Enumeration of spanning trees and forests in graphs

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Introduction

The results of this exposition are joint with my colleagues Young Soo Kwon, Lilya Grünewald and Ilya Mednykh. In this presentation we investigate the infinite family of circulant graphs $C_n(s_1, s_2, \ldots, s_k)$. We present an explicit formula for the number of spanning trees, rooted spanning forests and the Kirchhoff index for this family of graphs. Then we investigate arithmetical and asymptotic properties of the obtained numbers. All formulas are given in terms of the Chebyshev polynomials. We start with some basic definitions.

Spanning trees and forests

Consider a finite undirected graph G without loops, possibly with multiple edges.

A *spanning forest* F in G is an uncyclic subgraph that contains all vertices of G. All connected components of F are trees. A spanning forest F is called *rooted* if any tree in F has a *root*, that is a labeled vertex.

Connected spanning forest is a *spanning tree*.

Number of rooted spanning trees in a connected graph G is $n\tau(G)$, where $\tau(G)$ is the number of all spanning trees or just complexity of graph G and n is the number of vertices of G. This simple observation is not true anymore for the number of spanning forests.

To count the number of rooted spanning forests in a graph G and to count the number of all spanning forests in G are completely different problems. In spite of there are about one thousand papers devoted to enumeration of spanning trees, there are just a very few papers devoted to spanning forests.

Spanning trees and forests

Consider a finite graph G without loops. We denote the vertex and edge set of G by V(G) and E(G), respectively. Given $u, v \in V(G)$, we set a_{uv} to be equal to the number of edges between vertices u and v. The matrix $A = A(G) = \{a_{uv}\}_{u,v \in V(G)}$ is called the adjacency matrix of the graph G. The degree d(v) of a vertex $v \in V(G)$ is defined by $d(v) = \sum_{u \in V(G)} a_{uv}$. Let D = D(G) be the diagonal matrix indexed by the elements of V(G)with $d_{vv} = d(v)$. The matrix L = L(G) = D(G) - A(G) is called the Laplacian matrix, or simply Laplacian, of the graph G. By I_n we denote the identity matrix of order n = |V(G)|. Let $\chi_G(\lambda) = \det(\lambda I_n - L(G))$ be the characteristic polynomial of the Laplacian matrix of the graph G.

Laplacian. Useful observation

Let $f:V(G)=\{v_1,v_2,\ldots,v_n\}\to\mathbb{C}$ be a function defined on the vertices of graph G. Suppose that function f is harmonic, that is

$$L(G).(f(v_1), f(v_2), \ldots, f(v_d))^t = 0.$$

Then for each vertex $v \in V(G)$ of degree d = d(v) and its neighbors w_1, w_2, \ldots, w_d we have

$$f(v) = \frac{1}{d}(f(w_1) + f(w_2) + \cdots + f(w_d)).$$

Spanning trees and forests

Recall geometrical meaning of coefficients of the characteristic polynimial

$$\chi_G(\lambda) = \lambda^n + c_{n-1}\lambda^{n-1} + \ldots + c_2\lambda^2 + c_1\lambda.$$

The theorem by Kelmans and Chelnokov (1974) states that the absolute value of coefficient c_k of $\chi_G(\lambda)$ coincides with the number of rooted spanning k—forests in the graph G. By Bezout's theorem, the sequence c_k is alternating. So, the number of rooted spanning forests of the graph G can be found by the formula

$$f_G(n) = f_1 + f_2 + \ldots + f_n = |c_1 - c_2 + c_3 - \ldots + (-1)^{n-1}|$$

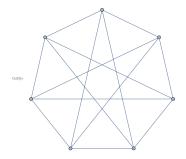
= $(-1)^n \chi_G(-1) = \det(I_n + L(G)).$

This result was independently obtained by many authors (P. Chebatorev, E. Shamis, O. Knill and others).

The famous Kirchhoff's Matrix Tree Theorem (1847) states that $c_1 = n \tau(G)$, where $\tau(G)$ is the number of spanning trees in G.

Circulant graphs

A typical example of circulant graphs is graph $C_n(1,3)$.



Circulant graphs

Circulant graphs can be described in a few equivalent ways:

- (a) The automorphism group of the graph includes a cyclic subgroup that acts transitively on the graph's vertices.
- (b) The graph has an adjacency matrix that is a circulant matrix.
- (c) The graph is a Cayley graph of a cyclic group.

Isomorphism problem for circulant graphs

In spite of simple definition, the isomorphism problem for circulant graphs was solved just recently:

M. Muzychuk, "A solution of the isomorphism problem for circulant graphs". Proc. Lond. Math. Soc. (3) 88 (2004) 1–41.

Also, it was shown that circulant graphs are recognizable from the set of all graphs in polynomial time:

Evdokimov, Sergei; Ponomarenko, Ilia . "Recognition and verification of an isomorphism of circulant graphs in polynomial time". St. Petersburg Math. J. 15: (2004) 813–835.

- (a) The circulant graph $C_n(s_1, \ldots, s_k)$ with jumps s_1, \ldots, s_k is a graph with n vertices labeled $0, 1, \ldots, n-1$ where each vertex i is adjacent to 2k vertices $i \pm s_1, \ldots, i \pm s_k \mod n$.
- (b) *n*-cycle graph $C_n = C_n(1)$.
- (c) *n*-antiprism graph $C_{2n}(1,2)$.
- (d) *n*-prism graph $Y_n = C_{2n}(2, n)$, *n* odd.
- (e) The Moebius ladder graph $M_n = C_{2n}(1, n)$.
- (f) The complete graph $K_n = C_n(1, 2, \dots, \lfloor \frac{n}{2} \rfloor)$.
- (g) The complete bipartite graph $K_{n,n} = C_n(1,3,\cdots,2[\frac{n}{2}]+1)$.

Kirchhoff theorem

By the celebrated Kirchhoff theorem, the number of spanning trees $\tau(n)$ is equal to the product of nonzero eigenvalues of the Laplacian of a graph $C_n(s_1,s_2,\ldots,s_k)$ divided by the number of its vertices n. To investigate the spectrum of Laplacian matrix, we denote by $T=circ(0,1,\ldots,0)$ the $n\times n$ shift operator. Consider the Laurent polynomial

$$L(z) = 2k - \sum_{i=1}^{k} (z^{s_i} + z^{-s_i}).$$

Then the Laplacian of $C_n(s_1, s_2, \ldots, s_k)$ is given by the matrix

$$\mathbb{L} = L(T) = 2kI_n - \sum_{i=1}^{k} (T^{s_i} + T^{-s_i}).$$

Kirchhoff theorem

Recall that circulant matrix T is diagonisable and conjugate to $\mathbb{T}=diag(1,\varepsilon_n,\ldots,\varepsilon_n^{n-1})$, where $\varepsilon_n=\exp(2\pi i/n)$. Hence, all the Laplacian eigenvalues of G are given by the formula

$$\lambda_j = L(\varepsilon_n^j) = 2k - \sum_{i=1}^k (\varepsilon_n^{js_i} + \varepsilon_n^{-js_i}), j = 0, 1, \dots, n-1.$$

By the Kirhhoff theorem we get

$$\tau(n) = \frac{1}{n} \prod_{j=1}^{n-1} L(\varepsilon_n^j).$$

This is a very beautiful formula, but absolutely useless for computations for large values of n.

How to make it suitable for numerical and analytical calculation?



Enumeration of spanning trees

Theorem

The number of spanning trees in the circulant graph $C_n(s_1, s_2, ..., s_k)$ is given by the formula

$$\tau(n) = \frac{n}{q} \prod_{p=1}^{s_k-1} |2 T_n(w_p) - 2|,$$

where $q = s_1^2 + s_2^2 + \ldots + s_k^2$ and w_p , $p = 1, 2, \ldots, s_k - 1$ are different from 1 roots of the equation $\sum_{j=1}^k T_{s_j}(w) = k$, and $T_k(w)$ is the Chebyshev polynomial of the first kind.

The Chebyshev polynomial of the first kind is defined as

$$T_n(z) = \cos(n \arccos(z)).$$

Enumeration of spanning forests

A similar result take a place for the numbers of rooted spanning forests of circulant graph $C_n(s_1, s_2, ..., s_k)$ in terms of Chebyshev polynomials.

Theorem

The number of rooted spanning forests $f_G(n)$ in the circulant graph $G=C_n(s_1,s_2,\ldots,s_k),\, 1\leq s_1< s_2<\ldots< s_k<\frac{n}{2},$ is given by the formula

$$f_G(n) = \prod_{p=1}^{s_k} |2T_n(w_p) - 2|,$$

thereby w_p , $p=1,2,\ldots,s_k$ are roots of the algebraic equation $\sum_{j=1}^k (2T_{s_j}(w)-2)=1$, where $T_s(w)$ is the Chebyshev polynomial of the first kind.

The main idea of the proof

The matrix $I_n + L(G)$ has the following eigenvalues

$$\mu_{j} = P(\varepsilon_{n}^{j}) = 2k + 1 - \sum_{i=1}^{k} (\varepsilon_{n}^{js_{i}} + \varepsilon_{n}^{-js_{i}}), j = 0, \dots, n-1.$$

Hence we have
$$f_G(n) = \det(I_n + L(G)) = \prod_{j=0}^{n-1} P(\varepsilon_n^j)$$
.

As $P(z) = P(\frac{1}{z})$, its roots are $z_1, \frac{1}{z_1}, \dots, z_{s_k}, \frac{1}{z_{s_k}}$ and we obtain

$$\prod_{i=0}^{n-1} P(\varepsilon_n^i) = \operatorname{Res}(P(z), z^n - 1) = |\operatorname{Res}(z^n - 1, P(z))|$$

$$= |\prod_{p=1}^{s_k} (z_p^n - 1)(z_p^{-n} - 1)| = |\prod_{p=1}^{s_k} (2T_n(w_p) - 2)|.$$

Finally, we use the identity $T_n(\frac{1}{2}(z+z^{-1})) = \frac{1}{2}(z^n+z^{-n})$.

Here $w_p = \frac{1}{2}(z_p + \frac{1}{z_p}), \ p = 1, \dots, s_k$. These numbers are the roots of

algebraic equation
$$\sum\limits_{j=1}^{k}(2T_{j}(w)-2)=1.$$



Generating function for the number of spanning trees

We also have the following theorem.

Theorem

Let $\tau(n)$ be the number of spanning trees in the circulant graph $C_n(s_1, s_2, \ldots, s_k)$ of even valency. Then

$$F(x) = \sum_{n=1}^{\infty} \tau(n) x^n$$

is a rational function with integer coefficients. Moreover, F(x) = F(1/x).

(This result was initiated by S.K. Lando).

Generating function. Examples

Graph $C_n(1,2)$. We have $\tau_{1,2}(n) = nF_n^2$, where F_n is the *n*-th Fibonacci number. Hence,

$$\sum_{n=1}^{\infty} \tau_{1,2}(n) x^n = \frac{1 - 2w + 2w^2}{(1+w)(-3+2w)^2}, \text{ where } w = \frac{1}{2}(x+\frac{1}{x}).$$

Graph $C_n(1,3)$. Here we have

$$\sum_{n=1}^{\infty} \tau_{1,3}(n) x^n = \frac{(1+w)(1-w-2w^2+11w^3+8w^4-16w^5+4w^7)}{2(-1+w)(-1-3w-3w^2+2w^4)^2}.$$

Arithmetic properties of the complexity for circulant graphs

It was noted in some recent papers that in many cases the complexity of circulant graphs is given by the formula $\tau(n) = na(n)^2$, where a(n) is an integer sequence. In the same time, this is not always true.

The aim of the next theorem is to explain this phenomena. Recall that any positive integer p can be uniquely represented in the form $p=q\,r^2$, where p and q are positive integers and q is square-free. We will call q the square-free part of p.

Theorem

Let $\tau(n)$ be the number of spanning trees in the circulant graph $C_n(s_1,s_2,\ldots,s_k),\ 1\leq s_1< s_2<\ldots< s_k<\frac{n}{2}.$ Denote by p the number of odd elements in the sequence s_1,s_2,\ldots,s_k and let q be the square-free part of p. Then there exists an integer sequence a(n) such that

$$1^0$$
 $\tau(n) = n a(n)^2$, if n is odd;

$$2^0$$
 $\tau(n) = q n a(n)^2$, if n is even.

Arithmetic properties of the number of rooted spanning forests

The main idea from the previous theorem gives us the following result.

Theorem

Let $f_G(n)$ be the number of spanning forests in the circulant graph

$$C_n(s_1, s_2, \ldots, s_k).$$

Denote by p the number of odd elements in the sequence s_1, s_2, \ldots, s_k and let q be the square-free part of 4p+1. Then there exists an integer sequence a(n) such that

- $1^0 \ f_G(n) = a(n)^2$, if n is odd;
- 2^{0} $f_{G}(n) = q a(n)^{2}$, if n is even.

The sketch of the proof

Since $\mu_j = P(\varepsilon_n^j) = P(\varepsilon_n^{n-j}) = \mu_{n-j}, j = 0, \dots, n-1,$ all eigenvalues of the matrix $I_n + L(G)$ (possibly, except the middle ones)

are coming twice. Hence $f_G(n) = \prod_{j=0}^{n-1} \mu_j$ is equal to $\left(\prod_{j=0}^{\frac{n-1}{2}} \mu_j\right)^2$ if n is odd

and to $\mu_{\frac{n}{2}} \left(\prod_{j=0}^{\frac{n}{2}-1} \mu_j\right)^2$ if n is even. In both cases, the squaring numbers are products of Galois conjugate algebraic numbers. So, they are integers.

To finish the proof, we note the middle term $\mu_{\frac{n}{2}} = P(-1) = 4p + 1$, where p the number of odd elements in the sequence s_1, s_2, \ldots, s_k .

Then the result follows.

Asymptotic for the number of spanning trees

In this section we give asymptotic formulas for the number of spanning trees in circulant graphs.

Theorem,

Let $\gcd(s_1, s_2, \ldots, s_k) = 1$. Then the number of spanning trees in the circulant graph $C_n(s_1, s_2, \ldots, s_k)$, $1 \le s_1 < s_2 < \ldots < s_k < \frac{n}{2}$ has the following asymptotic

$$au(n) \sim rac{n}{q} A^n$$
, as $n o \infty$,

where $q=s_1^2+s_2^2+\ldots+s_k^2$ and $A=\exp(\int_0^1\log|L(e^{2\pi it})|dt)$ is the

Mahler measure of Laurent polynomial $L(z) = 2k - \sum_{i=1}^{k} (z^{s_i} + z^{-s_i})$.



Asymptotics for the number of rooted spanning forests

Now we present asymptotic formulas for the number of rooted spanning forests in circulant graphs.

Theorem

The number of rooted spanning forests in the circulant graph $G = C_n(s_1, s_2, \ldots, s_k), 1 \le s_1 < s_2 < \ldots < s_k < \frac{n}{2}$ has the following asymptotic

$$f_G(n) \sim A^n$$
, as $n \to \infty$

where $A = \exp(\int_0^1 \log(L(e^{2\pi it}))dt)$ is the Mahler measure of Laurent polynomial $P(z) = 2k + 1 - \sum_{i=1}^k (z^{s_i} + z^{-s_i})$.

Kirhhoff index for circulant graphs

The Kirchhoff index of G originally was defined by Klein and Randić (1993) as a new distance function named resistance distance framed in terms of electrical network theory. More precisely, let vertices of the graph G are labeled by $1, 2, \ldots, n$. Then the resistance distance between vertices i and j, denoted by $r_{ij} = r_{ij}(G)$ is defined to be the effective electrical resistance between them when unit resistors are placed on every edge of G. Define

$$Kf(G) = \sum_{1 \le i < j \le n} r_{ij}$$

to be the Kirchhoff index of ${\it G}$. The motivation for such a definition was a famous Wiener

$$W(G) = \sum_{1 \leq i < j \leq n} d_{ij},$$

where d_{ij} is the distance between vertices i and j. Klein and Randić proved that $Kf(G) \leq W(G)$ with equality, if and only if G is a tree.

There is a a nice relationship discovered independently by I.Gitman, B.Mohar (1996) and by H.Y.Zhu, D.J.Klein, I.Lukovits (1996) between the Laplacian spectrum and the Kirchhoff index given by the formula

$$Kf(G) = n \sum_{j=1}^{n-1} \frac{1}{\lambda_j}.$$

Here, $0 = \lambda_0 < \lambda_1 \leq \ldots \leq \lambda_{n-1}$ are the Laplacian eigenvalue of G.

In this section, we give an explicit formula for the Kirchhoff index $Kf(G_n)$ in the circulant graph $G_n = C_n(s_1, s_2, \ldots, s_k)$, $1 \le s_1 < s_2 < \ldots < s_k < n/2$. We present the formula for $Kf(G_n)$ as a sum of s_k terms, each given by a combination of the n-th Chebyshev polynomials evaluated at the roots of some prescribed polynomial of degree s_k .

Theorem

$$Kf(G_n) = \frac{n}{6\sum_{j=1}^k s_j^2} (n^2 - \frac{\sum_{j=1}^k s_j^4}{\sum_{j=1}^k s_j^2}) + \sum_{p=2}^{s_k} \frac{n U_{n-1}(w_p)}{(1 - T_n(w_p))Q'(w_p)},$$

where w_p are all the roots different from 1 of the polynomial $Q(w) = \sum_{j=1}^k (2 - 2T_{s_j}(w)), \quad T_n(w) = \cos(s \arccos w)$ and $U_{n-1}(w) = \sin(n \arccos w)/\sin(\arccos w)$ are the Chebyshev polynomials of the first and the second kinds respectively.

The main idea of the proof. Use residues!

Lemma

Let P(z) and Q(z) be polynomials of degree n and m respectively with simple roots. Denote the rootes of P(z) by $\alpha_1, \alpha_2, \ldots, \alpha_n$, and roots of Q(z) by $\beta_1, \beta_2, \ldots, \beta_m$. Suppose that P(z) and Q(z) share the unique common root $\alpha_1 = \beta_1 = 1$. Then

$$\sum_{j=2}^{n} \frac{1}{Q(\alpha_j)} = -\operatorname{Res}_{z=1} \frac{1}{Q(z)} \frac{P'(z)}{P(z)} - \sum_{j=2}^{m} \frac{1}{Q'(\beta_j)} \frac{P'(\beta_j)}{P(\beta_j)}.$$

Proof easily follows from the identity

$$\frac{1}{2\pi i} \int\limits_{|z|=R} \frac{1}{Q(z)} \frac{P'(z)}{P(z)} dz = 0.$$

In our case,
$$P(w) = T_n(w) - 1$$
 and $Q(w) = \sum_{i=1}^k (2 - 2T_{s_i}(w))$.

As a corollary, we obtain that the asymptotical behavior of the Kirchhoff index is for the graph $G_n = C_n(s_1, s_2, ..., s_k)$ given by the formula

Corollary

$$Kf(G_n) = \frac{n}{6\sum_{j=1}^k s_j^2} (n^2 - \frac{\sum_{j=1}^k s_j^4}{\sum_{j=1}^k s_j^2}) + \sum_{p=2}^{s_k} \frac{2n^2}{Q'(w_p)\sqrt{w_p^2 - 1}} + O(\frac{n^2}{A^n}), n \to \infty,$$
 where w_p are all the roots different from 1 of the polynomial $Q(w) = \sum_{j=1}^k (2 - 2T_{s_j}(w)), \quad T_s(w)$ is the Chebyshev polynomial of the first kind and $A, A > 1$ is a constant depending only of s_1, s_2, \ldots, s_k .

Similar results are also obtained for the circulant graph $C_{2n}(s_1, s_2, \ldots, s_k, n)$ with odd valance of vertices and for direct product $C_n(s_1, s_2, \ldots, s_k) \times P_2$, where P_2 is the path graph on two vertices.

Cyclic graph C_n .

- (i) Number of trees: $\tau(C_n) = n$
- (ii) Number of rooted spanning forests:

$$f(C_n) = 2(T_n(3/2) - 1) = \tau(W_n),$$

where W_n is the wheel graph.

(iii) Kirchhoff index: $Kf(C_n) = \frac{n^2 - n}{12}$.

(i) Möbius Ladder $M_n = C_{2n}(1, n)$.

$$Kf(M_n) = \frac{n^3-n}{6} + \frac{n^2 \tanh(\frac{n}{2}\operatorname{arccosh} 2)}{\sqrt{3}}.$$

(G. Baiganakova, A. Mednykh (2019) and Z. Cinkir (2016)).

(ii) Prism graph $Pr_n = C_n \times P_2$.

$$Kf(Pr_n) = \frac{n^3 - n}{6} + \frac{n^2 \coth(\frac{n}{2}\operatorname{arccosh} 2)}{\sqrt{3}}.$$

(G. Baiganakova, A. Mednykh (2019) and Z. Cinkir (2017)).

Graph $C_n(1,2)$. By the above Theorems, we have $\tau(n) = nF_n^2$, where F_n is the n-th Fibonacci number.

Set
$$w_1 = \frac{1}{4}(-1 + \sqrt{29})$$
 and $w_2 = \frac{1}{4}(-1 - \sqrt{29})$. Then

$$f_{C_n(1,2)} = |2T_n(w_1) - 2| \cdot |2T_n(w_2) - 2| \sim A^n, n \to \infty,$$

where $A = \frac{1}{4}(7 + \sqrt{5} + \sqrt{38 + 14\sqrt{5}}) \simeq 4.3902568...$

Also, the Kirchhoff index is given by the formula

$$Kf_{C_n(1,2)}(n) = \frac{1}{300}n(5n^2 - 17)F_n^2 + \frac{n^2F_{2n}}{25F_n^2}.$$

We note that $F_{2n}/F_n^2 = \sqrt{5} + O(1/\phi^{2n})$, where $\phi = (1 + \sqrt{5})/2$ is the golden ratio.



Graph $C_n(1,3)$. Kirchhoff index of $C_n(1,3)$ has the following asymptotics

$$Kf(C_n(1,3)) = \frac{n}{600}(5n^2 + 6\sqrt{110 + 50\sqrt{5}}n - 41) + O(\frac{n^2}{A^n}), \ n \to \infty,$$

where
$$A = \sqrt{\frac{1}{2}(1+\sqrt{5}+\sqrt{2(1+\sqrt{5})})} \simeq 1.700015\ldots$$

By the above theorem, we have an explicit formula for the number of spanning trees

$$\tau(n) = \frac{2n}{5} \left(T_n \left(-\frac{1}{2} - \frac{i}{2} \right) - 1 \right) \left(T_n \left(-\frac{1}{2} + \frac{i}{2} \right) - 1 \right)$$

and the formula for the number of rooted spanning forests

$$f(n) = (2T_n(w_1) - 2)(2T_n(w_2) - 2)(2T_n(w_3) - 2),$$

where w_1 , w_2 and w_3 are the roots of $8w^3 - 4w - 5 = 0$. This leads to the interesting observation: $f(n) = a(n)^2$, where a(n) is an integer sequence.

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