Switching Checkerboards

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Workshop on Graph Modification

Zagreb Indices

Let $G = (V, E)$ be a simple graph with n vertices and m edges.

$$M_1 = \sum_{i \in V} d_i^2 \qquad M_2 = \sum_{\{ij\} \in E} d_i d_j,$$

$$Z_1 = \sqrt{\frac{M_1}{n}} \leq \lambda_1 \qquad Z_2 = \sqrt{\frac{M_2}{m}}$$

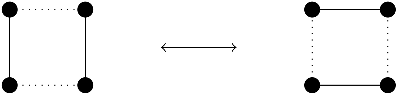
- Z_1 is the quadratic average of the degrees and a lower bound of the spectral radius λ_1.
- Z_2 is an average over the edges of $\sqrt{d_i d_j}$ and gives a loose approximation of λ_1.

Description of the problem

- We consider simple undirected graphs.
- We fix a degree distribution.
- How does the topology of the graph affect its eigenvalues?

Checkerboard

A *checkerboard* in a graph is an alternating cycle of 2 edges and 2 non-edges. The operation of *switching* a checkerboard consists of switching the edges and non-edges.



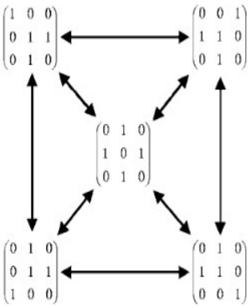
In the adjacency matrix, the switch affects a 2×2 sub-matrix and its symmetric:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \longleftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Graph of matrices

Theorem (Ryser, 1963)

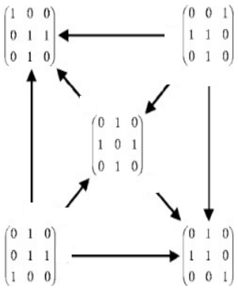
Any two graphs with identical degree distribution can be linked through sequence of switches.



From Y. Artzy-Randup,L. Stone, 2005

Orienting the Graph of matrices

By distinguishing positive checkerboards $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and negative checkerboards $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and only allowing switches from negative to positive, we define an orientation for the graph of matrices.



Proposition

The directed graph of matrices is acyclic.

Idea of proof: The quantity $I(A) = \sum ij\ a_{ij}$ increases along the edges.

Effect of a switch

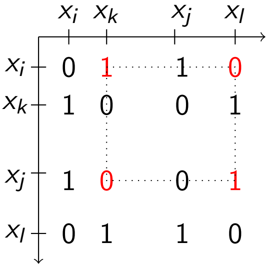
Let A' be obtained from A by switching a checkerboard of coordinates (i, j, k, l). Let X and X' be the normalised principal eigenvectors of A and A', respectively.

We have:

$$\lambda'_1 - \lambda_1 = {}^tX'A'X' - {}^tXAX$$
$$\geq {}^tXA'X - {}^tXAX = {}^tX(A' - A)X.$$

Thus $\lambda'_1 - \lambda_1 \geq 2(x_i - x_j)(x_k - x_l)$.

Similarly, $M'_2 - M_2 = (d_i - d_j)(d_k - d_l)$.



Remark

If the rows and columns of A are ordered increasingly (or decreasingly), M_2 increases with each positive switch and λ_1 increases with most positive switches.

Sources and Sinks

Theorem

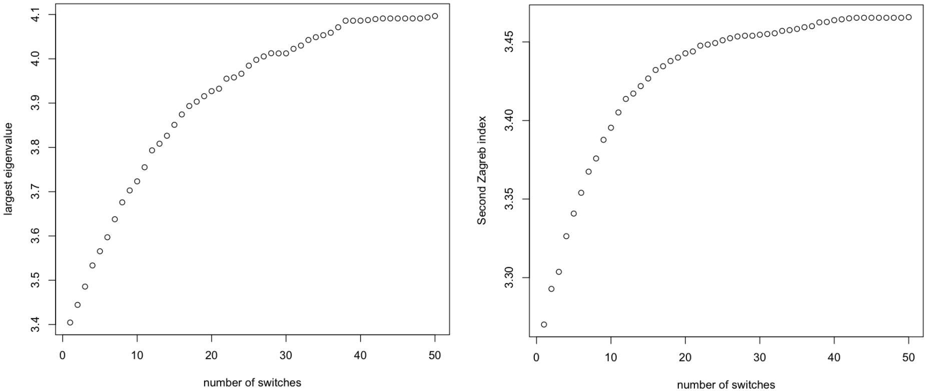
The sources and sinks of the directed graph of matrices are, respectively, the local minima and maxima for M_2 and Z_2.

Theorem

The global maximum of λ_1 is reached at a sink of the directed graph of matrices.

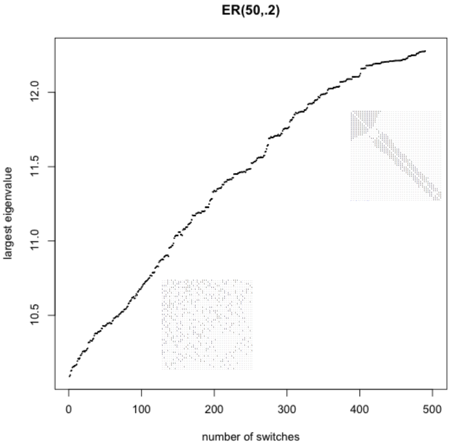
Key to the proof: If λ_1 is maximised, the coefficients of the principal eigenvector are in the same order as the degrees.

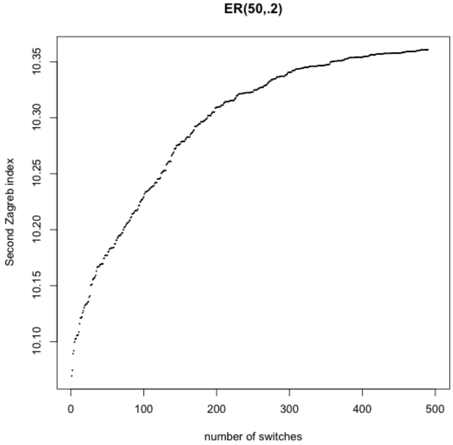
Simulations



Starting from a random graph with 20 vertices and 25 edges, successive random positive switches are applied.

Simulations





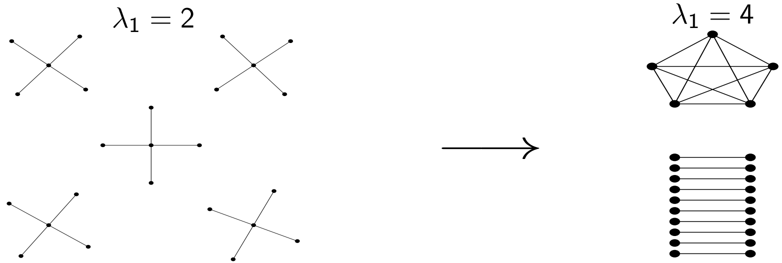
Starting from an Erdős-Rényi graph with 50 vertices ($p = .2$), successive random positive switches are applied.

Observations

- Z_2 is non-decreasing, but λ_2 may locally decrease slightly. (As expected)
- Generally, for large graphs, the amplitude of the total variation is fairly small. However, some theoretical examples yield arbitrarily large variations.

  For regular graphs, λ_1 and Z_2 do not vary at all.
- The variations of λ_1 and Z_2 are concavely shaped.

Large variations of λ_1



Degree distribution
$\{4,4,4,4,4,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1\}$

$$nK_{1,n-1} \quad \longrightarrow \quad K_n + \frac{n(n-1)}{2}K_2$$

$$\lambda_1 = Z_2 = \sqrt{n-1} \quad << \quad \lambda_1 = n-1, Z_2 \approx \frac{n-1}{\sqrt{2}}$$

Concavity

The observed concavity of λ_1 may be explained by the following result:

Theorem

For an Erdős-Rényi graph, the average variation of λ_1 caused by a positive switch decreases on average after a positive switch.

Elements of proof: The average variation of λ caused by a switch is twice the average checkerboard area $(x_i - x_j)(x_k - x_l)$. After a positive switch, some remaining checkerboards have their area reduced, but some small checkerboards disappear. The key is to verify that the former has a greater effect than the latter on the average checkerboard area.

Note that some carefully crafted pathological examples yield a convex increase of λ_1.

Discrepancy between Z_2 and λ_1

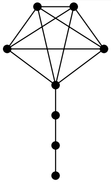
For kite graphs, λ_1 can be arbitrarily greater than Z_2. (Stevanović & Hansen, 2008)

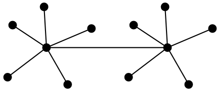
For double stars, $\frac{Z_2}{\lambda_1}$ can be arbitrarily close to $\sqrt{\frac{3}{2}}$. (Abdo et al., 2014)

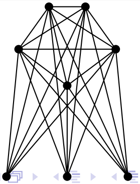
For certain cographs also, $\frac{Z_2}{\lambda_1}$ can be arbitrarily close to $\sqrt{\frac{3}{2}}$.

Conjecture: Revisiting a problem by Nikiforov (2006)

For any graph, $\frac{Z_2}{\lambda_1} < \sqrt{\frac{3}{2}}$. Furthermore, for a fixed n, the maximum of $\frac{Z_2}{\lambda_1}$ is reached for a split graph.







Questions

Thank you for your attention!