Spectral Invariants from Embeddings

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Outline

1. Polynomials from Good Cycles
   - Characteristic Polynomial
   - The Matching Polynomial
   - The Psicle Polynomial
2. Discrete Quantum Walks
   - Arc Reversal
   - Two Reflections

Outline

Remark

The work in this section is joint with Krystal Guo and Harmony Zhan.

Coefficients

The characteristic polynomial $\phi(X, t)$ of a graph X is $\det(tI - A)$.

Definition

A basic subgraph of a graph is a subgraph such that each component is an edge or a cycle. The weight $\mathrm{wt}(\beta)$ of a basic subgraph β with k components, of which c are cycles, is $(-1)^k 2^c$.

Theorem

The coefficient of t^{n-r} in $\phi(X, t)$ is the sum of the weights of the basic subgraphs of X with exactly r vertices.

Closed walks

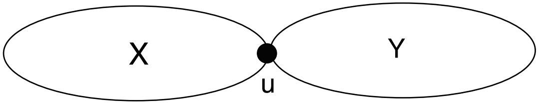
If $u \in V(X)$, the number of closed walks in X of length k starting u is $(A^k)u, u$. We denote the generating function for these walks by $W_{u,u}(X, t)$ it can be expressed in terms of characteristic polynomials:

Theorem

If $u \in V(X)$, then

$$t^{-1}W_{u,u}(X, t^{-1})\frac{\phi(X \setminus u, t)}{\phi(X, t)}.$$

1-Sums



Definition

If Z is a graph with induced subgraphs X and Y such that $V(Z) = V(X) \cup V(Y)$ and $V(X) \cap V(Y) = \{u\}$ for some vertex u, we say Z is the 1-sum of X and Y at u.

Characterisitic polynomial of a 1-sum

If Z is the 1-sum of X and Y at the vertex u, then $\phi(Z,t)$ is equal to

$$\phi(X \setminus u,t)\phi(Y,t) + \phi(X,t)\phi(Y \setminus u,t) - t\phi(X \setminus u,t)\phi(Y \setminus u,t).$$

Zeros

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(How many proofs of this can you provide?)

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Hence if X is a tree, $\phi(X, t) = \mu(X, t)$.

Splitting closed walks into loops

Definition

Consider a closed walk in a graph. Each time the walks returns to a vertex it creates a directed cycle of length at least two. We refer to the sequence of cycles created by a closed walk as its loop decomposition.

A loop of length two is just an edge. A walk with no edges in its loops decomposition is often referred to as a reduced walk.

Tree-like Walks

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As we might hope, any closed walk in a tree is tree-like.

Generating functions for tree-like walks

Theorem

If $C_u(X,t)$ is the generating function for the closed tree-like walks in X that start at u, then

$$t^{-1}C(X,t^{-1}) = \frac{\mu(X\setminus u,t)}{\mu(X,t)}.$$

Zeros

Theorem (Heilmann and Lieb)

The zeros of the matching polynomial are real.

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Good cycles from embeddings

Assume that we are given a cellular embedding of our graph X in some surface. The good cycles relative to this embedding are the cycles that are contractible. Let $\mathcal{B}$ denote the set of basic graphs of X that consist of edges and good cycles relative to the embedding.

Definition

The psicle polynomial of X relative to an embedding is

$$\psi(X,t) = \sum_{\beta \in \mathcal{B}} \mathrm{wt}(\beta).$$

Properties of the psicle polynomial

- Since every graph has a cellular embedding with no faces, $\mu(X,t)$ is a cycle polynomial.
- There is a 1-sum recurrence.
- The psicle polynomial gives rise to a generating function for a class of walks.

One problem

Question

What can we say about the distribution of the zeros of psicle polynomials.

The zeros need not be real, so we are asking about the distribution in the complex plane.

Outline

Remark

This section is joint work with Harmony Zhan (mostly from Godsil, Zhan: arXiv:1701.04474).

Random walks

A random walk on a graph X is specified by a matrix P, with rows and columns indexed by $V(X)$. More precisely it is determined by the sequence of matrices P^k for $k = 0, 1, \ldots$.

Each of these matrices is row stochastic, hence each row specifies a probability density on $V(X)$.

Quantum walks

To specify a quantum walk we start with a unitary matrix U. In place of the matrices P^k we work with the Schur products

$$M(k) = U^k \circ \overline{U}^k.$$

Since U is unitary, $M(k)$ is doubly stochastic and so, for each non-negative integer k the rows of $M(k)$ describe probability densities on $V(X)$. We call U the transition matrix of the quantum walk, and the matrices $M(k)$ are the mixing matrices of the walk.

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By way of example, we might ask if there is a time k such that entries of the u-row are all equal?

A constraint

- For physical reasons, our transition matrix U should be sparse.
- An obvious approach would be to use a weighted adjacency matrix but, in general, it is not possible to produce a unitary matrix by weighting an adjacency matrix. [Severini]
- In practice, most quantum walks are defined on the arcs of some graph.

Arc-reversal walks

For an arc-reversal walk on a graph X, the transition matrix U is a product of two unitary matrices S and C.
The first matrix S is a permutation that maps each arc to its reverse.
The second matrix C is block-diagonal, with blocks indexed by the vertices of X. The i-th block C_i is unitary matrix of order $d_i \times d_i$, where d_i is the valency of vertex i. One simple and useful choice is

$$C_i = \frac{2}{d_i} J - I.$$

The matrices C_i are usually referrred to as coins, and the choice just given is known as the Grover coin.

Some parameters of a discrete walk

- Mixing time.

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- The average mixing matrix:

$$\widehat{M} = \lim_{L\to\infty} \frac{1}{L} \sum_{k\leq L} U^k \circ \overline{U}^k.$$

- The rows of $\widehat{M}$ provide one probablity density for each vertex of X, and hence each vertex of X has an entropy associated with it.

Graph invariants

If we take all coins in the arc-reversal walk to be the Grover coin, we can view the spectrum of U as a graph invariant.

Emms et al proposed an algorithm for isomorphism of strongly regular graphs. It is based on a walk using the Grover coin: their invariant is the characteristic polynomial of the matrix obtained from U^3 by setting positive entries equal to 1 and non-positive entries to 0.

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It doesn't work. [Godsil, Guo, Myklebust: arXiv:1511.01962]

Shunt decompositions

For regular graphs there is a generalization of the arc-reversal model. Suppose X is d-regular. A shunt decompostion of X is a collection of permutation matrices $P_1, \ldots, P_d$ such that

$$A = P_1 + \cdots + P_d$$

Now let S be the permutation matrix with $P_1, \ldots, P_d$ as diagonal blocks and let C be a coin matrix as before. Then $U = SC$ describes a quantum walk.

Outline

A difficulty

- To successfully analyse properties of a discrete quantum walk, we need to work in the algebra generated by S and C. For general graphs this currently impossible, unless each coin is an involution, whence $C^2 = I$.

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- To successfully analyse properties of a discrete quantum walk, we need to work in the algebra generated by S and C. For general graphs this currently impossible, unless each coin is an involution, whence $C^2 = I$.
- If we use Grover coins, then the coin matrix C in the arc-reversal walk is an involution.
- For shunt decompositions neither S nor C has order two in general. The permutation matrix S is an involution if and only if the shunt decomposition is a 1-factorization.

Why two reflections help

Suppose $U = MN$, where M and N are symmetric involutions. Then U is diagonalizable.

Lemma

If z is an eigenvector for U with eigenvalue λ, then the span of $\{z, Nz\}$ is invariant under $\langle M, N\rangle$.

Proof.

Since $N^2 = I$, the set $\{u, Nu\}$ is N-invariant. As $MNz = \lambda z$ and $\lambda \neq 0$, we have $Mz = \lambda^{-1} Nz$. As $MNz = \lambda z$, we see that $\{z, Nz\}$ is M-invariant. □ □

Reflections from partitions

If π is a partition of a set E, we define P_π to be orthogonal reflection onto the space of functions on E that are constant on the cells of π.
If P is a projection then $P^2 = P$ and $(2P - I)^2 = I$.

Lemma

If π_1 and π_2 are partitions of E with corresponding projections P_1 and P_1, then

$$U = (2P_1 - I)(2P_2 - I)$$

is unitary and hence determines a discrete quantum walk on E.

Face-vertex walks

[The following construction is due to H. Zhan.]

Suppose we have a cellular embedding of X in an oriented surface. Let π_1 be the partition whose cells are the sets of arcs with a given start vertex. Let π_2 be the partition whose cells are the set of arcs for which a given face lies on the left (as move along the arc). Then this pair of partitions determines a discrete quantum walk.

We call this a face-vertex walk.

The Problem

The description of a discrete quantum walk on a graph requires that we specify extra structure—in fact, a linear order on the arcs leaving a vertex. We can provide this extra structure by shunt decompositions or embeddings.

The basic task is to relate properties of the walk with the underlying combinatorial structure.

The End(s)