Brain Networks and Topology

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Ma191b: Geometry of Neuroscience

Some References

- Alex Fornito, Andrew Zalesky, Edward Bullmore, *Fundamentals of Brain Network Analysis*, Elsevier, 2016
- Olaf Sporns, *Networks of the Brain*, MIT Press, 2010
- Olaf Sporns, *Discovering the Human Connectome*, MIT Press, 2012
- Fan Chung, Linyuan Lu, *Complex Graphs and Networks*, American Mathematical Society, 2004
- László Lovász, *Large Networks and Graph Limits*, American Mathematical Society, 2012

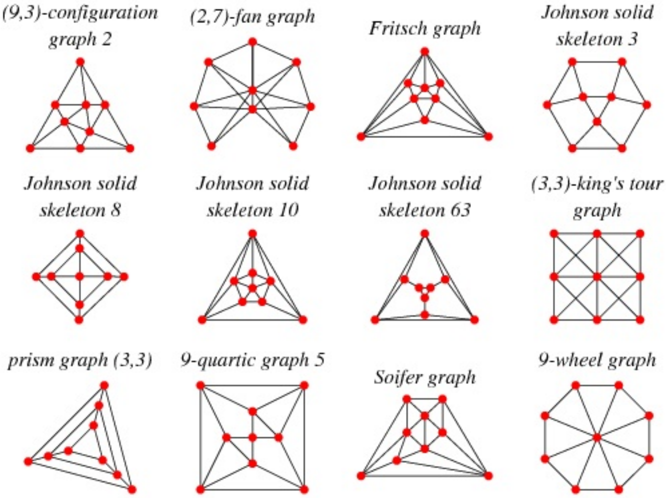
Graphs $G = (V, E, \partial)$

- $V = V(G)$ set of vertices (nodes)
- $E = E(G)$ set of edges (connections)
- boundary map $\partial : E(G) \to V(G) \times V(G)$, boundary vertices $\partial(e) = \{v, v'\}$
- directed graph (oriented edges): source and target maps

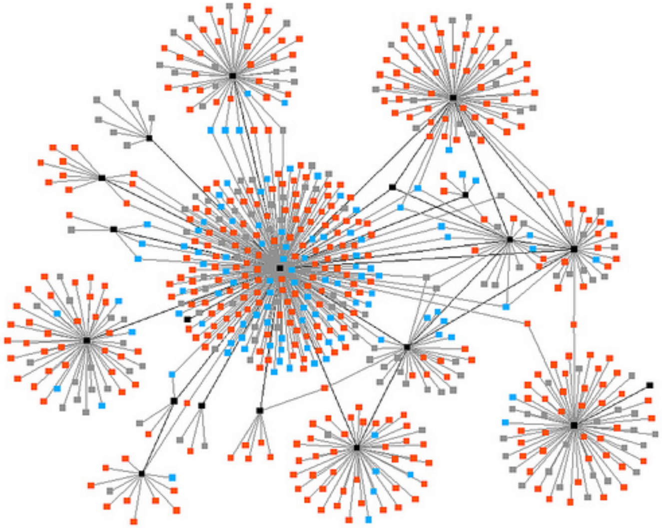
$$s : E(G) \to V(G), \quad t : E(G) \to V(G), \quad \partial(e) = \{s(e), t(e)\}$$

- *looping edge*: $s(e) = t(e)$ starts and ends at same vertex; *parallel edges*: $e \neq e'$ with $\partial(e) = \partial(e')$
- simplifying assumption: graphs G with no parallel edges and no looping edges (sometimes assume one or the other)
- additional data: label functions $f_V : V(G) \to L_V$ and $f_E : E(G) \to L_E$ to sets of vertex and edge labels L_V and L_E

Examples of Graphs

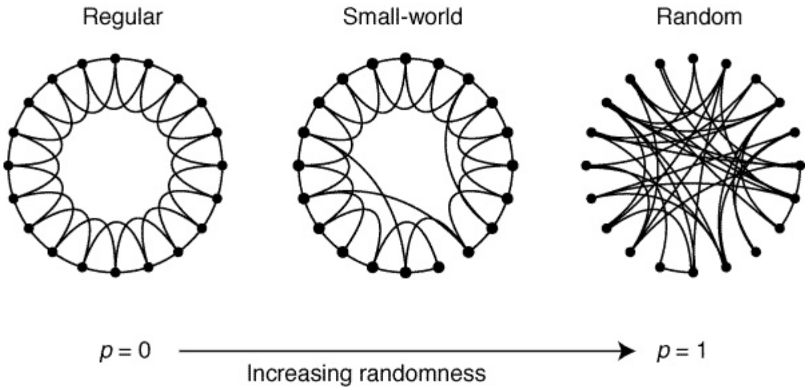


Network Graphs



(Example from Facebook)

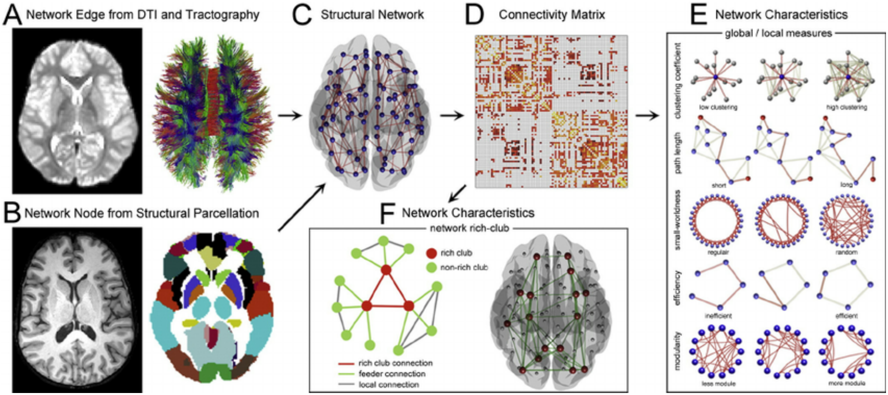
Increasing Randomness



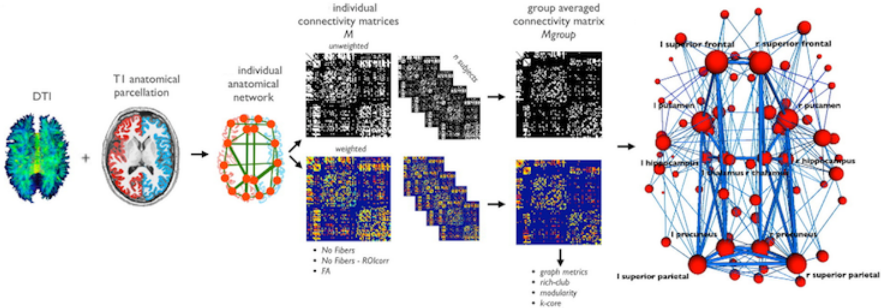
rewiring probability p

with probability p edges are disconnected and attached to a randomly chosen other vertex (Watts and Strogatz 1998)

Brain Networks: Macroscopic Scale (brain areas)

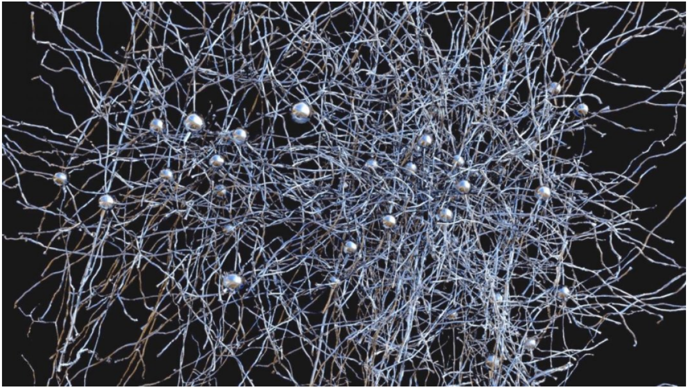


Brain Networks: Macroscopic Scale (brain areas)



Heuvel & Sporns (2011)

Brain Networks: Microscopic Scale (individual neurons)



(Clay Reid, Allen Institute; Wei-Chung Lee, Harvard Medical School; Sam Ingersoll, graphic artist; largest mapped network of individual cortical neurons, 2016)

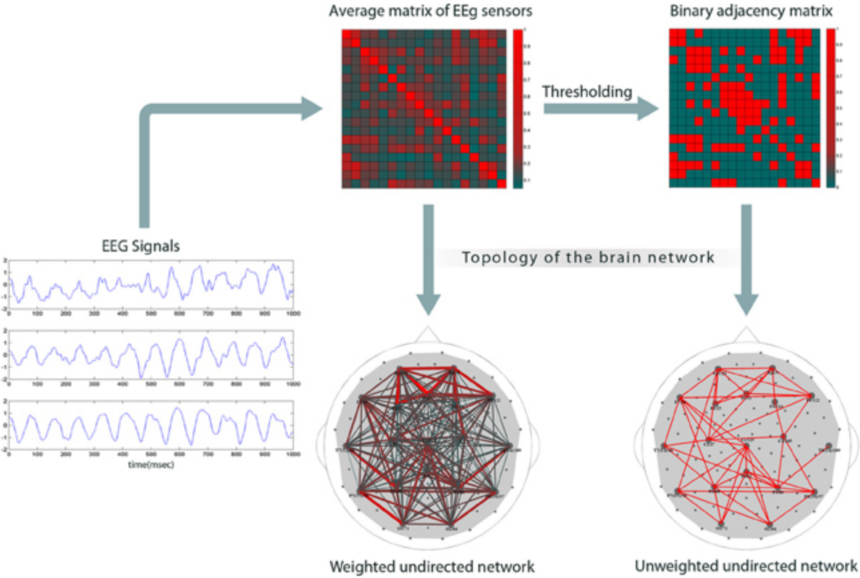
Modeling Brain Networks with Graphs

1. Spatial embeddings (embedded graphs $G \subset S^3$, knotting and linking, topological invariants of embedded graphs)
2. Vertex labels (heterogeneity of node types): distinguish different kinds of neurons/different areas
3. Edge labels (heterogeneity of edge types)
4. Orientations (directionality of connections): directed graphs
5. Weights (connection strengths)
6. Dynamical changes of network topology

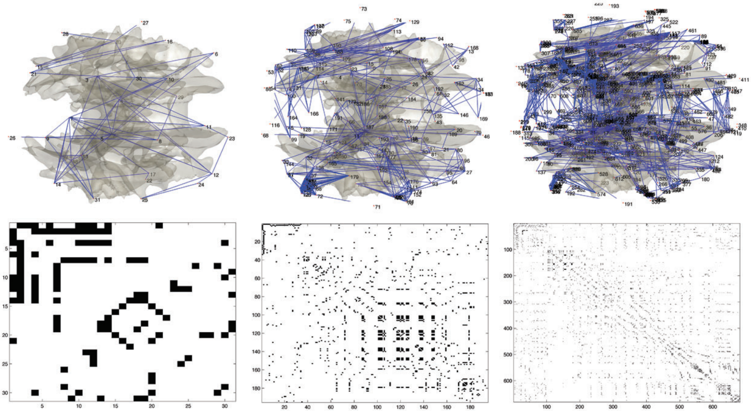
Connectivity and Adjacency Matrix

- connectivity matrix $C = (C_{ij})$ matrix size $N \times N$ with $N = \#V(G)$, with $C_{ij} \in \mathbb{R}$ connectivity strength for oriented edge from v_i to v_j
- sign of C_{ij}: excitatory/inhibitory connection
- $C_{ij} = 0$ no oriented connecting edges between these vertices
- in general $C_{ij} \neq C_{ji}$ for directed graphs, while $C_{ij} = C_{ji}$ for non-oriented
- can use $C_{ij} \in \mathbb{Z}$ for counting multiple parallel edges
- $C_{ii} = 0$ if no looping edges
- adjacency matrix $A = (A_{ij})$ also $N \times N$ with $A_{ij} = 1$ if there is (at least) an edge from v_i to v_j and zero otherwise
- $A_{ij} = 1$ if $C_{ij} \neq 0$ and $A_{ij} = 0$ if $C_{ij} = 0$
- if no parallel (oriented) edges: can reconstruct G from $A = (A_{ij})$ matrix

Connectivity and Adjacency Matrix



Filtering the Connectivity Matrix



various methods, for example pruning weaker connections: threshold

• connection density

$$\kappa = \frac{\sum_{ij} A_{ij}}{N(N-1)}$$

density of edges over choices of pairs of vertices

• total weight $W^{\pm} = \frac{1}{2}\sum_{ij} w_{ij}^{\pm}$ (for instance strength of connection positive/negative $C_{ij}^{\pm}$)

• how connectivity varies across nodes: valence of vertices (node degree), distribution of values of vertex valence over graph (e.g. most vertices with few connections, a few hubs with many connections: airplane travel, math collaborations)

• in/out degree $\iota(v) = \#\{e : v \in \partial(e)\}$ vertex valence; for oriented graph in-degree $\iota^{+}(v) = \#\{e : t(e) = v\}$ and out-degree $\iota^{-}(v) = \#\{e : s(e) = v\}$

$$\#E = \sum_v \iota^{+}(v) = \sum_v \iota^{-}(v)$$

• mean in/out degree
$\langle \iota^{+} \rangle = \frac{1}{N}\sum_v \iota^{+}(v) = \frac{\#E}{N} = \frac{1}{N}\sum_v \iota^{-}(v) = \langle \iota^{-} \rangle$

Degree Distribution

- $\mathbb{P}(\deg(v) = k)$ fraction of vertices (nodes) of valence (degree) k

Erdös–Rényi graphs: generate random graphs by connecting vertices randomly with equal probability p: all graphs with N vertices and M edges have equal probability

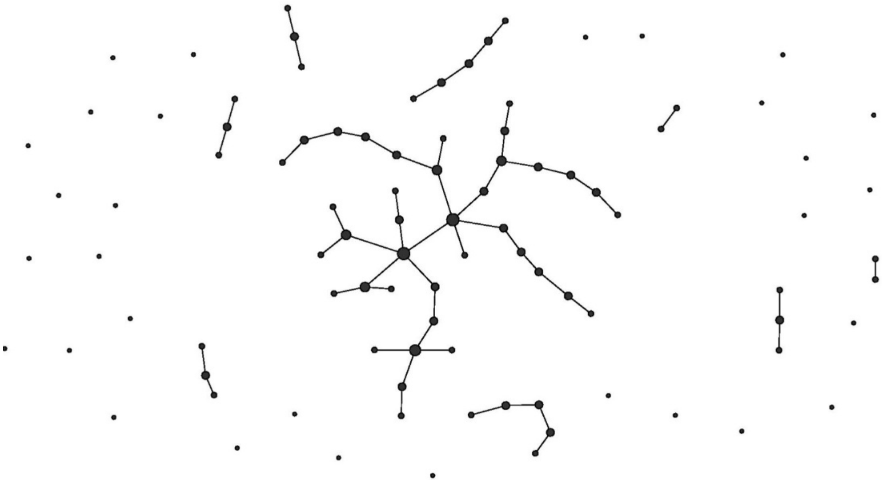
$$p^M (1-p)^{\binom{N}{2} - M}$$

- for Erdös–Rényi graphs degree distribution

$$\mathbb{P}(\deg(v) = k) = \binom{N-1}{k} p^k (1-p)^{N-1-k}$$

second exponent $N - 1 - k$ remaining possible connection from a chosen vertex (no looping edges) after removing a choice of k edges

- $p =$ connection density of the graph (network)



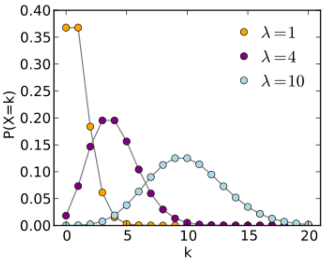
An Erdös–Rényi graph generated with $p = 0.001$

- the Erdös–Rényi degree distribution satisfies for $n \to \infty$

$$\mathbb{P}(\deg(v) = k) = \binom{N-1}{k} p^k (1-p)^{N-1-k} \sim \frac{(np)^k e^{-np}}{k!}$$

- so for large n the distribution is Poisson

$$\mathbb{P}(k) = \frac{\lambda^k e^{-\lambda}}{k!}$$



- .... but Erdös–Rényi graphs not a good model for brain networks

Scale-free networks ... power laws

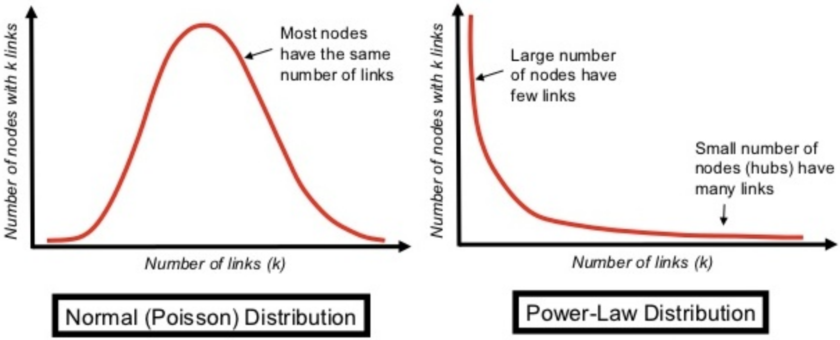
$$\mathbb{P}(\deg(v) = k) \sim k^{-\gamma} \qquad \text{for some } \gamma > 0$$

• slower decay rate than in binomial case: fat tail ... higher probability than in Erdös–Rényi case of highly connected large k nodes

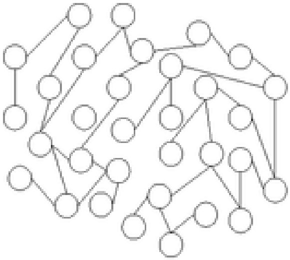
• Erdös–Rényi case has a peak in the distribution: a characteristic scale of the network

• power law distribution has no peak: no characteristic scale... scale free (typical behavior of self-similar and fractal systems)

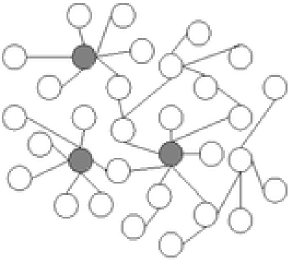
Poisson versus Power Law degree distributions



(nodes = vertices, links = edges, number of links = valence)



(a) Random network



(b) Scale-free network

Broad Scale Networks

• intermediate class: more realistic to model brain networks

• exponentially truncated power law

$$\mathbb{P}(\deg(v) = k) \sim k^{-\gamma} e^{-k/k_c}$$

• cutoff degree k_c: for small k_c quicker transition to an exponential distribution

• range of scales over which power law behavior is dominant

• so far measurements of human and animal brain networks consistent with scale free and broad scale networks

For weighted vertices with weights $w \in \mathbb{R}_+^*$

• weight distribution: best fitting for brain networks log-normal distribution

$$\mathbb{P}(\mathrm{weight}(v) = w) = \frac{1}{w\sigma\sqrt{2\pi}} \exp\left(\frac{-(\log w - \mu)^2}{2\sigma^2}\right)$$

Gaussian in log coordimates

• why log-normal? model based on properties:

1. geometry of embedded graph with distribution of interregional distances $\sim$ Gaussian
2. distance dependent cost of long distance connections

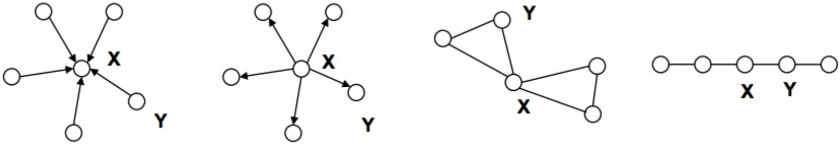
drop in probability of long distance connections with strong weights

Centrality

- a node is more "central" to a network the more
  - it is highly connected (large valence) – degree
  - it is located on the shortest path between other nodes – betweenness
  - it is close to a large number of other nodes (eg via highly connected neighbors) – closeness

- valence $\deg(v)$ is a measure of centrality (but not so good because it does not distinguish between highly or sparsely connected neighbors)

In each of the following networks, X has higher centrality than Y according to a particular measure



indegree outdegree betweenness closeness

Perron–Frobenius centrality

- Perron–Frobenius theorem (version for non-negative matrices)
  - $A = (A_{ij})$ non-negative $N \times N$ matrix: $A_{ij} \geq 0, \forall i, j$
  - A is primitive if $\exists k \in \mathbb{N}$ such that A^k is positive
  - A irreducible iff $\forall i, j, \exists k \in \mathbb{N}$ such that $A^k_{ij} > 0$ (implies $I + A$ primitive)
  - Directed graph G_A with N vertices and edge from v_i to v_j iff $A_{ij} > 0$: matrix A irreducible iff G_A strongly connected (every vertex is reachable through an oriented path from every other vertex)
  - Period h_A: greatest common divisor of lengths of all closed directed paths in G_A

Assume A non-negative and irreducible with period h_A and spectral radius ρ_A, then:

1. $\rho_A > 0$ and eigenvalue of A (Perron–Frobenius eigenvalue); simple
2. Left eigenvector V_A and right eigenvector W_A with all positive components (Perron–Frobenius eigenvector): only eigenvectors with all positive components
3. h_A complex eigenvectors with eigenvalues on circle $|\lambda| = \rho_A$
4. spectrum invariant under multiplication by $e^{2\pi i/h_A}$

Take $A =$ adjacency matrix of graph G

• $A =$ adjacency matrix of graph G

• vertex $v = v_i$: PF centrality

$$\mathcal{C}_{PF}(v_i) = V_{A,i} = \frac{1}{\rho_A} \sum_j A_{ij} V_{A,j}$$

ith component of PF eigenvector V_A

• high centrality if high degree (many neighbors), neighbors of high degree, or both

• can use V_A or W_A, left/right PF eigenvectors: centrality according to in-degree or out-degree

Page Rank Centrality (google)

- $D =$ diagonal matrix $D_{ii} = \max\{\deg(v_i)^{out}, 1\}$
- α, β adjustable parameters

$$\mathcal{C}_{PR}(v_i) = ((I - \alpha A D^{-1})^{-1} \beta 1)_i$$

with 1 vector of N entries 1

- this scales contributions of neighbors of node v_i by their degree: dampens potential bias of nodes connected to nodes of high degree

Delta Centrality

• measure of how much a topological property of the graph changes if a vertex is removed

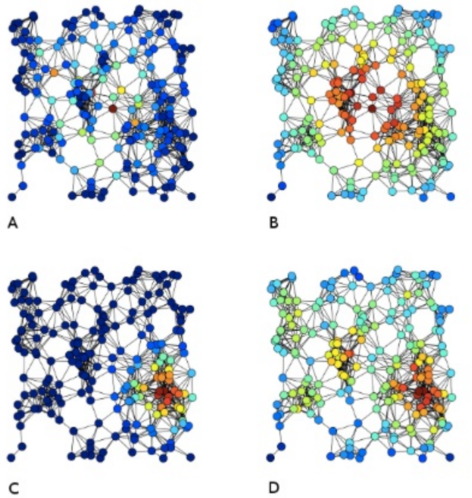
• graph G and vertex $v \in V(G)$: remove v and star $S(v)$ of edges adjacent to v

$$G_v = G \smallsetminus S(v)$$

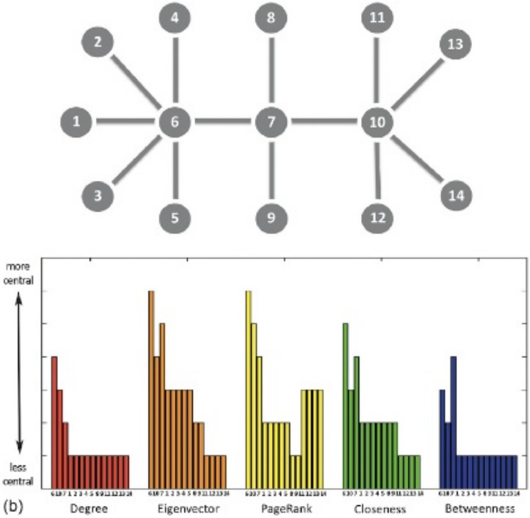
• topological invariants of (embedded) graph $M(G)$ (with integer or real values)

• delta centrality with respect to M

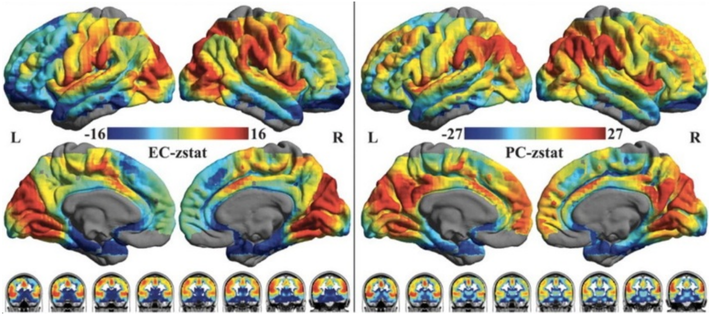
$$\mathcal{C}_M(v) = \frac{M(G) - M(G_v)}{M(G)}$$



(A) betweenness; (B) closeness; (C) eigenvector (PF); (D) degree


1
2
3
4
5
6
7
8
9
10
11
12
13
14
more central
less central
(b)
Degree
Eigenvector
PageRank
Closeness
Betweenness

Eigenvalue and PageRank centrality in brain networks



X.N.Zuo, R.Ehmke, M.Mennes, D.Imperati, F.X.Castellanos, O.Sporns, M.P.Milham, *Network Centrality in the Human Functional Connectome*, Cereb Cortex (2012) 22 (8): 1862-1875.

Connected Components

• what is the right notion of "connectedness" for a large graph? small components breaking off should not matter, but large components becoming separated should

• is there one large component?

• Erdös–Rényi graphs: size of largest component ($N = \#V(G)$)

- sharp increase at $p \sim 1/N$
- graph tends to be connected for $p > \frac{\log N}{N}$
- for $p < \frac{1}{N}$ fragmented graph: many connected components of comparable (small) size
- for $\frac{1}{N} \leq p \leq \frac{\log N}{N}$ emergence of one giant component; other components still exist of smaller size

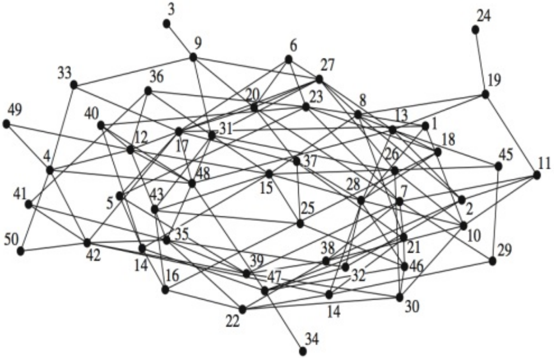


Figure: Emergence of connectedness: a random network on 50 nodes with $p = 0.10$.

(from Daron Acemoglu and Asu Ozdaglar, Lecture Notes on Networks)

How to prove the emergence of connectedness?

(Argument from Daron Acemoglu and Asu Ozdaglar, Lecture Notes on Networks)

• threshold function $\tau(N)$ for a property $\mathcal{P}(G)$ of a random graph G with $N = \#V(G)$, with probability $p = p(N)$:

$$\mathbb{P}(\mathcal{P}(G)) \to 0 \quad \text{when } \frac{p(N)}{\tau(N)} \to 0$$

$$\mathbb{P}(\mathcal{P}(G)) \to 1 \quad \text{when } \frac{p(N)}{\tau(N)} \to \infty$$

with $\mathbb{P}(\mathcal{P}(G))$ probability that the property is satisfied

• show that $\tau(N) = \frac{\log N}{N}$ is a threshold function for the property $\mathcal{P} =$connectedness

- for $\mathcal{P}$ =connectedness show that for $p(N) = \lambda \frac{\log N}{N}$:

$$\mathbb{P}(\mathcal{P}(G)) \to 1 \quad \text{for } \lambda > 1$$

$$\mathbb{P}(\mathcal{P}(G)) \to 0 \quad \text{for } \lambda < 1$$

- to prove graph disconnected for $\lambda < 1$ show growing number of single node components

- in an Erdös–Rényi graph probability of a given node being a connected component is $(1-p)^{N-1}$; so typical number of single node components is $N \cdot (1-p)^{N-1}$

- for large N this $(1-p)^{N-1} \sim e^{-pN}$

- if $p = p(N) = \lambda \frac{\log N}{N}$ this gives

$$e^{-p(N)\,N} = e^{-\lambda \log N} = N^{-\lambda}$$

- for $\lambda < 1$ typical number of single node components

$$N \cdot (1-p)^{N-1} \sim N \cdot N^{-\lambda} \to \infty$$

• for $\lambda > 1$ typical number of single vertex components goes to zero, but not enough to know graph becomes connected (larger size components may remain)

• probability of a set S_k of k vertices having no connection to the rest of the graph (but possible connections between them) is $(1-p)^{k(N-k)}$

• typical number of sets of k nodes not connected to the rest of the graph

$$\binom{N}{k}(1-p)^{k(N-k)}$$

• Stirling's formula $k! \sim k^k e^{-k}$ gives for large N and k

$$\binom{N}{k}(1-p)^{k(N-k)} \sim (\frac{N}{k})^k e^k e^{-k\lambda \log N} = N^k N^{-\lambda k} e^{k(1-\log k)} \to 0$$

for $p = p(N) = \lambda \frac{\log N}{N}$ with $\lambda > 1$

Phase transitions:

- at $p = \frac{\log N}{N}$: graph becomes connected
- at $p = \frac{1}{N}$: emergence of one giant component

• use similar method: threshold function $\tau(N) = \frac{1}{N}$ and probabilities $p(N) = \frac{\lambda}{N}$ with either $\lambda > 1$ or $\lambda < 1$

Case $\lambda < 1$:

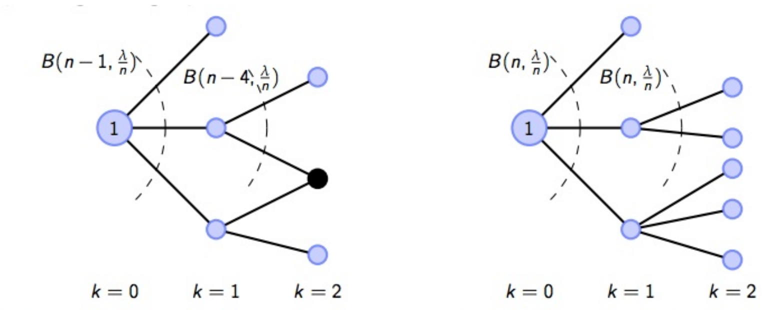
• starting at a vertex approximate counting of connected vertices in an Erdös–Rényi graph with a branching process $B(N, \frac{\lambda}{N})$

• replaces graph by a tree (overcounting of vertices) with typical number of descendants $N \times \frac{\lambda}{N}$ so in k steps from starting vertex expected number of connections λ^k

• so typical size of the component connected to first vertex is bounded above by size obtained from branching process

$$\sum_k \lambda^k = \frac{1}{1-\lambda}$$

small sized components



(a) Erdos-Renyi graph process. (b) Branching Process Approx.

Branching process approximation to an Erdös–Rényi graph process (from Daron Acemoglu and Asu Ozdaglar, Lecture Notes on Networks)

Case $\lambda > 1$:

• process $B(N, \frac{\lambda}{N})$ asymptotically Poisson with probability (k steps)

$$e^{-\lambda} \frac{\lambda^k}{k!}$$

• probability ρ that tree obtained via this process is finite: recursive structure (overall tree finite if each tree starting from next vertices finite)

$$\rho = \sum_k e^{-\lambda} \frac{\lambda^k}{k!} \rho^k$$

fixed point equation $\rho = e^{\lambda(\rho-1)}$

• one solution $\rho = 1$ but another solution inside interval $0 < \rho < 1$

• however... the branching process $B(n, p)$ produces trees, but on the graph G fewer vertices...

• after δN vertices have been added to a component via the branching process starting from one vertex, to continue the process one has $B(N(1-\delta), p)$ correspondingly changing $\lambda \mapsto \lambda(1-\delta)$ (to continue to approximate same p of Erdös–Rényi process)

• progressively decreases $\lambda(1-\delta)$ as δ increases so branching process becomes more likely to stop quickly

• typical size of the big component becomes $(1-\rho)N$ where $\rho = \rho(\lambda)$ as above probability of finite tree, solution of $\rho = e^{\lambda(\rho-1)}$

Robustness to lesions

• Remove a vertex $v \in V(G)$ with its star of edges $S(v) = \{e \in E(G) : v \in \partial(e)\}$

$$G_v = G \smallsetminus S(v)$$

measure change: e.g. change in size of largest component

• when keep removing more $S(v)$'s at various vertices, reach a threshold at which graph becomes fragmented

• in opposite way, keep adding edges with a certain probability, critical threshold where giant component arises, as discussed previously

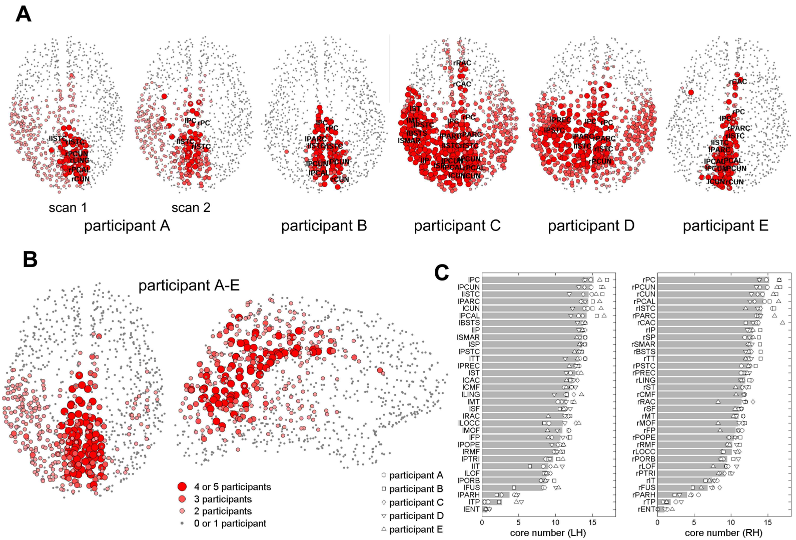
Core/Periphery

- *core*: subset of vertices highly connected to each other (hubs)
- *periphery*: nodes connected to core vertices but not with each other
- *maximal cliques*: maximally connected subsets of nodes

k-core decomposition: remove all $S(v)$ with $\deg(v) < k$, remaining graph $G^{(k)}$ *k-core*

- *core index* of $v \in V(G)$: largest k such that $v \in V(G^{(k)})$

s-core $G^{(s)}$: remove all $S(v)$ of vertices with weight $w(v) < s$



k-core decomposition, from P.Hagmann, L.Cammoun, X.Gigandet, R.Meuli, C.J.Honey, V.J.Wedeen, O.Sporns, "Mapping the Structural Core of Human Cerebral Cortex", PLOS bio 2008

Topology and flow of information along directed graphs

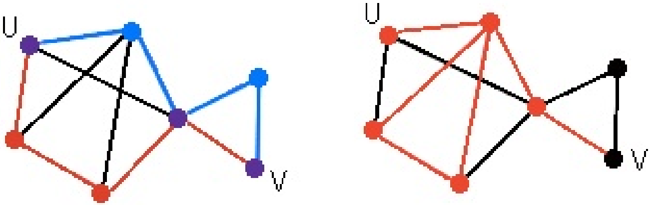
• networks with characteristic path length (close to min in a random graph)

• path length = min number of oriented edges or minimum total weight of these edges

walks, trails, paths

- *walk*: sequence of oriented edges (target of one source of next): revisiting vertices and edges allowed
- *trail*: same but no edge repetitions (edges visited only once)
- *path*: no edge and no vertex repetitions (both vertices and edges visited only once)

Warning: terminology varies in the literature



two paths from U to V and a trail from U to V

- shortest path = geodesics (with edge weights as metric)
- average of path length over all shortest path in the graph
    - at vertex v_i average ℓ_i of lengths $\ell_{ij} = \ell(v_i, v_j)$ of shortest paths starting at v_i (and ending at any other vertex v_j)
    - average over vertices

$$L = \frac{1}{N} \sum_i \ell_i = \frac{1}{N(N-1)} \sum_{i \neq j} \ell_{ij}$$

• main idea: brain networks with the shortest average path length integrate information better

• in case of a graph with several connected components, for v_i and v_j not in the same component usually take $\ell_{ij} = \infty$, then better to use harmonic mean

$$N(N-1)\left(\sum_{i\neq j}\ell_{ij}^{-1}\right)^{-1}$$

or its inverse, the global efficiency:

$$\frac{1}{N(N-1)}\sum_{i\neq j}\ell_{ij}^{-1}$$

The Graph Laplacian   measuring flow of information in a graph

- $\delta = (\delta_{ij})$ diagonal matrix of valencies $\delta_{ii} = \deg(v_i)$
- adjacency matrix A (weighted with w_{ij})
- Laplacian $\Delta_G = \delta - A$
- normalized Laplacian $\hat{\Delta}_G = I - A\delta^{-1}$ or symmetrized form $\hat{\Delta}^s_G = I - \delta^{-1/2} A \delta^{-1/2}$
- $w_{ij}/\delta_{ii} =$ probability of reaching vertex v_j after v_i along a random walk search
- dimension of $\mathrm{Ker}\hat{\Delta}_G$ counts connected components
- eigenvalues and eigenvectors give decomposition of the graph into "modules"

Dynamics

• in brain networks fast dynamics $\sim$ 100 millisecond timescale: variability in functional coupling of neurons and brain regions, underlying functional anatomy unchanged; also slow dynamics: long lasting changes in neuron interaction due to plasticity... growth, rewiring

• types of dynamics: diffusion processes, random walks, synchronization, information flow, energy flow

• topology of the graph plays a role in the spontaneous emergence of global (collective) dynamical states

• multiscale dynamics: dynamics at a scale influenced by states and dynamics on larger and smaller scales

• mean field model: dynamics at a scale averaging over effects at all smaller scales

• synchronization of a system of coupled oscillators at vertices with coupling along edges

• if graph very regular (eg lattice) difficult to achieve synchronized states

• small-world networks are easier to synchronize

• fully random graphs synchronize more easily but synchronized state also very easily disrupted: difficult to maintain synchronization

• more complex types of behavior when non-identical oscillators (different weights at different vertices) and additional presence of noise

• still open question: what is the role of topology and topology changes in the graph in supporting self-organized-criticality

Return to discuss expander Graphs: heuristic properties

- spectral property: like Ramanujan graphs if M matrix associated to G then $\mathrm{Spec}(M)$ contained in spectrum of analogous operator on covering tree
- pseudo-random behavior: G behaves in some sense like a random graph
- information is passed easily through the network
- random walk: a random walker on the graph gets lost quickly
- boundary: every subset of the vertices that is not "too large" has a "large" boundary
- different ways of formalizing these: edge expanders, vertex expanders, spectral expanders
- how to detect good expander property? via other data (especially spectral and zeta function)

Expansion Constant

- sets of vertices S, T of G
- $E(S,T)$ = edges of G with one vertex in S and the other in T
- $\partial S = E(S, G \smallsetminus S)$
- expansion constant of G

$$h(G) := \min_{S \subset V, \# S \leq n/2} \frac{\# \partial S}{\# S}$$

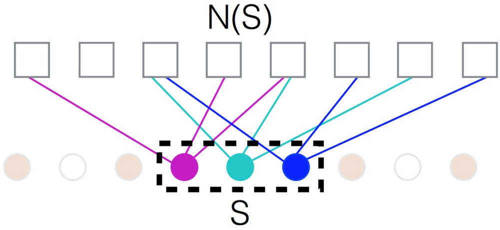
- analog of the Cheeger constant for differentiable manifolds
- relation to the spectral gap (Chung)

$$2h(G) \geq \lambda_G \geq h(G)^2/2$$

with $\lambda_G = \min\{\lambda_1, 2 - \lambda_{n-1}\}$ for
$\mathrm{Spec}(1 - D^{-1/2} A D^{-1/2}) = \{0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_n\}$

- various other Cheeger-type inequalities in terms of spectral data
- similar notion of edge expansion

- expander graph has large expansion parameter and low degree
- bipartite expander graphs

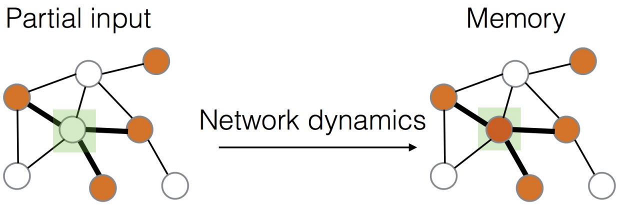


- $(\gamma, 1-\epsilon)$-expander: all sets S with $\deg = z$ and $\#S \leq \gamma N$ (fraction of total number of vertices) have $\#N(S) = \#\partial S > (1-\epsilon) z \#S$
- bipartite expander graphs are good for constructing codes with good error-correcting properties (number of errors corrected $> \beta N$ with $\beta = \gamma(1-2\epsilon)N$

Expander Graphs in Neuroscience

(work of Rishidev Chaudhuri and Ila Fiete)

- bipartite expander Hopfield networks
- Hopfield networks: models for neural memory
- stored states recovered from noisy/partial input

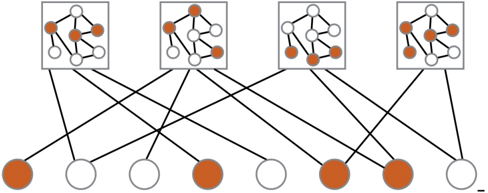


- good error correcting properties of expander bipartite graphs

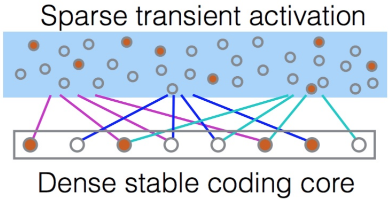
Expander Graphs in Neuroscience

(work of Rishidev Chaudhuri and Ila Fiete)

- Hopfield networks with stable states determined by sparse constraints with expander structure

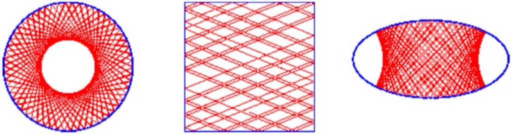


- modelling of neural codes: higher order correlations (better coding properties) unlike neural code with many neurons that are rarely activated and pairwise decorrelated

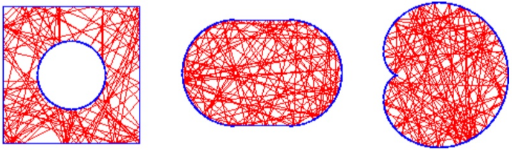


Quantum Chaos: the basic idea

- Classical (continuous) dynamical systems: regular and chaotic behavior

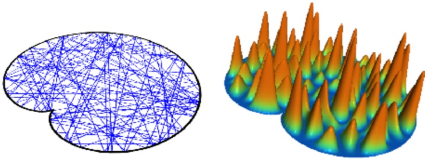


Integrable billiard: regular motion.



Chaotic billiard: irregular motion.

- Properties of Schrödinger equation associated to chaotic classical systems



Pictures Arnd Bäcker: http://www.physik.tu-dresden.de/~baecker/

- spectral properties related to counting of periodic orbits for chaotic classical system and to Random Matrix Theory
- quantum version of classical integrable systems have Poisson distribution of eigenvalues
- quantum version of chaotic classical systems follow eigenvalue distribution of Random Matrix Theory (Dyson's circular ensemble)

Quantum Chaos on Graphs

- Tsampikos Kottos and Uzy Smilansky, *Periodic orbit theory and spectral statistics for quantum graphs*, Annals of Physics 274 (1999) 76–124
- Uzy Smilansky, *Quantum chaos on discrete graphs*, J. Phys. A 40 (2007) no. 27, F621–F630

- Summary
  - quantum (metric) graphs versus discrete graphs
  - Schrödinger operator on quantum graphs spectral statistics similar to Random Matrix Theory (which describes generic quantum Hamiltonians)
  - similarity with chaotic Hamiltonian dynamical systems: a similar *trace formula* describing spectral densities in terms of sums over periodic orbits
  - zeta function for a Perron–Frobenius operator on the graph: same expression in terms of periodic orbits (like Ruelle dynamical zeta function for Hamiltonian dynamical systems)
  - discrete graphs: spectral properties from Ihara zeta function

- Quantum graphs case: quick overview
  - Schrödinger equation on quantum graphs good for modelling traveling waves in networks
  - assign a coordinate x_e to each oriented edge of a graph, from 0 to ℓ_e length
  - Hilbert space $\mathcal{H} = \oplus_e L^2([0, \ell_e])$ and wave functions $\Psi = (\Psi_e(x_e))_{e \in E}$
  - Schrödinger equation (with magnetic vector potential $A = (A_e)$

$$(-i \frac{d}{dx_e} - A_e)^2 \Psi_e(x_e) = k^2 \, \Psi_e(x_e)$$

    with matching boundary conditions at vertices
  - self-adjoint with unbounded discrete spectrum

- spectrum from $\zeta_E(k) = \det(I - S_E(k)) = 0$ with edge scattering matrix $S_E(k)$ (unitary $2\#E \times 2\#E$ matrix)
- Fredholm determinant

$$\log \det(I - S_E(k)) = -\sum_{n=1}^{\infty} \frac{1}{n} \mathrm{Tr}(S_E^n(k))$$

- traces $\mathrm{Tr}(S_E^n(k))$ in terms of a sum over n-periodic orbits on the graph of a "magnetic flux" along that orbit (depending on magnetic potential A)
- symbolic dynamics: subshift of finite type with Markov/Bernoulli measure (chaotic dynamical system)

Case of discrete graphs

- Laplacian L of the discrete graph: (weighted) connectivity matrix and diagonal matrix of vertex valencies
- zeta functions and trace formulae for discrete graphs
- eigenvalues of the graph Laplacian related to nontrivial poles of the Ihara zeta function of the graph
- again zeta function related to counting of periodic orbits of a subshift of finite type dynamics

Zeta Functions of Graphs and Chaos Theory

- Audrey Terras, *Zeta functions and Chaos*, A Window Into Zeta and Modular Physics, MSRI Publications, Volume 57, 2010
- Model zeta function: Riemann Zeta Function

$$\zeta(s) = \sum_{n\geq 1} n^{-s} = \prod_p (1-p^{-s})^{-1}$$

sum over $n \in \mathbb{N}$ or Euler product over primes

- What plays the role of primes for a graph?
- another model example: Selberg Zeta Function

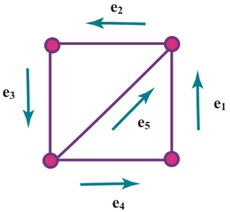
$$Z(s) = \prod_C \prod_{\ell\geq 1} (1 - e^{-(s+\ell)\nu(C)})$$

primitive closed geodesics C in $X = \mathrm{SL}_2(\mathbb{Z})\backslash\mathbb{H}^2$ modular curve with length $\nu(C)$

- expect closed paths to play role of geodesics on a graph with length the number of oriented edges

Paths on Graphs and "Primes"

- start from an undirected graph and assign arbitrary orientations



- path in directed graph has backtrack if $C = e_1 \dots e_s$ with some $e_{j+1} = e_j^{-1}$
- path in directed graph has tail if $C = e_1 \dots e_s$ with $e_s = e_1^{-1}$
- equivalence class of a closed path $C = e_1 \dots e_n$ consists of all cyclically permuted ordering of the oriented edges in the path: $e_2, \dots, e_n, e_1$ etc.
- closed path primitive if no backtracking and $C \neq D^k$
- "primes": equiv classes of taill-less primitive closed paths

Ihara Zeta Function

- Ihara Zeta:

$$\zeta(u,G) = \prod_P (1 - u^{\nu(P)})^{-1}$$

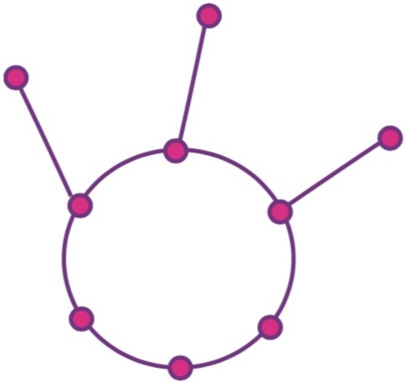
- P ranges over primes, equiv classes of tail-less primitive closed paths in G
- $\nu(P)$ is the length (number of edges) in the path
- Bass Determinant Formula

$$\zeta(u,G)^{-1} = (1-u^2)^{r-1}\det(I - Au + Qu^2)$$

$r = \#E - \#V + 1$ rank of fundamental group $\pi_1(G)$

- $A =$ vertex adjacency matrix: $\#V \times \#V$ matrix with (i,j)-entry $\#$ directed edges from v_i to v_j
- $Q =$ diagonal matrix with j-th entry $\mathrm{val}(v_j) - 1$
- tetrahedron graph K_4

$$\zeta(u, K-4)^{-1} = (1-u^2)^2(1-u)(1+u+2u^2)(1-u^2-2u^3)$$



An example of a bad graph for zeta functions.

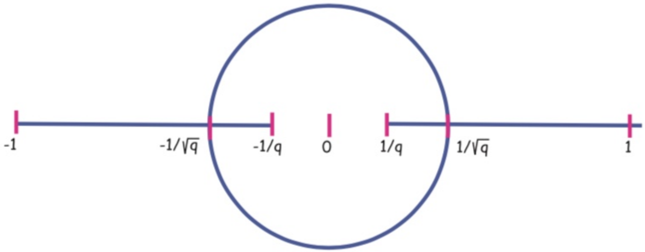
valence one vertices are not good for zeta function because of tails (but loops and multiple edges are OK)

Riemann Hypothesis for the Ihara Zeta Function
(Lubotzky, Phillips and Sarnak)

- case of $(q+1)$-regular graphs
- Ihara Riemann Hypothesis $\zeta(q^{-s}, G)$ has no poles with $0 < \Re(s) < 1$ unless $\Re(s) = 1/2$
- for a graph equivalent to being a Ramanujan graph
- this property means that nontrivial spectrum of adjacency matrix of the graph contained in spectrum of adjacency operator on universal covering tree, which is interval $[-2\sqrt{q}, 2\sqrt{q}]$
- Ramanujan graphs provide efficient communication networks: best expander properties

Pole locations for regular graphs

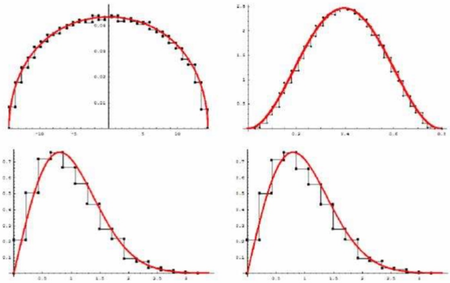
- using the determinant formula for the Ihara zeta function
- possible location of poles for a $(q+1)$-regular graph



- poles on the circles: those that satisfy Riemann Hypothesis
- non-trivial poles $(\neq \pm 1, \pm q^{-1})$ on other lines: non-RH poles
- $1/q$ always the closest pole to 0 for $(q+1)$-regular graph
- Alon conjecture: RH *approximately* true for most regular graphs (and asymptotically 27% of regular graphs satisfy exactly)

Spectra of random real symmetric matrices

- similar behavior of statistics of spectra of random real symmetric matrices and statistics of imaginary parts of s at poles of Ihara zeta $\zeta(q^{-s}, G)$ for a $(q+1)$-regular graph G



- pseudo-random regular graph deg=53 and 2000 vertices: top row distrib of eigenvalues of adjacency matrix (left) and imaginary part of Ihara poles (right); level spacings on second row
- red line: Wigner law for GOE random matrices

Beyond regular case

- R_G = radius of largest circle of convergence of Ihara zeta function (conv abs for $|u| < R_G$, pole order 1 at $u = R_G$ for G connected)
- $1/R_G$ is spectral radius of edge adjacency matrix ($W_{ij} = 1$ if $t(e_i) = s(e_j)$)
- poles of Ihara zeta = reciprocals of eigenvalues of edge adjacency matrix
- for $(q+1)$-regular G have $R_G = 1/q$
- Ihara Riemann Hypothesis for irregular graphs

$$\text{no poles of } \zeta(u, G) \text{ in region } R_G < |u| < \sqrt{R_G}$$

- no good functional equation for Ihara in this case, so $u = R_G^s$ and $0 < \Re(s) < 1$ too large and only half-strip for RH
- still a way of detecting good expander properties

Ruelle zeta function

- dynamical system iterates of $f : M \to M$ on a compact manifold with finite sets of fixed points $\mathrm{Fix}(f^m)$ for all $m \geq 1$
- assign a weight function (matrix valued) $\phi : M \to M_{D\times D}(\mathbb{C})$
- Ruelle zeta function:

$$\zeta(u) := \exp\Big(\sum_{m\geq 1} \frac{u^m}{m} \sum_{x\in \mathrm{Fix}(f^m)} \mathrm{Tr}\big(\prod_{k=0}^{m-1} \phi(f^k(x))\big)\Big)$$

- generalization of the Artin–Mazur zeta function

$$\zeta(u) = \exp\Big(\sum_{m\geq 1} \frac{u^m}{m} \#\mathrm{Fix}(f^m)\Big)$$

which in turn generalizes case of the Frobenius on varieties over finite fields (counting points over finite fields as fixed points of powers of Frobenius)

Subshift of finite type

- $\mathcal{I}$ set of directed edges of a graph G (alphabet)
- transition matrix (W_{ij}) entries $\{0,1\}$ is edge adjacency matrix
- admissible words $(a_k)_{k\in\mathbb{N}} \in \mathcal{I}^{\mathbb{N}}$ with $W_{a_k a_{k+1}} = 1$ are (infinite) paths in G without backtracking
- shift map $\sigma : \mathcal{I}^{\mathbb{N}} \to \mathcal{I}^{\mathbb{N}}$ mapping $a_0 a_1 a_2 \cdots$ to $a_1 a_2 a_3 \cdots$
- $\mathrm{Fix}(\sigma^m) =$ closed paths of length m without tails or backtracking
- Ihara zeta function is a special case of Ruelle zeta function

$$\log \zeta(u, G) = \sum_{m\geq 1} \frac{N_m}{m} u^m$$

with number of closed paths of length m

$$N_m = \#\mathrm{Fix}(\sigma^m) = \mathrm{Tr}(W^m)$$

Matrices associated to graphs

- $A =$ vertex adjacency matrix
- $L = D - A$ Graph Laplacian (with D diagonal matrix of degrees of vertices)
- $W =$ edge adjacency matrix: $2 \cdot \#E \times 2 \cdot \#E$ matrix with (i,j) entry 1 if e_i feeds into e_j (counting edges and their inverses)

Hashimoto Determinant Formula

- $W =$ edge adjacency matrix
- Ihara Zeta Function

$$\zeta(u, G)^{-1} = \det(I - uW)$$

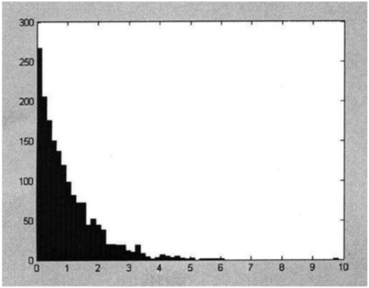
- poles of the Ihara Zeta Function are reciprocals of eigenvalues of the edge adjacency matrix W

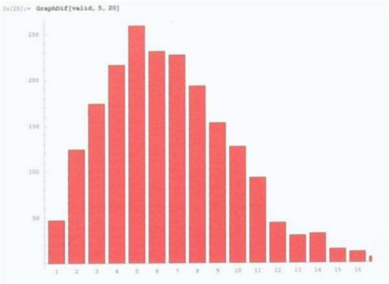
- Kotani-Sudana: connected graph G with $\mathrm{rank}\pi_1(G) > 1$, no $\deg = 1$ vertices, min degree $p+1$, max deg $q+1$: every non-real pole of Ihara zeta $\zeta(u, G)$

$$q^{-1/2} \leq |u| \leq p^{-1/2}$$

and poles on circle $|u| = R_G$ are $u = R_G e^{2\pi i a/\Delta_G}$ with $a = 1, \ldots, \Delta_G$ and $\Delta_G =$ gcd lengths of prime paths (tail-less primitive closed paths)

Spacing of Ihara Poles





difference between Euclidean graph (Cayley graph of an abelian group) and random regular graph: the Euclidean case looks like a Poisson distribution while the random case looks like Wigner's law for GOE

$$\frac{1}{2}\pi x \exp(-\pi x^2/4)$$

when arranging eigenvalues of a symmetric matrix in decreasing order and normalize them so that mean of level spacing is 1

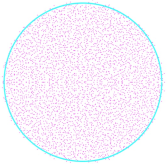
Spectral properties of edge adjacency W

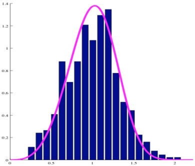
- Girko circle law: eigenvalues of a set of random $n \times n$ real matrices with independent entries with a standard normal distribution approximately uniformly distributed in a circle of radius $\sqrt{n}$ for large n
- random matrix that, like W has form

$$W = \begin{pmatrix} A & B \\ C & A^t \end{pmatrix}$$

with B, C symmetric real, A real with transpose A^t

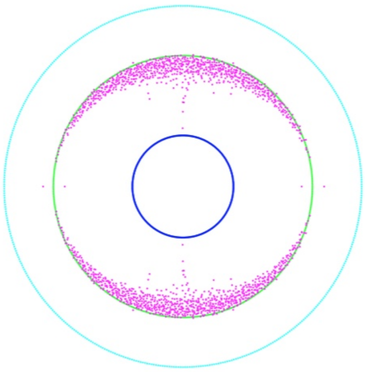
- construct random matrices with this same structure: then circle radius not same as Girko's: spectrum and spacings

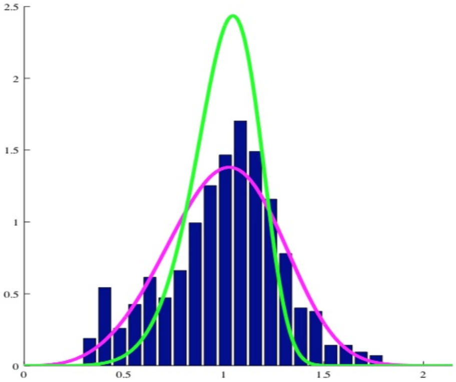




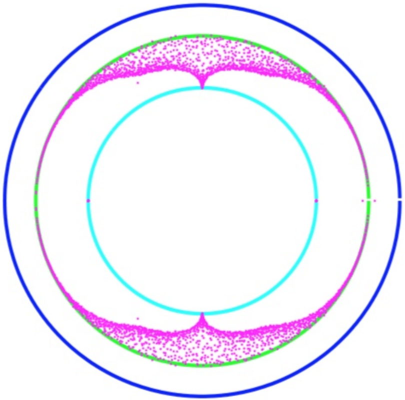
- What shape of the spectrum for actual W?

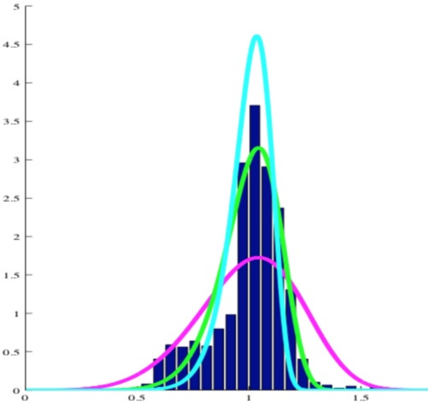
• by Kotani-Sudana spectrum cannot fill a disk: in an annulus



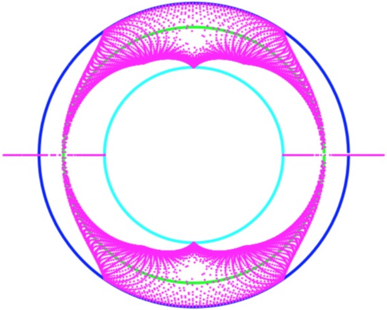


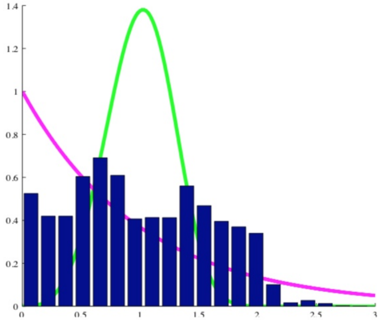
eigenvalues (pink points) of edge adjacency matrix W for a random graph with 800 vertices mean deg 13.125 and edge probability $p \sim 0.0164$; green circle RH; histogram of nearest neighbor spacings in $\mathrm{Spec}(W)$





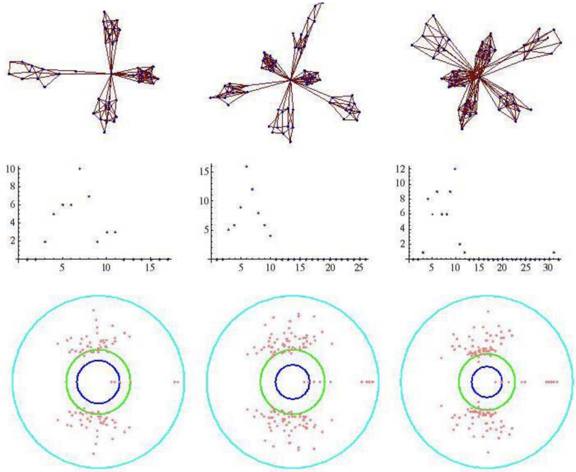
eigenvalues (pink points) and spacings of edge adjacency matrix W for a random cover of the graph with two loops and one extra vertex on one loop (801 sheets of cover, each a copy of a spanning tree)





eigenvalues (pink points) and spacings of edge adjacency matrix W for an abelian covering of same graph (Galois group $\mathbb{Z}/163 \times \mathbb{Z}/45$)

detecting poor or good expander properties



graphs, histogram of degrees, poles of Ihara zetas (green RH circle, and outer/inner Kotani-Sudana circles