Spectral density of random graphs: convergence properties and application in model fitting

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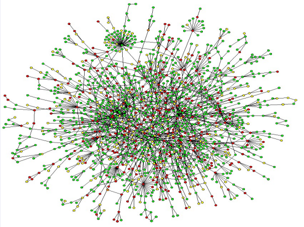
Outline

1. Model selection for statistical analysis of random graphs
2. The empirical spectral density of a graph
3. Model selection procedure
4. Results and some experiments

Outline

Data: networks, their properties and beyond I

Some networks characteristics



- Potentially large number n of interacting entities,
- Potentially **sparse** networks: number of edges $\ll O(n^2)$,
- **Scale-free property** : Degree distribution has a power law $\mathbb{P}(D_i = k) = ck^{-\gamma}, (\gamma > 0)$,
- **Small world property**: shortest path length is small on average (less than 6),
- **Transitivity/clustering property**: is there a large amount of triangles?
- ...

Data: networks, their properties and beyond II

Some challenges

- Go beyond these (local) descriptors and capture **higher-level structures**, such as topological patterns, cliques, nodes groups, etc,
- Propose relevant models that will capture those structures **without any a priori information on which structures we are looking for**,
- Go from static to **dynamic** models,
- Go from pairwise interactions to **higher order** interactions,
- ...

Random graphs models for networks

Random graphs are the mathematical tools that model the networks.

Some existing models, advantages and drawbacks

- Erdös-Rényi, **simple and mathematically well-understood**, too homogeneous;

$$\textit{edges are i.i.d.} \sim \mathcal{B}(p)$$

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  Nodes degrees are fixed, samples obtained through rewiring algorithm

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- Generative processes (like preferential attachment), **dynamic model**, depends on parameters that may not be inferred from data (initialisation, stop, exact procedure, . . .),

  Start from a small graph, add nodes and connect them with higher prob. to nodes with large degrees

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- Exponential random graph, **natural from a statistical point of view**, big inference issues ;

$$\mathbb{P}_\theta(\mathbf{Y} = \mathbf{y}) = c(\theta)^{-1} \exp(\theta^\intercal S(\mathbf{y}))$$

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Model selection issue

- For a fixed model, specific statistical procedures fit the model to the data through parameter inference algorithms ;
- **Issue**: how do you compare 2 different models?
  - Model selection procedures are required.
  - Criteria such as estimated likelihood can't be used (at least without penalization terms)

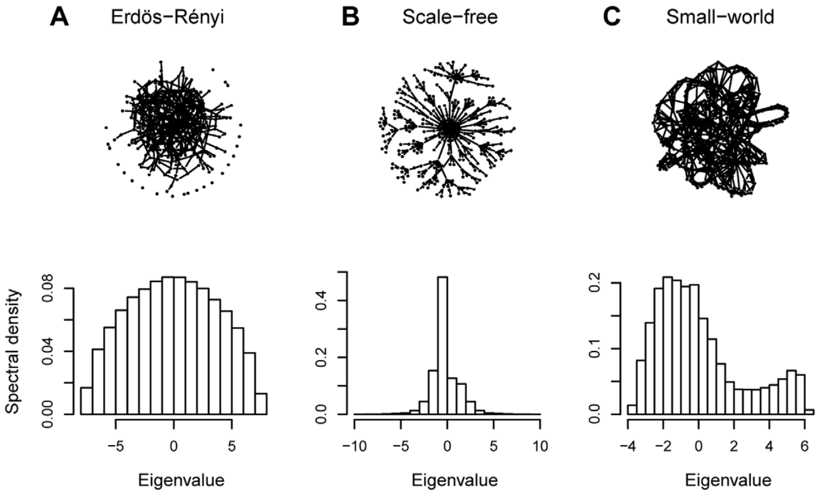
Outline

Empirical spectral density (ESD) I

Spectrum of a matrix

- The spectrum of a matrix is the set of its eigenvalues;
- The adjacency matrix of an undirected graph is a real symmetric matrix, hence its spectrum is real valued.
- The empirical spectral density (ESD) is the empirical distribution over the set of (normalized) eigenvalues.
- **Characteristic:** a lot of the graph's information is contained in its ESD.

Empirical spectral density (ESD) II



Picture from [TSFF12].

Empirical spectral density (ESD) III

Adjacency or Laplacian?

- Laplacian matrices L are 'normalized' versions of adjacency matrices A, e.g $L = I - D^{-1/2}AD^{-1/2}$ where D diagonal with degrees.
- In the following, we focus on adjacency matrices.

Beware: Random graphs induce random ESD

- Once we fix a random graph model, the entries of the adjacency matrix are random variables. Thus the eigenvalues are also random and the ESD becomes a random measure.
- Behaviour of the random ESD, as the number of nodes increases, relates to **random matrix theory**.

Empirical spectral density (ESD) IV

Notation

- A adjacency matrix of (undirected) graph G over n nodes
- $\lambda_1^G \geq \lambda_2^G \geq \cdots \geq \lambda_n^G$ the eigenvalues of A
- ESD and corresponding cumulative distr function (CDF):

$$\mu^G(\cdot) = \frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i^G/\sqrt{n}}(\cdot); \quad F^G(x) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\left\{ \frac{\lambda_i^G}{\sqrt{n}} \leq x \right\},$$

In other words, for any function f, we have
$\mu^G(f) = \int_{\mathbb{R}} f(\lambda)\mu^G(d\lambda) = \frac{1}{n}\sum_{i=1}^{n} f(\lambda_i^G/\sqrt{n})$.

ESD as a tool to estimate a random graph model

Principle and Questions

- It is **easy to compute** the ESD of a random graph from the observation of its adjacency matrix
- AND a lot of the **graph's information** is contained in its spectral density.
- Thus, a natural idea is to use this ESD to discriminate between 2 random graphs models.

Our goals

Takahashi's *et al.* [TSFF12] have proposed such a procedure.

- Better understand the theoretical properties of such a procedure
- For this we need to understand more about the limiting behaviour of the ESD.

Convergence properties of the ESD

Wigner's law

If the entries of A are **iid with zero mean and unit variance**, then the ESD converges (weakly in expectation) to the semicircle law

$$\mu_{sc}(dx) = \frac{1}{2\pi}\sqrt{4 - x^2}\mathbf{1}\{|x| \leq 2\}dx. \tag{1}$$

- Important issues in random matrix theory: in more general contexts,
  - does the ESD still converge to some limit?
  - If yes, what is this limit?
- **Question here**: can we use these results to prove that the model selection procedure based on ESD is consistant?

Spectral densities of random graph models I

Spectral density

- A (parametric) random graph model is a collection of graphs $\mathcal{G}$ together with a family of distributions $\{\mathbb{P}_\theta, \theta \in \Theta\}$ over $\mathcal{G}$.
- Consider a sequence of graphs $(G_n)_{n\geq 1}$ with distribution $\mathbb{P}_\theta$, whenever the limit of the sequence of ESDs $(\mu^{G_n})_{n\geq 1}$ exists, we denote it μ_θ. It's the **spectral density associated to the probability measure** $\mathbb{P}_\theta$.

Example

The Erdös-Rényi (ER) model $\mathcal{G}(n,p)$ is a family of distributions over the set of graphs with n nodes. Here $\theta = p$ is the parameter of the model and it is known that the ER spectral density is

$$\mu_{p,sc}(dx) = \frac{1}{2\pi p(1-p)}\sqrt{4p(1-p)-x^2}\mathbf{1}\{|x| \leq 2\sqrt{p(1-p)}\}dx.$$

Spectral densities of random graph models II

How do you compute the spectral density?

- Recall that the spectral density is defined as the **limit** of ESDs.
- Either you have an analytic formula for the spectral density
- Or you can sample many different graphs from $\mathbb{P}_\theta$ with large size and approximate the spectral density through the ESDs of these graphs.

State of the art about existing spectral densities

Model	Matrix	Limit
ER	$\mathbf{A}/\sqrt{n}$	$\mu_{p,sc}(x) = \frac{1}{2\pi p(1-p)}\sqrt{[4p(1-p)-x^2]_+}$
	$\mathbf{A}/\sqrt{np(1-p)}$	$\mu_{sc}(x) = \frac{1}{2\pi}\sqrt{[4-x^2]_+}$
DR	$\mathbf{A}$	$\mu_d(x) = \frac{d}{2\pi(d^2-x^2)}\sqrt{[4(d-1)-x^2]_+}$
	$\mathbf{A}/\sqrt{d-1}$	$\tilde{\mu}_d(x) = \left(1+\frac{1}{d-1}-\frac{x^2}{d}\right)^{-1}\frac{1}{2\pi}\sqrt{[4-x^2]_+}$
BM	$(\mathbf{A}-\mathbb{E}(\mathbf{A}))/\sqrt{np^\star(1-p^\star)}$	expression through Stieltjes transform

Table: Convergences of ESD in different models.

DR : d-regular graphs ; BM: blockmodel graphs (+ some constraints).
Remark: Very few results compared to variety of models.

Outline

Model selection by Takahashi's *et al.* [TSFF12]

General idea

- For a fixed parametric model $\{\mathbb{P}_\theta, \theta \in \Theta\}$ and a grid of values $\theta \in \tilde{\Theta}$, compute (the kernel estimator of) the ESD μ_θ under parameter θ.
- Compare each μ_θ with (the kernel estimator of) the ESD μ^G of the observed graph G, through some distance D.
- Select the model and corresponding parameter value with closest distance.

Advantages

- No need for a model specific inference procedure;
- Compares models with completely different number of parameters, with no need to penalize for these numbers.

Algorithm's description

Input: Graph $\mathcal{G}$, a list of random graph models $\{P^i_\theta; \theta \in \Theta^i \subset \mathbb{R}^d\}$, a finite subset $\tilde{\Theta}^i \subset \Theta^i$, for $i = 1, 2, \ldots, N$.

Output: Return model and parameter with best fit.

Compute the kernel density estimator $\mu^{\mathcal{G}}$.

for each parameterized random graph model $\{P^i_\theta; \theta \in \Theta^i\}$, $i = 1, 2, \cdots, N$, **do**

  for each $\theta^j \in \tilde{\Theta}^i$ **do**

    if the limit of ESD from $P^i_{\theta^j}$, denoted by $\mu^i_{\theta^j}$, is known analytically **then**

      $D_{i,j} \leftarrow D(\mu^{\mathcal{G}}, \mu^i_{\theta^j})$.

    else

      Sample M graphs $\mathcal{G}_1, \mathcal{G}_2, \cdots, \mathcal{G}_M$ from $P^i_{\theta^j}$.

      for each graph $\mathcal{G}_m$ **do**

        Compute the kernel density estimator $\mu^{\mathcal{G}_m}$.

      end for

      $\hat{\mu}^i_{\theta^j} \leftarrow \frac{1}{M} \sum_{m=1}^{M} \mu^{\mathcal{G}_m}$.

      $D_{i,j} \leftarrow D(\mu^{\mathcal{G}}, \hat{\mu}^i_{\theta^j})$

    end if

  end for

end for

return Model and parameter (i, j) with smallest $D_{i,j}$ value

Outline

Consistency results

Theorem

Let $\{P_\theta; \theta \in \Theta\}$ denote a parameterized random graph model and assume that for any $\theta \in \Theta$ there exists μ_θ the limiting ESD with respect to weak, almost sure convergence. We assume that $\mu_\theta \in \mathcal{M}_1(\Lambda)$, where Λ is a bounded set. Consider $(\mathcal{G}_n)_{n\geq 1}$ a sequence of random graphs from distribution $P_{\theta^\star}$. If the map $\theta \mapsto \mu_\theta(d\lambda)$ is injective, continuous and Θ is compact, then the minimizer

$$\hat{\theta}_n = \underset{\theta \in \Theta}{Argmin} \|\mu^{\mathcal{G}_n} - \mu_\theta\|_1$$

converges in probability to $\theta^\star$ as $n \to \infty$.

Consequence: Using D the $\mathbb{L}_1$-norm, [TSFF12]'s procedure will recover the true parameter value.

Block model spectral density - beyond [ACK15] I

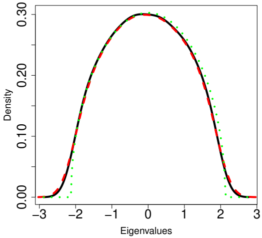
ESD convergence for BM is established in [ACK15] under the particular case of equal size groups ; equal probability p_0 of connecting vertices from different groups ; and intra group probability $p_m > p_0$ for each $1 \leq m \leq M$.

Settings - 5 scenarios

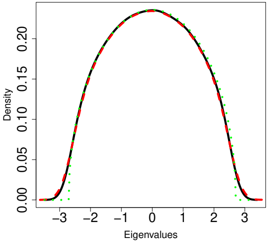
$K=$ bloc sizes ; $M=$ nb groups ; p_0 inter-group probability ; p_m intra-groups probabilities

	K	M	p_0	p_m
S1	300	3	0.2	(0.8,0.5,0.6)
S2	300	10	0.2	$(0.8, 0.5, 0.6, 0.7, 0.4, 0.9, 0.55, 0.42, 0.38, 0.86)$
S3	100,80,300	3	0.2	(0.8,0.5,0.6)
S4	300	3	0.9	(0.8,0.5,0.6)
S5	300	3		$\begin{pmatrix} 0.8 & 0.1 & 0.2 \\ \star & 0.5 & 0.05 \\ \star & \star & 0.6 \end{pmatrix}$

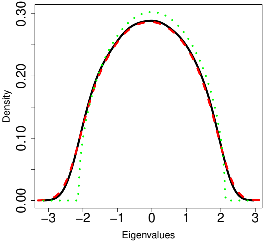
Block model spectral density - beyond [ACK15] II



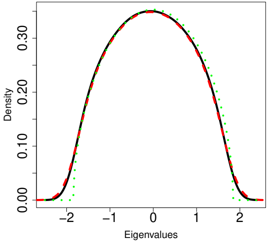
(a) Scenario 1



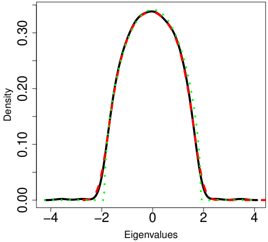
(b) Scenario 2



(c) Scenario 3



(d) Scenario 4



(e) Scenario 5

Block model spectral density - beyond [ACK15] III

Notation $\gamma(n) = \sqrt{np_\star(1-p_\star)}$; $\tilde{A} = (A - E(A))/\gamma(n)$ and $p_\star = \max_{m \geq 1} p_m$.

Comments

- For all the scenarios, the ESDs of $\mathbf{A}/\gamma(n)$ and $\tilde{\mathbf{A}}$ were very close
- For scenarios 1, 2, 4, and 5, the ESD of $\tilde{\mathbf{A}}$ and $\mathbf{A}/\gamma(n)$ are close to the theoretical distribution from [ACK15] ;
- For scenario 3 the ESD are farther from the theoretical density. This might be due to numerical errors during ESD estimation or might indicate that Avrachenkov *et al.*'s results do not apply to graphs with blocks of different sizes.

Conclusions

- We reviewed known results about the limiting behaviour of ESD in different random graphs models
  - Very few results exist compared to the variety of models (difficult problems)
  - For BlockModels, only partial results are known and in some cases (eg different block sizes), the limiting behaviour seems to differ
- We wanted to establish the convergence of the procedures from [TSFF12]
  - Our result is only partial and establishes consistency of parameter estimation within a parametric model ;
  - but not the convergence of the model selection procedure.

Thank you for your attention!

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[ACK15] K. Avrachenkov, L. Cottatellucci, and A. Kadavankandy. Spectral properties of random matrices for stochastic block model. In *The 2015 4th International Workshop on Physics-Inspired Paradigms in Wireless Communications and Networks*, pages 537–544, 2015.

[TSFF12] Daniel Yasumasa Takahashi, João Ricardo Sato, Carlos Eduardo Ferreira, and André Fujita. Discriminating Different Classes of Biological Networks by Analyzing the Graphs Spectra Distribution. *PLoS ONE*, 7(12):e49949, 2012.