Zeta functions of graphs and Kirchhoffian indices

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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 $G$: $v_1, ..., v_n$

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

  $$a_{ij} = \text{number of edges between } v_i \text{ and } v_j$$
  $$a_{ii} = \text{twice the number of loops at vertex } v_i.$$  

  $A$ is a symmetric matrix so it has real eigenvalues.

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

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

- **Laplacian matrix** \( L = D - A \)
  - \( L \) is not affected by loops
  - \( L \) is symmetric with row sums = 0
  - \( L \) is positive semidefinite so its eigenvalues \( \mu_1, ..., \mu_n \) are \( \geq 0 \).
  - \( \mu_1 = 0 \) is an eigenvalue of \( L \) with multiplicity 1.

- **Normalized Laplacian matrix** \( N = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} \)
  - \( N \) is symmetric
  - \( N \) is positive semidefinite so its eigenvalues \( \nu_1, ..., \nu_n \) are \( \geq 0 \)
  - \( \nu_1 = 0 \) is an eigenvalue of \( N \) 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 $L$.***
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)

\[ Z(u)^{-1} = (1 - u^2)^{m-n} \det(I_n - uA + u^2(D - I_n)) \]

Consequence: \( Z(u) \) is the reciprocal of a polynomial of degree \( 2m \).
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
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 $\tau$
- 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 \textit{Wiener index} of $G$ as

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

Modified Wiener indices:

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

Regard $G$ as an electrical network with unit resistors placed on each edge. Define the \textit{resistance distance} function on $G$ by

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

\textbf{Theorem (Bapat)}

The resistance distance on a simple connected graph $G$ satisfies

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

where $\tau$ is the number of spanning trees and $L^{(ij)}$ is the matrix obtained from the Laplacian by deleting its $i^{th}$ and $j^{th}$ rows and columns.
Define a random walk on a simple connected graph $G$ as the $n$-state Markov chain with transition matrix $P = (p_{ij})$, 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 $W$ be the $n \times n$ matrix whose rows are all equal to $\pi$. 
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

$$Z = (I_n - P + W)^{-1}$$
Kirchhoff Index

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

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

**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 $\{\mu_1 = 0 < \mu_2 \leq \ldots \leq \mu_n\}$ 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 $d_1, \ldots, d_n$ are the degrees of the vertices $v_1, \ldots, v_n$ then define  

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

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

$$Kf^+(G) = \sum_{1 \leq i < j \leq n} (d_i + d_j)r_{ij}.$$
Let $\mathbf{N}$ be the normalized Laplacian matrix of $G$ and $\nu_1 = 0 < \nu_2 \leq \ldots \leq \nu_n$ 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

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

<table>
<thead>
<tr>
<th>Index</th>
<th>Crab</th>
<th>Squid</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_f$</td>
<td>607/7</td>
<td>593/7</td>
</tr>
<tr>
<td>$K_f^+$</td>
<td>9,166/21</td>
<td>8,956/21</td>
</tr>
<tr>
<td>$K_f^*$</td>
<td>22,843/42</td>
<td>22,339/42</td>
</tr>
</tbody>
</table>

**Table:** Kirchhoffian indices
Recall that

\[ Z(u)^{-1} = (1 - u^2)^{m-n} \det(I_n - uA + u^2(D - I_n)) \]

Let \( f(u) = \det(I_n - uA + u^2(D - I_n)) \).

\[ f(1) = \det(L) = 0 \]
Recall that
\[ Z(u)^{-1} = (1 - u^2)^{m-n} \det(I_n - uA + u^2(D - I_n)) \]
\[ f(u) = \det(I_n - uA + u^2(D - I_n)). \]

**Theorem (Northshield, 1998)**

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

**Corollary (Northshield)**

\[ \lim_{u \to 1^-} Z(u)(1 - u)^{m-n+1} = -\frac{1}{2^{m-n+1}(m - n)\tau} \]
Question: Does $f''$ contain any information about the graph?

**Theorem (MS)**

If $f(u) = \det(I_n - uA + u^2(D - I_n))$ then

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

where

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

$Kf^z =$ the zeta Kirchhoff index of the graph.
Recall:

\[
K_f = \sum_{1 \leq i < j \leq n} r_{ij}
\]

\[
K_f^* = \sum_{1 \leq i < j \leq n} d_i d_j r_{ij}
\]

\[
K_f^+ = \sum_{1 \leq i < j \leq n} (d_i + d_j) r_{ij}
\]

and

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

Thus,

\[
K_f^z = K_f^* - 2K_f^+ + 4K_f
\]
# Kirchhoffian indices of the crab and the squid

<table>
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<th>Squid</th>
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**Table:** Kirchhoffian indices

Both graphs have $Kf^z = \frac{249}{14}$
\[ Kf^z = \sum_{1 \leq i < j \leq n} (d_i - 2)(d_j - 2)r_{ij} \]

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.
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 ($Kf = \frac{5}{3}$).
**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)**

\[
Kf^*(S(G)) = 8Kf^*(G) + 2m(2m - 2n + 1)
\]
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?
Figure: Same zeta function (Setyadi and Storm)
Setyadi and Storm’s graphs:

<table>
<thead>
<tr>
<th>Index</th>
<th>Left graph</th>
<th>Right graph</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_f$</td>
<td>19.70</td>
<td>19.75</td>
</tr>
<tr>
<td>$K_f^*$</td>
<td>220.4</td>
<td>220.2</td>
</tr>
<tr>
<td>$K_f^+$</td>
<td>132.6</td>
<td>132.6</td>
</tr>
</tbody>
</table>

**Table:** Kirchhoffian indices

Both graphs have $K_f^z = 34$. 
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