Zeta functions of graphs and Kirchhoffian indices

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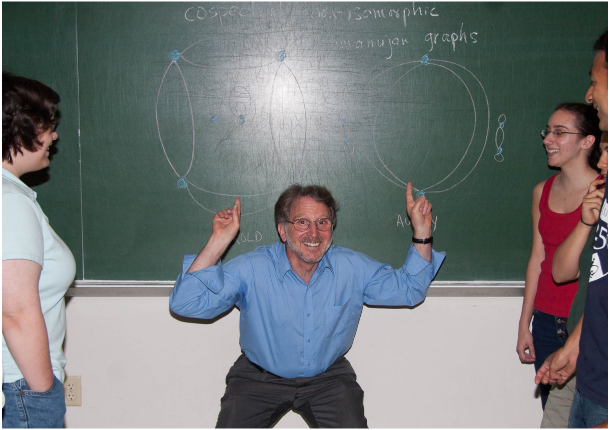
graphs

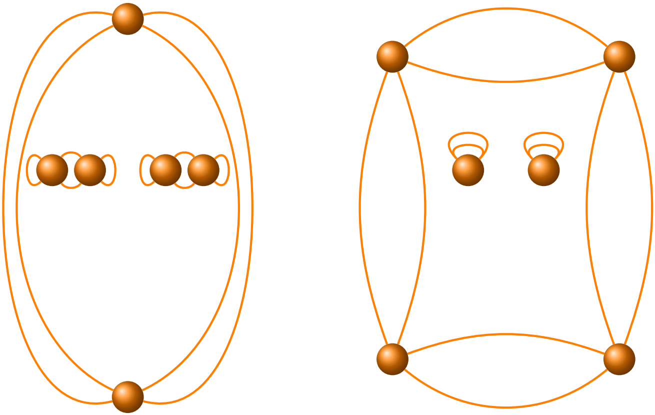

Figure: Audrey and Harold

Non-isomorphic, cospectral graphs; same zeta function

Important matrices

$G = (V(G), E(G))$ is an undirected connected graph.
May have multiple edges and/or loops.
$|V(G)| = n$; $|E(G)| = m$
Label the vertices of G: $v_1, \ldots, v_n$

- *Adjacency matrix* $\mathbf{A} = (a_{ij})$ with

$$a_{ij} = \text{number of edges between } v_i \text{ and } v_j$$

$$a_{ii} = \text{twice the number of loops at vertex } v_i.$$

  $\mathbf{A}$ is a symmetric matrix so it has real eigenvalues.

- *Degree matrix* $\mathbf{D} = \text{diag}(d_1, \ldots, d_n)$ where d_i = degree of vertex v_i.

$$d_i = \text{number of neighbors of } v_i \text{ plus twice number of loops at } v_i$$

Important matrices

- *Laplacian matrix* $\mathbf{L} = \mathbf{D} - \mathbf{A}$
  $\mathbf{L}$ is not affected by loops
  $\mathbf{L}$ is symmetric with row sums $= 0$
  $\mathbf{L}$ is positive semidefinite so its eigenvalues $\mu_1, ..., \mu_n$ are ≥ 0.
  $\mu_1 = 0$ is an eigenvalue of $\mathbf{L}$ with multiplicity 1.
- *Normalized Laplacian matrix* $\mathbf{N} = \mathbf{D}^{-\frac{1}{2}}\mathbf{L}\mathbf{D}^{-\frac{1}{2}}$
  $\mathbf{N}$ is symmetric
  $\mathbf{N}$ is positive semidefinite so its eigenvalues $\nu_1, ..., \nu_n$ are ≥ 0
  $\nu_1 = 0$ is an eigenvalue of $\mathbf{N}$ with multiplicity 1

Spanning trees

Spanning tree of G: a connected subgraph on all the vertices of G, that contains no closed paths (tree)

Theorem (Matrix tree theorem)

The number of spanning trees of G equals any cofactor of $\mathbf{L}$.

Ihara zeta function

Analogous to the Dedekind zeta function: for a connected graph G, the Ihara zeta function of G is

$$Z(u) = \prod_{[C]} (1 - u^{|C|})^{-1}$$

where $[C]$ runs over all prime cycles of G and $|C|$ is the length of C.
Prime cycles:

- Starting point does not matter
- Direction matters
- No backtracking or tails
- Primitive

Pendant edges don't matter.

Ihara zeta function

Theorem (Bass, 1992)

$$Z(u)^{-1} = (1-u^2)^{m-n}\det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D}-\mathbf{I}_n))$$

Consequence: $Z(u)$ is the reciprocal of a polynomial of degree $2m$.

Dedekind zeta function

The Dedekind zeta function of a number field encodes:

- the degree
- the discriminant
- the number of roots of unity
- the number of real and complex embeddings
- the product of the class number and the regulator
- the list of residual degrees of the extension primes

Ihara zeta function

If G is md2 then $Z(u)$ encodes:

- the size (number of edges) m
- the order (number of vertices) n
- the number of loops
- the girth (length of shortest closed path in G)
- the number of spanning trees τ
- whether the graph is regular
- whether the graph is bipartite
- whether the graph is a cycle
- the adjacency spectrum (only for certain families of graphs, e.g. regular, biregular-bipartite)

How do we construct pairs of (non-isomorphic) graphs that have the same zeta function?

- GM^* switching: change certain edges of a graph to get a cospectral mate (Haemers and Spence; Setyadi and Storm)
- Gassmann triples: the resulting graphs appear as covers of a given graph (Terras and Stark)
- Computer search

Wiener index

The usual distance function on a simple connected graph G:

$$d(v_i, v_j) = \text{the length of the shortest path from } v_i \text{ to } v_j$$

Molecular graphs
Define the *Wiener index* of G as

$$W(G) = \sum_{1 \le i < j \le n} d(v_i, v_j).$$

Modified Wiener indices:

- *Schultz index* (1989): $S(G) = \sum_{1 \le i < j \le n} (d_i + d_j) d(v_i, v_j)$
- *Gutman index* (1994): $S^*(G) = \sum_{1 \le i < j \le n} (d_i d_j) d(v_i, v_j).$

Resistance distance

Regard G as an electrical network with unit resistors placed on each edge. Define the *resistance distance* function on G by

$$r_{ij} = r(v_i, v_j) = \text{the effective resistance between } v_i \text{ to } v_j.$$

Theorem (Bapat)

The resistance distance on a simple connected graph G satisfies

$$r_{ij} = \frac{\det \mathbf{L}^{(ij)}}{\tau}$$

where τ is the number of spanning trees and $\mathbf{L}^{(ij)}$ is the matrix obtained from the Laplacian by deleting its i^{th} and j^{th} rows and columns.

Resistance distance - a probabilistic approach

Define a random walk on a simple connected graph G as the n-state Markov chain with transition matrix $\mathbf{P} = (p_{ij})$, where $p_{ij} = \frac{1}{d_i}$, if vertices v_i and v_j are neighbors, and 0 otherwise.
The chain has a stationary distribution: $\pi = (\pi_i)_{1 \leq i \leq n}$ where

$$\pi_i = \frac{d_i}{2m}$$

Let $\mathbf{W}$ be the $n \times n$ matrix whose rows are all equal to π.

Resistance distance - a probabilistic approach

Let $E_i T_j$ be the expected number of steps in a walk that starts at vertex v_i and ends when first reaching v_j. Then

$$r_{ij} = \frac{1}{2m}(E_i T_j + E_j T_i)$$

and

$$E_i T_j = \frac{z_{jj} - z_{ij}}{\pi_j}$$

where z_{ij} are the entries of the fundamental matrix

$$\mathbf{Z} = (\mathbf{I}_n - \mathbf{P} + \mathbf{W})^{-1}$$

Kirchhoff Index

Define the *Kirchhoff index* of a simple connected graph G (Klein and Randic, 1993)

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

Theorem (Gutman and Mohar, 1996)

The Kirchhoff index of a simple connected graph G satisfies

$$Kf(G) = n \sum_{i=2}^{n} \frac{1}{\mu_i}$$

where $\{\mu_1 = 0 < \mu_2 \le \ldots \le \mu_n\}$ is the Laplacian spectrum of G.

- complete graphs K_n: $Kf = n - 1$
- star graphs S_n: $Kf = (n-1)^2$

Modified Kirchhoff Indices

Multiplicative degree-Kirchhoff index of G (Chen, Zhang, 2007)
If $d_1, ..., d_n$ are the degrees of the vertices $v_1, ..., v_n$ then define

$$Kf^*(G) = \sum_{1 \leq i < j \leq n} d_i d_j r_{ij}.$$

Additive degree-Kirchhoff index of G (Gutman, Feng, Yu, 2012)

$$Kf^+(G) = \sum_{1 \leq i < j \leq n} (d_i + d_j) r_{ij}.$$

Multiplicative degree-Kirchhoff Index

Let **N** be the normalized Laplacian matrix of G and $\nu_1 = 0 < \nu_2 \leq ... \leq \nu_n$ be its spectrum.

Theorem (Chen, Zhang, 2007)

The multiplicative degree-Kirchhoff index of a simple connected graph G satisfies

$$Kf^*(G) = 2m \sum_{i=2}^{n} \frac{1}{\nu_i}$$

Compare to:

$$Kf(G) = n \sum_{i=2}^{n} \frac{1}{\mu_i}$$

Additive degree-Kirchhoff index

For a simple connected graph G: Palacios (2013):

$$Kf^{+}(G) = \sum_{i=1}^{n} \sum_{j=1}^{n} \pi_j E_i T_j + \sum_{j=1}^{n} \sum_{i=1}^{n} \pi_i E_i T_j.$$

Revisiting the other two indices

Theorem (Palacios, Renom, 2011)

$$Kf^*(G) = 2m \sum_{j=1}^{n} \pi_j E_i T_j = 2mK$$

where K is Kemeny's constant.

Theorem

$$Kf(G) = \frac{1}{2m} \sum_{i<j} (E_i T_j + E_j T_i).$$

Zeta function and Kirchhoffian indices

Question: Does the zeta function $Z(u)$ encode Kf, Kf^+, or Kf^*?

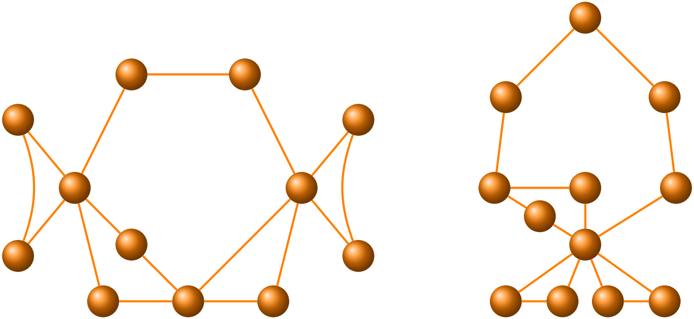

Figure: The crab (left) and the squid (right), found by Durfee and Martin

Kirchhoffian indices

Index	Crab	Squid
Kf	$\frac{607}{7}$	$\frac{593}{7}$
Kf^{+}	$\frac{9,166}{21}$	$\frac{8,956}{21}$
Kf^{*}	$\frac{22,843}{42}$	$\frac{22,339}{42}$

Table: Kirchhoffian indices

Zeta function and graph complexity

Recall that

$$Z(u)^{-1} = (1-u^2)^{m-n}\det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D}-\mathbf{I}_n))$$

Let $f(u) = \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D}-\mathbf{I}_n))$.

$$f(1) = \det(L) = 0$$

Zeta function and graph complexity

Recall that

$$Z(u)^{-1} = (1-u^2)^{m-n} \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D} - \mathbf{I}_n))$$

$f(u) = \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D} - \mathbf{I}_n))$.

Theorem (Northshield, 1998)

$$f'(1) = 2(m-n)\tau$$

Corollary (Northshield)

$$\lim_{u \to 1^-} Z(u)(1-u)^{m-n+1} = -\frac{1}{2^{m-n+1}(m-n)\tau}$$

Second derivative of zeta function

Question: Does f'' contain any information about the graph?

Theorem (MS)

If $f(u) = \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D} - \mathbf{I}_n))$ *then*

$$f''(1) = 2(Kf^z + 2mn - 2n^2 + n)\tau$$

where

$$Kf^z = \sum_{1 \le i < j \le n} (d_i - 2)(d_j - 2) r_{ij}$$

Kf^z = the zeta Kirchhoff index of the graph.

Zeta Kirchhoff index

Recall:

$$Kf = \sum_{1 \leq i < j \leq n} r_{ij}$$

$$Kf^* = \sum_{1 \leq i < j \leq n} d_i d_j r_{ij}$$

$$Kf^+ = \sum_{1 \leq i < j \leq n} (d_i + d_j) r_{ij}$$

and

$$Kf^z = \sum_{1 \leq i < j \leq n} (d_i - 2)(d_j - 2) r_{ij}$$

Thus,

$$Kf^z = Kf^* - 2Kf^+ + 4Kf$$

Kirchhoffian indices of the crab and the squid

Descriptor	Crab	Squid
Kf	$\frac{607}{7}$	$\frac{593}{7}$
Kf^+	$\frac{9,166}{21}$	$\frac{8,956}{21}$
Kf^*	$\frac{22,843}{42}$	$\frac{22,339}{42}$

Table: Kirchhoffian indices

Both graphs have $Kf^z = \frac{249}{14}$

Zeta Kirchhoff index

$$Kf^z = \sum_{1 \le i < j \le n} (d_i - 2)(d_j - 2) r_{ij}$$

If G is k-regular then

$$Kf^z = (k-2)^2 Kf$$

If G has loops at all vertices then

$$Kf^z(G) = Kf^*(G')$$

where G' is obtained from G by deleting one loop from each vertex.

Graphs with loops

Corollary

If G and H have loops at each vertex and the same Ihara zeta function then $Kf^*(G') = Kf^*(H')$, where G' and H' are the graphs obtained by deleting one loop from each vertex.

Are there any such graphs?

Figure: Same Ihara zeta function (Czarneski)

Same Kirchhoff index ($Kf = \frac{5}{3}$).

Graphs with loops

Figure: Same $Kf^* = 43$ (and same $Kf = \frac{5}{3}$)

Subdivision graphs

$S(G)$ obtained from G (simple) by inserting one vertex in each edge.

Theorem (Yang, 2014)

$$Kf(S(G)) = 2Kf(G) + Kf^{+}(G) + \frac{1}{2}Kf^{*}(G) + \frac{m^2 - n^2 + n}{2}$$

Theorem (Yang, Klein, 2015)

$$Kf^{+}(S(G)) = 4Kf^{+}(G) + 4Kf^{*}(G) + (m+n)(m-n+1) + 2m(m-n)$$

Theorem (Yang, Klein, 2015)

$$Kf^{*}(S(G)) = 8Kf^{*}(G) + 2m(2m-2n+1)$$

Subdivision graphs

Corollary (MS)

$$Kf^z(S(G)) = 2Kf^z(G)$$

$$Kf(S(G)) = \frac{1}{2}Kf^z(G) + 2Kf^+(G) + \frac{m^2 - n^2 + n}{2}$$

Corollary (MS)

Let G and H have the same Ihara zeta function. Then $Kf(S(G)) = Kf(S(H))$ if and only if $Kf^+(G) = Kf^+(H)$.

Are there any such graphs?

Example

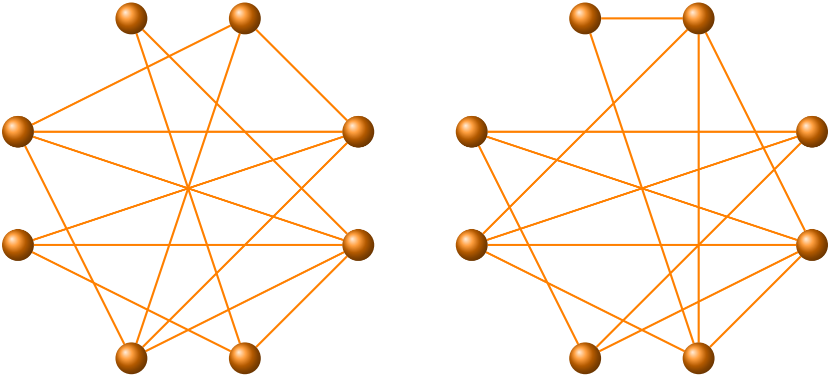

Figure: Same zeta function (Setyadi and Storm)

Example

Setyadi and Storm's graphs:

Index	Left graph	Right graph
Kf	19.70	19.75
Kf^*	220.4	220.2
Kf^+	132.6	132.6

Table: Kirchhoffian indices

Both graphs have $Kf^z = 34$.

Ihara zeta function

Recall that

$$Kf(S(G)) = \frac{1}{2}Kf^z(G) + 2Kf^+(G) + \frac{m^2 - n^2 + n}{2}$$

If G is md2 then its zeta function also encodes:

- the zeta Kirchhoff index $Kf^z(G)$
- the multiplicative Kirchhoff index $Kf^*(G')$ (for graphs with loops at all vertices)
- the difference $Kf(S(G)) - 2Kf^+(G)$

The End