now the result. \square

Proposition 3.4 explains the factor $q^2 - q + 1$ and one of the factors $q - 1$ of the polynomial $S(T) = (q-1)^2(q^2 - q + 1)(q^4 + 2q^3 + q^2 + 2q + 1)$ with T given by Figure 1. Since $S(T)$ is palindromic, the factor $q - 1$ divides $S(T)$ with even multiplicity. All cyclotomic factors in this examples have thus easy explanations.

3.3 Conjectural properties of roots of $S(T)$

3.3.1 Location of roots

Experimental observations (computation of examples) suggest the following result:

Conjecture 3.5 *All roots of $S(T)$ are on the union of the of the complex unit circle with the real negative half-line.*

Moreover, the number of real negative roots is at most equal to twice the number of vertices of degree at least 3.

In the case of rooted trees, the number of negative roots of the first polynomial a in the associated invariant $(a, b) = S(R) \in \mathbb{Z}[q]^2$ is at most equal to twice the number of non-root vertices of degree at least 3 in R .

Conjecture 3.5, if true, gives a method for constructing *Salem numbers*, defined as algebraic integers of absolute value > 1 having all conjugates in the closed complex unit disc and having at least one conjugate on the unit circle. Indeed, given k natural integers $l_1, \dots, l_k \geq 1$, we denote by $St(l_1, \dots, l_k)$ the generalized star-tree obtained by gluing k paths of length l_1, \dots, l_k along one of their extremal vertices. For $k \geq 3$, the resulting graph T with $1 - k + l_1 + \dots + l_k$ vertices has k leaves, $-k + l_1 + \dots + l_k$ vertices of degree 2 and a central vertex of degree $k \geq 3$. The polynomial $S(T)$ defines thus conjecturally in most cases a Salem number.

We describe now a construction showing that the last part of Conjecture 3.5 holds for generalized stars (trees having at most one vertex of degree > 2) as considered a few lines above.

Proposition 3.6 *Given a strictly positive natural number k , a complex number λ of norm at most 1 and non-negative real constants c_1, c_2, \dots such that $0 < \sum_j c_j < \infty$, the holomorphic function defined by*

$$\sum_{j=1}^{\infty} c_j \frac{1 + \lambda z^j}{1 + \lambda z^{j+k}}$$

has no roots in the open complex unit disc.

The same result holds for $\sum_{j=1}^{\infty} c_j \frac{1 + \lambda z^{j+k}}{1 + \lambda z^j}$.

Corollary 3.7 *Let $C(x) \in \mathbb{Q}[x]$ be a rational polynomial having only strictly positive real roots and let $L(x) \in \mathbb{Q}[x]$ be a polynomial having all its roots on the complex unit circle (ie. of norm 1). Given an integer $k \geq 1$ and n integers $j_1, \dots, j_n \geq 0$, the polynomials*

$$\prod_{c \in \mathbb{R}, C(c)=0} \prod_{\lambda \in \mathbb{C}, L(\lambda)=0} \left(\prod_{h=1}^n (1 + \lambda z^{j_h+k}) \right) \left(\sum_{h=1}^n c \frac{1 + \lambda z^{j_h}}{1 + \lambda z^{j_h+k}} \right)$$

and

$$\prod_{c \in \mathbb{R}, C(c)=0} \prod_{\lambda \in \mathbb{C}, L(\lambda)=0} \left(\prod_{h=1}^n (1 + \lambda z^{j_h}) \right) \left(\sum_{h=1}^n c \frac{1 + \lambda z^{j_h+k}}{1 + \lambda z^{j_h}} \right)$$

are rational polynomials having all their roots on the complex unit circle.

Corollary 3.7 is mainly an illustration and is not stated in the most general case.

Proof of Corollary 3.7 These polynomials are clearly rational polynomials. They have a leading coefficient of the same size as their constant coefficient. The product of all their roots is thus on the unit circle. Hence it is enough to prove that they have no root in the open unit disc. This follows from Proposition 3.6. \square

Proof of Proposition 3.6 We set $\mu = \lambda z^k$ for z in the open complex unit disc. The image of the map

$$\mathbb{N} \setminus \{0\} \ni n \mapsto \frac{1 + \lambda z^n}{1 + \lambda z^{n+k}} = \frac{1 + \lambda z^n}{1 + \mu z^n}$$

belongs then to the open disc or halfplane \mathcal{S} given by the image of the open unit disc under the homography

$$z \mapsto \frac{1 + \lambda z}{1 + \mu z}$$

which does not contain the origin. Non-trivial positive linear combinations of elements in \mathcal{S} are thus never zero. \square

The following result proves a particular case of the conjectural properties of the first polynomial a for R a rooted tree with $S(R) = (a, b)$.

Proposition 3.8 *Given a generalized star R , rooted at its central vertex with rays of arbitrary lengths, the polynomials a and b of $S(R) = (a, b)$ have all their roots on the unit circle.*

Proof The a -polynomial of such a rooted tree is a polynomial described by Corollary 3.7. The b -polynomial is a product of cyclotomic polynomials. \square

3.3.2 Real negative roots, subdivisions

Subdividing an edge into more edges by insertion of intermediary vertices of degree 2 does generally not augment the number of real negative roots of the polynomial S . Moreover, real negative roots do seemingly converge to some algebraic “limit-roots” in a sequence of graphs with a larger and larger number of subdivisions of an edge. Subdividing all edges by insertion of more and more intermediary vertices around a given vertex of degree $\alpha + 1 \geq 3$ leads to limit-roots $-\alpha, -1/\alpha$. This can be done at several vertices. In particular, subdivision of all edges by insertion of more and more intermediate

vertices leads seemingly to real limit-roots $-\alpha_1, \dots, -\alpha_k, -1/\alpha_1, \dots, -1/\alpha_k$ where $\alpha_1 + 1, \dots, \alpha_k + 1$ are the degrees of all vertices of degree at least 3.

It would be interesting to understand the behaviour of roots on the unit-circle under larger and larger edge-subdivisions. The number of these roots increases and the simplest possible behaviour would be convergency of the relative root density on the unit-circle to some continuous limit given by a probability-measure.

3.4 Proofs

A matrix M with rows and columns indexed by vertices of a simple graph G is a G -matrix if a non-diagonal coefficient $m_{s,t}$ of M is zero if and only if $\{s, t\}$ is not an edge of G . Diagonal entries of a G -matrix are arbitrary. Equivalently, a G -matrix is a matrix whose non-diagonal support (set of non-zero coefficients) encodes the edge-set of G . A G -matrix has a symmetric support but is not necessarily symmetric. We have:

Theorem 3.9 *The number of invertible T -matrices of a finite tree T having n vertices is given by $(q-1)^{2n-2}S(T)$ with $S(T)$ defined at the beginning of this Section.*

Proof of Theorem 3.2 Follows from the obvious action on T -matrices of the abelian group $(\mathbb{F}_q^*)^n \times (\mathbb{F}_q^*)^n$ of pairs of invertible diagonal matrices (with coefficients in \mathbb{F}_q) by left and right multiplication. \square

Proof of Theorem 3.9 An R -matrix for a rooted tree $R \in \mathcal{R}$ is a T -matrix for the underlying unrooted tree T with an unknown x on the diagonal corresponding to the root of R . The determinant of a R -matrix for $R \in \mathcal{R}$ over a finite field \mathbb{F}_q is thus an affine function of the form $ax + b \in \mathbb{F}_q[x]$.

We consider now a fixed rooted tree R . Given two subsets A, B of \mathbb{F}_q we denote by $N(A, B)$ the number of R -matrices of determinant $ax + b$ with $(a, b) \in A \times B$. We encode the natural integers $N(0, 0), N(0, \mathbb{F}_q^*), N(\mathbb{F}_q^*, 0), N(\mathbb{F}_q^*, \mathbb{F}_q^*)$ (with 0 denoting the singleton $\{0\}$) using the square matrix

$$\begin{pmatrix} N(0, 0) & N(0, \mathbb{F}_q^*) \\ N(\mathbb{F}_q^*, 0) & N(\mathbb{F}_q^*, \mathbb{F}_q^*) \end{pmatrix}.$$

Since right and left multiplications by invertible diagonal matrices preserve the set of R -matrices, we have $N(\lambda a, \mu b) = N(a, b)$ for invertible elements λ and μ . Elementary linear algebra shows now that the operators V, E, M, F correspond to the operators

$$\begin{aligned} v &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \\ e &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto (q-1)^2 \begin{pmatrix} qa & c+d \\ qb & (q-1)(c+d) \end{pmatrix}, \end{aligned}$$

$$\begin{aligned}
m &= \left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \right) \mapsto \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \\
f &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto qb + (q-1)(c+d)
\end{aligned}$$

where

$$\begin{aligned}
A &= a\alpha + a\beta + b\alpha + a\gamma + c\alpha + \\
&\quad + a\delta + d\alpha + b\beta, \\
B &= b\gamma + c\beta + b\delta + d\beta, \\
C &= c\gamma + \frac{1}{q-1}d\delta, \\
D &= c\delta + d\gamma + \frac{q-2}{q-1}d\delta.
\end{aligned}$$

We can neglect the values $N(0,0)$ and lump together $N(\mathbb{F}_q^*, 0)$ and $N(\mathbb{F}_q^*, \mathbb{F}_q^*)$. This leads to the formulae for $S(T)$ except for an extra factor of $(q-1)^2$ for every edge of T . \square

The following result will be used in the proof of Proposition 3.3:

Proposition 3.10 *Let $(a, b) = S(R) \in \mathbb{Z}[q]^2$ be the pair of polynomials associated to a rooted tree R with n vertices and a root of degree d . The polynomial a has then degree $n-2$ and is of the form $dq^{n-2} + O(q^{n-3})$. The polynomial b has degree $n-1$ and is of the form $q^{n-1} - dq^{n-2} + O(q^{n-3})$.*

The proof of Proposition 3.10 is an easy induction based on the formulae for v, e and m . We leave the details to the reader. \square

Proof of Proposition 3.3 An easy induction on the number n of vertices shows that the polynomials a and b of a rooted trees are palindromic, up to signs (given by $(-1)^{n-2}$ and $(-1)^{n-1}$). The polynomial b is moreover always monic by Proposition 3.10. This implies assertion(i).

Assertion (ii) follows from Proposition 3.10 and the easy computation

$$S(T) = f(a, b) = qa + (q-1)b = dq^{n-1} + q^n - q^{n-1} - dq^{n-1} + O(q^{n-2})$$

for $(a, b) = S(R)$ with R obtained from T by choosing a root-vertex (of degree d) among the vertices of T . \square

4 Trees with coloured vertices

A rooted tree with non-rooted vertices coloured (not necessarily properly, ie. adjacent vertices have not necessarily distinct colours) by a set \mathcal{C} can be constructed using the construction-operators V (creation of a root-vertex), M (merging of two rooted trees along their root) and replacing E by operators E_c (for $c \in \mathcal{C}$) depending on the final colour of the initial root-vertex.

For ordinary trees, one replaces F by operators F_c indexed by all possible colours of the last vertex.

Identity (1) is replaced by

$$F_s(M(A, E_t(B))) = F_t(M(E_s(A), B))$$

for all $s, t \in \mathcal{C}$ and $A, B \in \mathcal{R}$.

Denoting by E_b, E_w and F_b, F_w the coloured operators for trees with black and white vertices, the black-white coloured tree underlying Figure 1 is given by

$$F_b(M\{E_w(M\{E_b(M\{E_w(V), E_w(V)\}), E_b(E_w(V))\}), E_w(V)\}).$$

Local invariants for coloured trees are now defined in the obvious way.

A somewhat trivial method for creating coloured local invariants is given by choosing colour-constants $V_c \in \mathbb{E}$ and by replacing e , respectively f , by $e_c(A) = e(m(A, V_c))$, respectively, $f_c(A) = f(m(A, V_c))$. These invariants amount to attachments of “virtual trees” depending on the colour at all vertices of a tree.

A coloured variation of the characteristic polynomial of the adjacency matrix is given by computing the determinant of the matrix coinciding with the adjacency matrix outside the diagonal and with diagonal coefficients $-x$ or $-y$ according to the bipartite class of the corresponding vertex. The resulting determinant is well-defined in $\mathbb{Z}[x, y]$ up to exchanging x with y and can be computed as a local invariant. This construction works of course also for the combinatorial Laplacian of a tree.

4.1 Coloured Schrödinger operators

The enumeration of Schrödinger operators according to coloured diagonal zeros leads to a local invariant of coloured trees. It takes its values in $\mathbb{Z}[q, \mathcal{C}]$ with the coefficient (in $\mathbb{Z}[q]$) of a monomial $\prod_j c_j^{e_j} \in \mathcal{C}^*$ counting the number of Schrödinger operators with e_j zero terms on diagonal elements associated to vertices of colour c_j .

The corresponding operators are given by

$$\begin{aligned} v &= (0, 1, 0), \\ e_s(a, b, c) &= (sb + c, (q - 1 + s)a, (q - 1)b + (q - 2 + s)c), \\ m((a, b, c), (\alpha, \beta, \gamma)) & \\ &= (a\beta + b\alpha + a\gamma + c\alpha, b\beta + \frac{c\gamma}{q-1}, b\gamma + c\beta + \frac{q-2}{q-1}c\gamma) \\ f_s(a, b, c) &= (q - 1 + s)a + (q - 1)b + (q - 2 + s)c. \end{aligned}$$

(with (a, b, c) standing for $a = N(0, \mathbb{F}_q^*)$, $b = N(\mathbb{F}_q^*, 0)$ and $c = N(\mathbb{F}_q^*, \mathbb{F}_q^*)$ using the notation of the Proof of Theorem 3.9).

Skeptical readers are invited to check the identity

$$f_s(m((a, b, c), e_t(\alpha, \beta, \gamma))) = f_t(m(e_s(a, b, c), (\alpha, \beta, \gamma))).$$

4.2 A few examples of colourings for trees

Since trees are bipartite graphs, they have a unique proper colouring (up to colour permutation) with two colours, see Figure 1 for an example. More generally, given a symmetric subset \mathcal{M} of $\mathbb{N} \times \mathbb{N}$, colour the two endpoints s, t of an edge e with the same colour if $(\deg(s), \deg(t)) \in \mathcal{M}$ and with both colours (of a colour set with 2 elements) otherwise. The proper bipartite colouring corresponds to the case of two colours with $\mathcal{M} = \emptyset$.

A canonical proper colouring (up to colour permutations) with 3 colours is defined by requiring that a vertex of degree 2 and its two neighbours have all different colours. All other vertices have neighbours of the same colour (distinct from the colour of the central vertex).

An improper canonical colouring of trees with 3 colours appears in [3] and [1]. We describe it following [2]: Call a subset \mathcal{S} of vertices of a tree a *vertex cover* if \mathcal{S} intersects every edge. Minimal vertex cover have a minimal number of elements. Colour a vertex in green if it is contained in every minimal vertex cover, in orange if it is contained in some minimal vertex cover and in red if it is contained in no minimal vertex cover. See the references cited above for more properties of this colouring.

Trees with an odd number of vertices have a canonical orientation of edges: Removal of an edge e joining two vertices s and t in such a tree T determines two subtrees T_s , respectively T_t , containing s , respectively t . We orient e from s to t if the subtree T_s contains an even number of vertices. This leads to a proper \mathbb{Z} -colouring of T , well defined up to addition of a constant, by the requirement $c(t) = c(s) + 1$ if s and t are as above. This colouring is compatible with reduction modulo N for any natural integer N . Reduction modulo 2 gives the proper bipartite colouring.

In the case of a tree T with an even number of vertices, we get a partition of the edges of T into two classes \mathcal{E} and \mathcal{O} according to the parity of the number of vertices in the two subtrees T_s and T_t . This leads to a proper "dihedral" \mathbb{Z} -colouring of T , well defined up to the action of the infinite dihedral group: $c(t) = c(s) + (-1)^{c(s)}$ if the edge joining s to t is in \mathcal{E} and $c(t) = c(s) - (-1)^{c(s)}$ otherwise. The dihedral colouring is compatible with reduction modulo N for any even natural number N . The case $N = 2$ corresponds to the bipartite colouring.

One can also consider colourings where the colours of two adjacent vertices s, t depend not only on the parities of the two subtrees obtained by removing the edge $\{s, t\}$ but also on their sizes (and perhaps also on the degrees of s and t). More generally, a vertex v of a tree T with n vertices determines a partition of $n - 1$ by considering the number of vertices in connected components of the forest obtained by removing v from T . We can now colour v with the (colour of the) corresponding partition.

5 Plane trees

A *plane tree* is a tree embedded in the oriented plane, up to orientation-preserving homeomorphisms. Plane trees are abstract trees together with cyclic orders on edge sets incident at a common vertex.

A *rooted plane tree* is a rooted plane tree together with a refinement into a linear order of the cyclic order on edges incident at the root.

Rooted plane trees can be constructed using the operators V, E, M already considered, except that M is no longer commutative (but remains of course associative). When dealing with ordinary plane trees, we need moreover the operator F together with the identity $F(M(A, B)) = F(M(B, A))$.

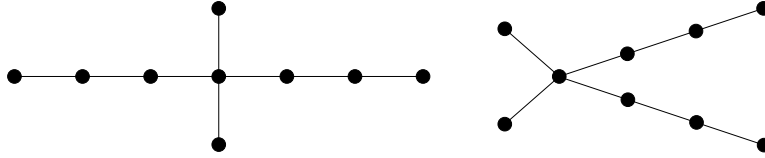


Figure 2: Two non-isomorphic plane trees.

Figure 2 shows two non-isomorphic plane trees, given for example by

$$F(M(M(E(E(E(V))), E(V)), M(E(E(E(V))), E(V))))$$

and

$$F(M(M(E(V), E(V)), M(E(E(E(V))), E(E(E(V))))))$$

with the same underlying abstract tree.

5.1 An example of a local invariant for plane trees coming from 2-coloured edges

A 2-colouring into black and red of all edges in a plane tree T is *admissible* if two red edges are never cyclically consecutive (ie. all letters b in the cyclic word in $\{b, r\}^*$ encoding the colours around a vertex are isolated). We want to compute the polynomial $\sum \alpha_j x^j$ counting the number a_j of admissible colourings with j red edges of a plane tree.

We consider six coefficients $a_1, \dots, a_6 \in \mathbb{N}[x]$: where $v = (1, 0, 0, 0, 0, 0)$ and $a_1 = 0$ whenever R is not a trivial rooted tree, a_2 counts situations with neither first nor last (not necessarily distinct) red edge issued from the root, a_3 first edge red but not last, a_4 last edge red but not first, a_5 first and last edge both red and distinct, a_6 root is the leaf of a red edge. We resume this information in the table

a_1	a_2	a_3	a_4	a_5	a_6
\emptyset	$b \dots b$ or b	$r \dots b$	$b \dots r$	$r \dots r$	r

We have

$$v = (1, 0, 0, 0, 0, 0),$$

$$e(a_1, a_2, a_3, a_4, a_5, a_6) = (0, a_1 + a_2 + a_3 + a_4 + a_5 + a_6, 0, 0, 0, x(a_1 + a_2)),$$

$$\begin{aligned} & m((a_1, \dots, a_6), (b_1, \dots, b_6)) \\ &= (a_1 b_1, c_2, c_3, c_4, c_5, a_1 b_6 + a_6 b_1) \end{aligned}$$

where

$$\begin{aligned} c_2 &= a_2 b_2 + a_2 b_3 + a_4 b_2 + a_1 b_2 + a_2 b_1 \\ c_3 &= a_3 b_2 + a_3 b_3 + a_5 b_2 + a_6 b_2 + a_1 b_3 + a_3 b_1 \\ c_4 &= a_2 b_4 + a_2 b_5 + a_2 b_6 + a_4 b_4 + a_1 b_4 + a_4 b_1 \\ c_5 &= a_3 b_4 + a_3 b_5 + a_3 b_6 + a_5 b_4 + a_6 b_4 + a_1 b_5 + a_5 b_1 \end{aligned}$$

and $f(a_1, a_2, a_3, a_4, a_5, a_6) = a_1 + a_2 + a_3 + a_4 + a_6$.

For the plane rooted tree underlying Figure 1, we get the polynomial $7x^3 + 13x^2 + 7x + 1$ enumerating also matchings. This is not surprising since all solutions for plane trees involving only vertices of degree ≤ 3 correspond to matchings of the underlying tree.

For the two plane trees of Figure 2 we get

$$5x^4 + 18x^3 + 20x^2 + 8x + 1 \quad \text{and} \quad 4x^4 + 18x^3 + 20x^2 + 8x + 1$$

showing that they are indeed non-isomorphic plane trees.

5.2 Generalizing the 2-edge-coloured example

The previous example just discussed has of course many variations giving rise to similar formulae. The next simple example is perhaps given by edge-colourings with three colours such that two cyclically consecutive edges have neither the same colour (weighting such colourings with $x^\alpha y^\beta z^\gamma$ where α, β, γ are the multiplicities of the colours (identified with) x, y, z , we get a symmetric polynomial in x, y, z). A set of values \mathbb{E} of the corresponding local invariant can be chosen as given by elements

$$(a, a_x, a_y, a_z, a_{xx}, a_{xy}, a_{xz}, a_{yx}, a_{yy}, a_{yz}, a_{zx}, a_{zy}, a_{zz})$$

of $\mathbb{N}[x, y, z]$ ¹³ with $a = 1$ if R is an isolated vertex and $a = 0$ otherwise, with $a_u = 0$ except if the root of R is a leaf attached to an edge of colour u , and with $a_{u,v}$ counting the number of admissible colourings as above where the root has a first edge of colour u and a distinct last edge of colour v . We have then $v = (1, 0, 0, \dots, 0)$. Formulae for the remaining operators are straightforward but tedious to write down.

5.3 Another family of examples

We consider a (multiplicative) group Γ together with a (generally non-symmetric) generating set \mathcal{S} . We consider edge-colourings with colours in Γ of trees such that $\alpha^{-1}\beta$ is always in \mathcal{S} for an edge of colour α followed cyclically (say in the trigonometric sense) around a non-leaf by an edge of colour β . The first interesting example is given by $\Gamma = \mathbb{Z}/3\mathbb{Z}$ with $\mathcal{S} = \{0, 1\}$. Colours of cyclically consecutive edges remain either the same or increase only by 1.

5.4 Vertex-colourings

The previous examples can be modified to deal with suitable (perhaps improper) vertex-colourings.

6 The language associated to V, E and M

Associativity of M and the fact that V, E, M have different numbers of arguments imply that parentheses are not necessary when constructing rooted trees in terms of the operators V, E and M . Elements of \mathcal{R} correspond thus (not uniquely) to a subset \mathcal{L} of words in $\{V, E, M\}^*$. Final non-empty factors of words in \mathcal{L} contain strictly more occurrences of V than of M . In particular, all words of \mathcal{L} end with V . Moreover, \mathcal{L} is closed under the operations $\mathcal{L} \ni A \mapsto EA$ and $\mathcal{L}^2 \ni (A, B) \mapsto MAB$. The language \mathcal{L} is the smallest language containing V which is closed under these two operations. We denote by \mathcal{L}' the subset of *reduced* words in \mathcal{L} , defined as those elements of \mathcal{L} which involve no trivial constructions of the form $M(V, A)$ or $M(A, V)$. We have $\mathcal{L}' = \mathcal{L} \cap (\{V\} \cup \{EV, E, M\}^*)$. The number e of occurrences of the letter E in an element of \mathcal{L} counts the number of edges in the corresponding rooted tree. The numbers v and m of occurrences of V and M satisfy $v = m + 1$. The set \mathcal{L}' of reduced words gives thus minimal constructions for rooted trees.

An element of \mathcal{L} can always be considered as a construction of a plane rooted tree. Reduced words are in bijection with plane rooted trees decorated by splittings of non-root vertices of (total) degree at least 4 into vertices of degree 3. The root vertex is either of degree at most 2 or is splitted into a root vertex of degree 2 and remaining vertices of degree 3. The number of such splittings at a vertex is given by Catalan numbers: A non-root vertex of degree $d \geq 3$ can be splitted in c_{d-2} different ways with $c_n = \frac{1}{n+1} \binom{2n}{n}$ (and a root vertex of degree $d \geq 2$ can be split in c_{d-1} different ways).

7 Variations

7.1 A definition of local operators reminiscent of operads

Rooted trees can also be constructed using the local operators V and M_k , $k \geq 1$ where $M_k : \mathcal{R}^k \rightarrow \mathcal{R}$ is symmetric in its arguments. It takes k rooted trees, attaches an additional edge at each root, glues the k new trees together at the new root corresponding to the k recently attached leaves. The operators M_k are defined recursively as $M_1 = E$ and

$$M_k = M(E(A_1), M_{k-1}(A_2, \dots, A_k))$$

in terms of the operators E and M considered above. The operators M_k are associative in the obvious sense and satisfy the identity

$$\begin{aligned} & F(M_{k+1}(A_1, \dots, A_k, M_l(B_1, \dots, B_l))) \\ &= F(M_{l+1}(M_k(A_1, \dots, A_k), B_1, \dots, B_l)) . \end{aligned}$$

Except for the absence of an identity, the operators M_k form an operade.

When working with plane trees, the operators M_k are no longer symmetric and we have to add invariance of cyclic permutations of the arguments for $F \circ M_k$.

Local invariants are defined in an obvious way in this context.

7.2 Arbitrary graphs

It is of course possible to define Schrödinger operators for arbitrary (perhaps oriented) simple graphs and to count invertible Schrödinger operators over finite fields. I ignore if there is an efficient way for computing the corresponding numbers.

In a few very small examples, the resulting functions seem also to be polynomial in q . I ignore if this holds in general.

There are two variations on this theme: One can count all invertible matrices with off-diagonal support defining the corresponding graph (diagonal elements are arbitrary). In the case of unoriented graphs, one can moreover require symmetry of all matrices.

Polynomiality gets lost for non-simple graphs: Doubling every edge of a tree we get Schrödinger operators which are diagonal matrices in characteristic 2 and which are, up to a factor 2, Schrödinger operators of the underlying simple trees otherwise. Since $S(T)(2)$ is in general different from 1, the number of such Schrödinger operators over \mathbb{F}_q is no longer polynomial in q .

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