POLYNOMIAL INVARIANTS FOR TREES.
A STATISTICAL MECHANICS APPROACH.

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Abstract

We introduce two "polynomial invariants" for rooted trees and discuss their properties. A statistical mechanics interpretation is pointed out. In particular we show that the partition function of the Ising model, in the simple surface separation ensemble, is a complete invariant.

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1. Introduction.

Trees are interesting objects in many areas of mathematics and physics. They appear not only in combinatorics but also in algebra, in geometry and in analysis. Their interest in physics is mainly due to their use as a geometric space for constructing statistical mechanics models. In this situation a classification theory is in order and, in fact, many beautiful results about their enumeration are well established starting from the classical works of Cayley and Polya [1].

In this brief note we consider a "polynomial strategy" in the same spirit of the polynomial invariants appearing in the theory of knots [2] [3]. One of the motivations of our work is to test that procedure in a simplified framework: trees in fact can be considered as multiple loops in $d = 2$ (Fig. 1):

$$S^1 \sqcup S^1 \sqcup \ldots \sqcup S^1 \hookrightarrow \mathbb{R}^2 \tag{1.1}$$

up to diffeomorphisms in the same way the links are in $d = 3$. The problem of classifying these two-dimensional "links" is enormously simpler than the three-dimensional one since it does not contains the superposition structure of three-dimensional loops projected on a plane; nevertheless, in spite of this simplified picture, the polynomial approach reveals some interesting features mainly because, like for knots, it turns out to be related to statistical mechanics models. For this reason we hope our work will be useful to understand more difficult concepts.

Recently, two interesting proposals on how to construct invariants for trees have appeared in the literature [4] [5]. In the first reference numerical invariants for oriented or rooted trees are discussed via the "contraction-deletion" procedure of graph theory analogous to the "skein" familiar from knot theory. In the second one, the authors present a powerful two-variable polynomial in the more general setting of greedoids which can be used, in particular, to distinguish rooted trees. Our approach is similar to the latter. We use a general algorithm to associate polynomials to rooted trees and we show how they are related to the Ising model. The main theorem we prove establishes a one to one correspondence between rooted trees and a particular two-variable polynomial.

The work is organized as follows: in section 2 we define for each rooted tree two "dually paired" polynomials C and C^* with positive integer coefficients. In section 3 we study the structural meaning of the coefficients of C and C^*; our main result is the injection theorem for the two-variable C polynomial which has the meaning of a "prime decomposition theorem". In section 4 we present some examples which give some insight on the combinatorial properties of the two polynomials, showing that C^* and a particular one-variable evaluation of C are not sufficient to distinguish rooted trees. In section 5 we consider the statistical mechanics interpretation of our polynomials in terms of Ising models; we show that the partition function and the two point correlation functions coincide essentially with our two polynomials. Section 6 collects some general remarks.

2. Polynomial invariants.

A tree is a connected acyclic graph with vertices connected by edges. In this work we consider only finite trees. A rooted tree $\lambda \in \Lambda_3$ is a tree with a marked vertex r called root. Conventionally, we consider an orientation along the edges of the tree directed from the root to the endpoints. It is possible to count elements in Λ_3 with the help of a functional equation for the generating function (see for instance [1]).

For each rooted tree λ there is a natural partial order between the vertices. One says that a vertex v follows a vertex v' ($v > v'$) if they are connected by an oriented path from v' to v. In this way each vertex has a set of first successor vertices $s_{v,1}$ and a set of successor vertices s_v. A vertex is called trivial if $|s_{v,1}| = 1$ and it is called final (leaf) if $|s_{v,1}| = 0$. It is useful to consider also two sets of vertices: the set p_v defined as the set of vertices which have v as successive vertex and ns_v defined as the set of nearest non-trivial successive vertices. For any vertex v of a given tree λ rooted at r we indicate with λ_v the rooted tree which has v as root and is the subgraph of λ induced by s_v; obviously $\lambda = \lambda_r$. We also denote with $\partial\lambda$ the set of final vertices of λ. In a tree there is a natural notion of distance between vertices: $d(v', v'')$ is equal to the number of edges of the shortest path connecting the vertices v' and v''. The presence of the root allows to define the height of a vertex v as its distance from the root $h(v) = d(v, r)$.

Our proposal is to associate to each $\lambda \in \Lambda_3$ the two–variable polynomial C_λ and the one–variable polynomial C^*_λ with positive integer coefficients. They are defined by a recursive procedure: fixed a vertex v we have

$$C_{\lambda_v}(t,a) = \prod_{v' \in s_{v,1}} (C_{\lambda_{v'}}(t,a) + t) \tag{2.1}$$

and

$$C^*_{\lambda_v}(t) = t \sum_{v' \in s_{v,1}} C^*_{\lambda_{v'}}(t) \tag{2.2}$$

with

$$C_{\lambda_{v'}}(t,a) = a, \qquad C^*_{\lambda_{v'}}(t) = 1 \qquad \text{if } v' \text{ is a final vertex} \tag{2.3}$$

and finally

$$C_\lambda(t,a) := C_{\lambda_r}(t,a), \qquad C^*_\lambda(t) := C^*_{\lambda_r}(t). \tag{2.4}$$

The procedure to obtain the C polynomials can be visualized on the tree: we associate to each edge the variable t and to each final vertex the initial condition a. Then, starting from one endpoint, we add the variables we meet going toward the root, until we reach a non trivial vertex where we multiply the polynomial we have obtained with all the polynomials obtained in a similar way along all the paths which meet in the same vertex. If we are arrived to the root, we stop. If not, we continue our procedure adding the new variable along the path, and so on (Fig. 2). The procedure to obtain the C^* polynomial is the same as above up to interchange of sums with products and restricting, without loss of generality, to the case $a = 1$ since $C^*_\lambda(t,a) = aC^*_\lambda(t,1)$.

The next section collects the main properties of our polynomials.

3. Properties.

We start discussing $C_\lambda(t) = C_\lambda(t,0)$ and $C^*_\lambda(t)$, then we consider the general case. Using the fact that the (2.1) and (2.2) give

$$C_{\lambda_v}(t) = \prod_{v' \in ns_v} (C_{\lambda_{v'}}(t) + d(v,v')t) \tag{3.1}$$

$$C^*_{\lambda_v}(t) = \sum_{v' \in ns_v} t^{d(v,v')} C^*_{\lambda_{v'}}(t) \tag{3.2}$$

respectively, it is easy to find the structural meaning of the coefficients of the two polynomials. Associating to each polymomial $C(t)$ the unique arithmetical function $c(n)$ given by the $C(t) = \sum_{n=1}^{\infty} c(n)t^n$ one immediately finds

$$c_{\lambda_v} = \prod_{v' \in ns_v}^{\star} (c_{\lambda_{v'}} + d(v,v')e_1) \tag{3.3}$$

where e_i is the arithmetical function corresponding to the polynomial t^i and the star product is the usual Cauchy convolution product defined by $f \star g(n) = \sum_{k=0}^{n} f(k)g(n-k)$, and

$$c^*_{\lambda_v} = \sum_{v' \in ns_v} (S^{d(v,v')} c^*_{\lambda_{v'}}) \tag{3.4}$$

where S is the one step shift of the arithmetic functions defined by $Se_k = e_{k+1}$. The recursive relation (3.4) can be explicitly integrated and gives:

$$C^*_\lambda(t) = \sum_{h=0}^{\infty} c^*_\lambda(h) t^h, \tag{3.5}$$

with

$$c^*_\lambda(h) = \#\{ \quad \text{final points at height } h \text{ in } \lambda \quad \}; \tag{3.6}$$

it follows that the trees with the same C^* polynomial are exactly those having the same number of final points at each height.

For the other polynomial it is not possible to find such a direct description; nevertheless the minimum and the maximum coefficients have a simple interpretation. Considering

$$C_\lambda(t) = \sum_{k=0}^{\infty} c_\lambda(k) t^k \tag{3.7}$$

one easily see from (3.3) that, defined $D = deg(C_\lambda)$, the following results hold:

$$D = C^*_\lambda(1) = \#\{ \quad \text{final points in } \lambda \quad \}, \tag{3.8}$$

and

$$c_\lambda(D) = \prod_{|s_{v,1}|=0} d(v, v'_v) \tag{3.9}$$

where the product runs over the final points and v'_v is the first nontrivial vertex (or the root) v' (with $v' < v$) which one encounter going from v toward the root.

Analogously, defined d as the minimum power of the variable t appearing in C, one finds that:

$$d = |s_{r,1}|, \tag{3.10}$$

and

$$c_\lambda(d) = \prod_{\{v\}} d(r, v) \tag{3.11}$$

where the product runs over the first nontrivial vertices (or final points) which one encounters along the $|s_{r,1}|$ paths emerging from the root. This results shows that the C polynomial contains the information on the number of final vertices and the number of the branching degree of the root. The meaning of the other coefficients is more involved since they result from sums of products of various contributions according to the convolution prescription.

Remark: for the particular class of trees which are made by a single linear path (a sequence of trivial vertices) with an arbitrary number of final vertices branching from it ("caterpillar" trees) there is an easy correspondence with the "up-right" paths starting from the origin on a square lattice (see Fig. 3); the duality between symmetrical paths with respect to the diagonal is then reflected in the values of $C(t, 0)$ and $C^*(t)$: if λ_1 and λ_2 are two dual caterpillar trees one has (see Fig. 3):

$$C_{\lambda_1}(t, 0) = C^*_{\lambda_2}(t) \tag{3.12}$$

Remark: from the properties above it is clear that the polynomial C^* is trivially bounded by the number n of edges both in the degree and in its value in one. The polynomial C has the same bound in the degree; its value in one can be easily bounded by k^n for some constant k, but this bound is attained only in particular cases.

It is interesting now to point out a result on the range of our maps $\lambda \to C_\lambda$ and $\lambda \to C^*_\lambda$. Calling P_C (resp. P_{C^*}) the set of all C (resp. C^*) polynomials, excluding the case corresponding to the trivial tree (the tree without edges), we have that P_C and P_{C^*} are the smallest subsets of $Z[t]$ satisfying the following properties:

$$
\begin{gathered}
t \in P_C, \\
\text{if} \quad C_1(t), C_2(t) \in P_C \qquad \text{then} \quad C_1(t)C_2(t) \in P_C \\
\text{if} \quad C(t) \in P_C \qquad \text{then} \quad C(t) + t \in P_C
\end{gathered}
\tag{3.13}
$$

and

$$
\begin{gathered}
t \in P_{C^*} \\
\text{if} \quad C^*_1(t), C^*_2(t) \in P_{C^*} \qquad \text{then} \quad C^*_1(t) + C^*_2(t) \in P_{C^*} \\
\text{if} \quad C^*(t) \in P_{C^*} \qquad \text{then} \quad tC^*(t) \in P_{C^*}.
\end{gathered}
\tag{3.14}
$$

Calling $I\!N_0[t]$ the set of all polynomials with positive integer coefficients, which vanish at zero, it can be easily proved that

$$I\!N_0[t] = P_C = P_{C^*}. \tag{3.15}$$

The proof is as follow: considering an element $N(t)$ of $I\!N_0[t]$ we construct a rooted tree λ such that $C_\lambda(t) = N(t)$. The construction is by iteration: being k the lowest power in t we define $N'(t)$ by $N(t) = t^{k-1}(at + N'(t))$ where a is an integer and $N'(t) \in I\!N_0[t]$. This permits us to construct the tree from the root with $k-1$ edges departing from it and an a-long branch. From the leaf of the branch we iterate the procedure to the polynomial $N'(t)$. The construction of a tree for which $C^* = N$ is trivial: for instance the tree without ramification points (other than the root) and with leaves according the theorem (3.5).

We observe that the results (3.8) (3.9) still hold for the two-variable C polynomial, together with the obvious generalizations of (3.13), (3.14).

It immediately follows that

$$C(0, a) = a^D. \tag{3.16}$$

Our main result is the following :

Theorem. The map $\lambda \to C_\lambda(t, a)$ is injective. In other words the two-variable polynomial $C(t, a)$ is a complete invariant for rooted trees.

Proof. Given a polynomial $C_\lambda(t, a)$ for some tree, we have to show that λ can be uniquely determined. We have just seen that we are able to recognize the degree of the root i.e. the number of branches emerging from it. Thus we know that C is the product of exactly d factors C_i of the form

$$a^{D_i} + c_i(t, a) + k_i t \tag{3.17}$$

where D_i, k_i are positive integers, c_i does not contain terms in t, it is of degree $D_i - 1$ (resp. D_i) in a (resp. t) and $c_i(0, a) = 0$. Moreover, C_i is the polynomial C_{λ_i} of a (sub-)tree λ_i with branching degree one. If every C_i is irreducible over the polynomial ring $Z[t, a]$, then the conclusion is a consequence of the fact that there exists a unique such decomposition of C (which corresponds to the decomposition into irreducible factors) and we may uniquely associate a polynomial to each branch. Taking one of these factors, subtracting t and repeating the procedure, the theorem follows by induction on the height of the tree. Therefore it is enough to prove the irreducibility of a polynomial of the form (3.17). This is easily established matching coefficients. In fact, let

$$C_i = (\alpha(a) + \beta(a)t + \gamma(a)t^2 + ...)(\epsilon(a) + \eta(a)t + \theta(a)t^2 + ...). \qquad (3.18)$$

Therefore $\alpha(a) = \alpha_h a^h, \epsilon(a) = \epsilon_k a^k, \alpha_h \epsilon_k = 1, h + k = D_i > 0$ so without loss of generality we may assume $h > 0$, and in the term $\pm(a^h \eta + a^k \beta)t$ the only possibility to get the monomial $k_i t$ is $k = 0, h = D_i$. Thus $\eta(a) = \eta_0$ must be independent of a. Next consider the term $(\alpha_{D_i} a^{D_i} \theta + \beta\eta_0 + \gamma)t^2$, and deduce that $\theta = \theta_0$ is independent of a, and so on. Therefore

$$C_i = (\alpha_{D_i} a^{D_i} + \beta(a)t + \gamma(a)t^2 + ...)(\epsilon_0 + \eta_0 t + \theta_0 t^2 + ...), \qquad (3.19)$$

and the only possibility is $\eta_0 = \theta_0 = ... = 0$ as may be easily recognized by rearranging the first polynomial in decreasing powers of a.

4. Some examples.

Looking at the polynomials $C(t)$, $C^*(t)$, it is easy to recognize that there exist different $\lambda \in \Lambda_3$ with the same $C^*(t)$ polynomial and other trees with the same $C(t)$. A more difficult and interesting problem is to see whether there exist two non isomorphic rooted trees with the same $C(t)$, $C^*(t)$: in Figure 4 we show that this is indeed the case with an example of two 13-vertices trees. This example has the minimum number of vertices since we have checked all trees up to 12 vertices by computer. Another question is whether in this case C and C^* characterize the "structure" of the trees, that is if there exist two trees with only non trivial vertices and the same $C(t, 0)$ and $C^*(t)$. Again the answer is affirmative: an example is given in Figure 5. In the last two examples (Fig. 4 and Fig. 5) the two trees have the same number of vertices, but also this property is not general. In fact in Figure 6 we show an example of a 17-vertex tree and an 18-vertex tree with the same $C(t)$ and $C^*(t)$.

Summarizing these examples: the map $\lambda \to (C_\lambda(t), C^*_\lambda(t))$ is not injective. Also the couple $C(t)$ and $C^*(t)$ not even characterize the number of vertices of a tree nor the trees without trivial vertices. Nevertheless it provide a complete system for rooted trees up to 12 vertices.

5. Ising models on rooted trees.

The Ising model on a general *finite* graph $G = (V, E)$ is usually defined by assigning its energy functional: one consider a spin $\sigma_v \in \{\pm 1\}$ associated to each vertex v and a coupling $j_e \in R$ associated to each edge e. The Hamiltonian, for a given configuration of spins and a fixed configuration of coupling constants, is

$$H(\sigma, j) = -\sum_{e \in E} j_e d\sigma_e \tag{5.1}$$

where $d\sigma_e = \sigma_i \sigma_j$ with $(i, j) = \partial e$; we use these symbols to stress the fact that to a vertex function σ (one-form) we associate an edge function $d\sigma$ (two-form) defined as above.

The statistical properties of the model are encoded in its partition function; for an assigned subset $\mathcal{E}$ (the statistical ensemble) of the full spin configuration space $2^V \equiv \{\pm 1\}^{|V|}$ the partition function is

$$Z_{\mathcal{E}} = \sum_{\sigma \in \mathcal{E}} e^{-\beta H(\sigma, j)} \tag{5.2}$$

where the parameter β, in the statistical mechanics interpetation, is usually understood as the inverse of the absolute temperature. The Gibbs prescription, used in equilibrium statistical mechanics, defines the mean values of the spin functions:

$$\langle f \rangle_{\mathcal{E}} = \sum_{\sigma \in \mathcal{E}} f(\sigma) e^{-\beta H(\sigma, j)} / Z_{\mathcal{E}} \tag{5.3}$$

The choice of the statistical ensemble completely defines the model: we consider here two natural cases for the Ising model on rooted trees. The free ensemble $\mathcal{E}_{C^*} = 2^V$ and the simple surface separation ensemble $\mathcal{E}_C$; this is defined as the set of all the spin configurations with positive value on the root, with negative values on all the final points, and fulfilling the condition that the sign of the spins changes only "once" moving along the paths ($\pi \in \Pi$) connecting the root to the final points; the set of edges on which the signs of the spins change is called the surface separation between the + and the - phase; it correspond to a "trim" ($\tau \in T$) on the tree. It is a classical result in statistical mechanics to express the partition function or the mean values as a series. Defining $\hat{\delta}$ by $\delta + \hat{\delta} = 1$, where δ is the usual Kronecker function, one has $d\sigma = -2\hat{\delta} + 1$. This identity gives the so called low temperature expansion for the partition function

$$Z_{\mathcal{E}_C} = \prod_{e \in E} e^{\beta j_e} \sum_{\tau \in T} \prod_{e \in \tau} e^{-2\beta j_e}, \tag{5.4}$$

which has first been obtained by Peierls ([6]). Considering the identity $e^{\beta d\sigma} = csh(\beta)(1 + d\sigma tgh(\beta))$ one has the high temperature expansion for the correlation which gives:

$$\sum_{p \in \partial\lambda} \langle \sigma(r)\sigma(p) \rangle_{\mathcal{E}_{C^*}} = \prod_{e \in E} csh(\beta j_e) \sum_{\pi \in \Pi} \prod_{e \in \pi} tgh(\beta j_e). \tag{5.5}$$

It is clear that the sums appearing in (5.4) and (5.5) reproduce respectively the C and the C^* algorithms. This is seen as follows: the indipendence of the Hamiltonians for the subtrees connected to a given vertex implies the factorization of the partition function which is just the product rule (2.1); as for C^* the (5.5) gives directly the characterization (3.6). One obtains exactly the two polynomials making the choice that the coupling variables j_e are of two types (j_1, j_2) on (5.4) and take the value j_1 on the final edges and j_2 on all the others. In this case the sum on (5.4) become the $C(t, a)$ polynomial with the identification $t + a = e^{-2\beta j_1}$ and $t = e^{-2\beta j_2}$. To identificate the C^* polynomial the choice to make is simply a coupling variable j on all the edges and the identification is $t = tgh(\beta j)$.

6. Some comments.

In this work we have analyzed two natural polynomials associated to rooted trees and we have discussed the statistical mechanics interpretation; our main result is the one-to-one correspondence between particular two-variable polynomials and rooted trees which result to be respectively the partition functions of an Ising model and the graphs on which that model lives. This interpretation opens the possibility of investigating the fruitful field of the relations between counting problems and statistical mechanics properties; in particular the search for the zeroes of our polynomial and the study of their nature (which is part of the "critical" problem in statistical mechanics), could be related to some of the unsolved counting problems in tree theory. Moreover our analysis has a natural continuation in the study of the behaviour of the "free energy density" function $|\lambda|^{-1} \log Z(\lambda)$ on increasing family of trees; our main theorem sounds as a strong indication that the simple surface separation ensemble should play an important role in the study of the coexistence phenomena for Ising model on rooted trees, like it does in classical cases (see for instance [7]). We hope to return on these questions elsewhere.

We conclude observing that the definitions of our polynomials for rooted trees admit a straightforward extension to labelled rooted trees; by label we mean some extra-structure appended to the vertices or to the edges of the tree which may depend on the structure of the tree (internal label) or may be put on by hand (external label). If one consider the Ising model previously defined, it is clear that one obtains a general external label choosing a generic family of coupling constants, for instance each different from the other. On the other hand one can consider a generic internally labeled C polynomial as

$$\tilde{C}_{\lambda_v} = \prod_{v' \in s_{v,1}} (\tilde{C}_{\lambda_{v'}} + f_{v'}), \tag{6.1}$$

where f_v is an algorithmically computable polynomial of the subtree with root v. In [5] the authors obtain the distinguishing polynomial for rooted directed arborescences with the step-dependent choice

$$f_v = t^{n+1}(z+1)^n \tag{6.2}$$

where n is the number of edges in the subtree of root v, and the initial condition

$$\tilde{C}_{\lambda_v} = t+1 \tag{6.3}$$

if λ_v is the tree with only one edge. We note that with this choice we have $\tilde{C}(t, \frac{1}{t}-1) = C(t,1)$.

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