Communicability and Bipartivity in Complex Networks at Negative Temperature

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Recent experiments (Kessels & Qualman 2004, Freisen et al. 2005) show SH3 involved in **trafficking of vesicles**.

[vesicle: small, enclosed compartment within a cell.]
Unweighted, undirected, with \( N \) nodes.
Adjacency matrix \( A \).

\((A^k)_{ij}\) counts the number of 
walks of length \( k \) from node 
i to node \( j \).

Communicability between distinct nodes \( i \) and \( j \)

\[
\left( A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots + \frac{A^k}{k!} + \cdots \right)_{ij}
\]
that is, \((e^A)_{ij}\).

Spectral form:

\[
\left( \sum_{s=1}^{N} e^{\lambda_s} x^{[s]} x^{[s]} \right)_{ij}.
\]
How can we characterize the idea that two nodes are in the **same bi-partite cluster**?

One answer: they favour **even** length walks over **odd**.

This motivates

\[ \left( -A + \frac{A^2}{2!} - \frac{A^3}{3!} + \frac{A^4}{4!} - \frac{A^5}{5!} + \cdots \right)_{ij} , \text{ that is, } \left( e^{-A} \right)_{ij} . \]

This suggests,

\[ \left( e^{-A} \right)_{ij} \begin{cases} \geq 0 & \Rightarrow \text{same cluster} \\ < 0 & \Rightarrow \text{different clusters} \end{cases} \]
A

\[ \exp(-A) \]
Communicability can be motivated through $e^{\beta A}$, where $\beta = \frac{1}{kT}$ is the inverse temperature:

- $k$ is the Boltzmann constant
- $T$ is the absolute temperature

Now we take $\beta = -1$. Negative absolute temperature.

“The temperature scale from cold to hot runs $+0K, \ldots , +300K, \ldots , +\infty K, -\infty K, \ldots , -300K, \ldots , -0K$”, Kittel and Kroemer, *Thermal Physics*, (1980).

As more energy is added, “neigbouring” particles will start to repel, and bipartite clusters will emerge.
To look for **quasi-bipartite clusters**, we introduce

\[
\Theta(x) = \begin{cases} 
1 & \text{if } x > 0 \\
0 & \text{if } x \leq 0
\end{cases}
\]

Node repulsion graph has adjacency matrix \( \Theta(e^{-A}) \).

Then look for cliques in the node repulsion graph. (We use Bron & Kerbosch algorithm.)

Features of this algorithm:

- focus on **communities** (rather than overall bipartivity or individual nodes/edges)
- tolerant to “errors”
- **several substructures** can be identified simultaneously
- no artificial parameters
Artificial Example: 2 quasi-bipartite groups
Artificial Example: 4 quasi-bipartite groups
Canton Creek Food Web: Reorganised

quasi-bipartite communities
Protein-Protein Interaction: herpes virus
What’s New?

Using $e^{-A}$ to discover **quasi-bipartite communities**, motivated by

- odd versus even length walks between nodes
- spectral transformation, $\lambda \mapsto e^{-\lambda}$
- communicability at negative absolute temperature

Computational task expressed as looking for cliques in the **node repulsion graph**.

Bipartite structure discovered in real complex networks.