Geometric clustering of a random graph

Antoine Channarond, Jean-Jacques Daudin, Stéphane Robin

4th Stochastic Geometry Days - August 27th 2015

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- 1 Introduction: from interaction networks to random graphs
- 2 Discussion about clustering
- 3 Fast count of the number of clusters in a non-parametric clustering setting

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Interaction networks

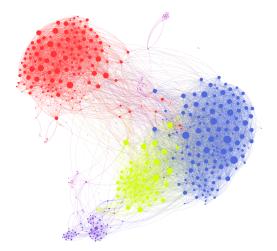


Figure: Friendship network (Source: griffsgraphs.com)

 $\mathsf{Graph}:$

• *n* nodes (individuals)



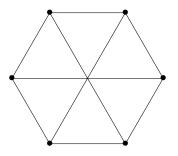
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n = 6

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Graph:

- n nodes (individuals)
- edges (interactions)
 - $X_{ij} = 1$ if nodes *i* and *j* interact.
 - $X_{ij} = 0$ if not.
- undirected edges: $X_{ij} = X_{ji}$
- $X = (X_{ij})$ symmetric adjacency matrix.



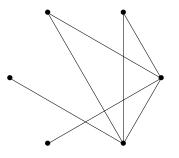
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Random Graph:

- n nodes (individuals)
- random edges (interactions)
 - $X_{ij} = 1$ if nodes *i* and *j* interact.
 - $X_{ij} = 0$ if not.
- undirected edges: $X_{ij} = X_{ji}$

 $X = (X_{ij})$ random symmetric adjacency matrix.



n = 6

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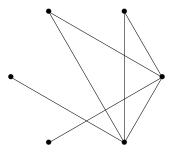
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Erdős-Rényi model:

$$X_{ij}$$
 i.i.d. $\sim \mathcal{B}(p)$

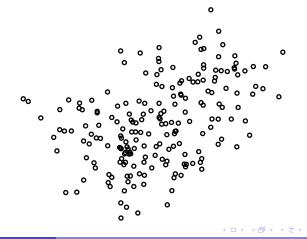


n = 6; p = 0.5

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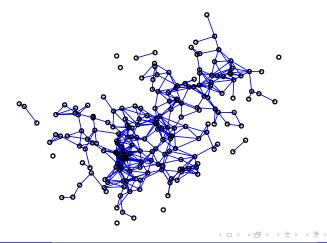
Paradigm: interactions induced by (unobserved) closeness

• Embedding of the individuals in a metric space; here the euclidean space \mathbb{R}^2



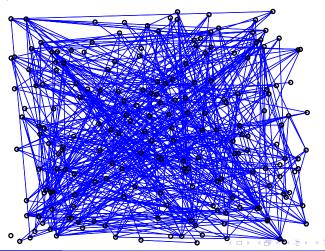
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- Probability of connection decreasing with respect to the euclidean distance



Paradigm: interactions induced by (unobserved) closeness

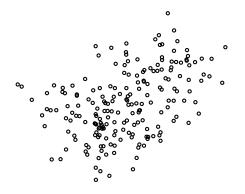
- $\bullet\,$ Embedding of the individuals in a metric space; here the euclidean space \mathbb{R}^2
- Probability of connection decreasing with respect to the euclidean distance
- Positions/distances are not observed.



Latent Position Models

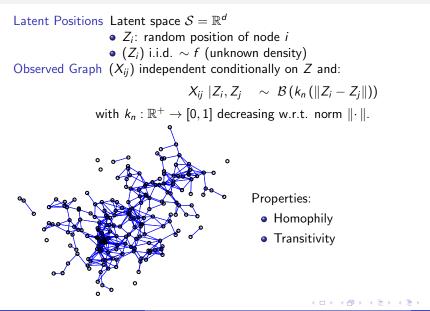
Latent Positions Latent space $S = \mathbb{R}^d$

- Z_i: random position of node i
- (Z_i) i.i.d. ~ f (unknown density)

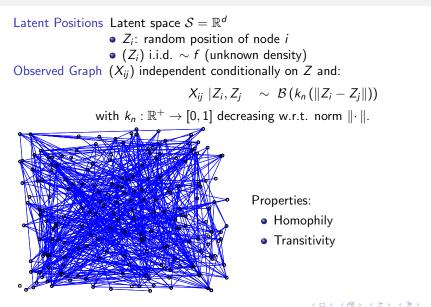


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Latent Position Models



Latent Position Models



Outline



2 Discussion about clustering

3 Fast count of the number of clusters in a non-parametric clustering setting

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Two ideas of clustering

Latent positions $(Z_i)_{i \in [n]}$ i.i.d. $\sim f$

Parametric clustering

• Gaussian Mixture with Q components: $f = \sum_{q=1}^{\infty} \pi_q \mathcal{N}_d(\mu_q, \sigma_q^2 I d).$

• Clusters defined by components of the mixture.

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Two ideas of clustering

Latent positions $(Z_i)_{i \in [n]}$ i.i.d. $\sim f$

Parametric clustering

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• Clusters defined by components of the mixture.

Non-parametric clustering

- f just assumed to be nice (regular).
- Clusters defined using level sets of *f*:

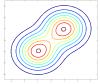


Figure: Level lines of a gaussian mixture

Statistical questions

How to get clustering information on the latent variables Z and their distribution, from the observed graph X only ?

Test Is the distribution of Z clustered ? Model choice How many clusters are there ? Classification Which nodes are in which cluster ? Estimation What are the characteristics of each cluster ?

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Latent Position Cluster Model (Handcock et al, 2007)

Positions Latent space \mathbb{R}^d . Parametric Gaussian mixture:

$$(Z_i)_{i\in[n]}$$
 i.i.d. $\sim f = \sum_{q=1}^Q \pi_q \mathcal{N}_d(\mu_q, \sigma_q^2 I d)$

Graph Logistic regression for the connection probability:

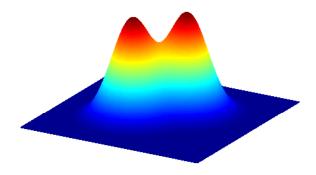
$$\mathsf{log-odds}(X_{ij} = 1 \mid Z_i, Z_j) = -\beta \|Z_i - Z_j\| \quad (\beta > 0)$$

Statistics

- Clustering structure defined by mixture components
 Unsupervised classification of the nodes:
 - **1** ML-Estimation of the distances $(||Z_i Z_j||)_{i,j \in [n]}$,
 - 2 Multidimensional scaling: estimating $(Z_i)_{i \in [n]}$ up to isometries,
 - O EM-algorithm: estimating mixture parameters α_q, μ_q, σ_q and constructing a classification rule.
 - (Estimation of the mixture parameters)
 - Model selection for Q.

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From parametric to non-parametric setting

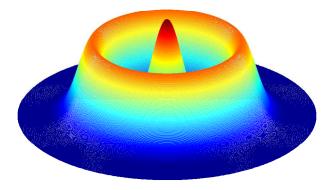


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From parametric to non-parametric setting



Definition of clustering in a non-parametric setting

Definition

Let t > 0 and $\mathcal{L}(t) = \{f \ge t\}$ be the t-level set of a function f. A connected component of $\mathcal{L}(t)$ is called t-cluster (Hartigan, 1975). Q(t) denotes the number of t-clusters.

- Clusters: connected regions of "high" density, i.e. higher than some level t
- Estimation of Q(t), number of such regions

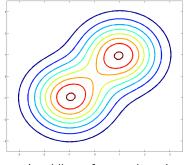
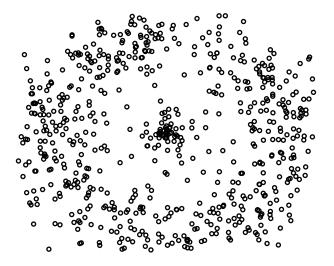
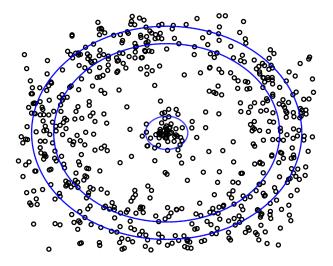


Figure: Level lines of a gaussian mixture

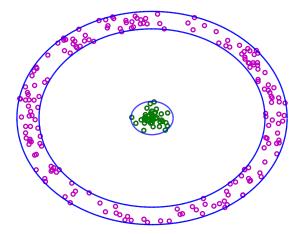


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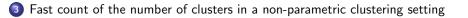


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Outline



2 Discussion about clustering

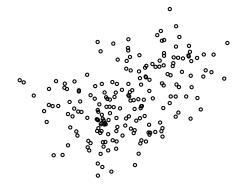


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Non-parametric latent position model

Latent Positions $Z = (Z_i)$ i.i.d. ~ f non-parametric density



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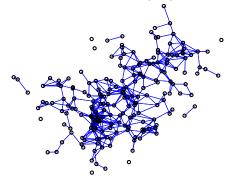
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Non-parametric latent position model

Latent Positions $Z = (Z_i)$ i.i.d. $\sim f$ non-parametric density Observed Graph (X_{ij}) independent conditionally on Z and:

$$X_{ij} | Z_i, Z_j \sim \mathcal{B}\left(k\left(\frac{Z_i-Z_j}{h_n}\right)\right)$$

with $k : \mathbb{R}^d \to [0, 1]$ isotropic and decreasing w.r.t. $\|\cdot\|$, with support B(0, 1), and $h_n > 0$ (connection radius).



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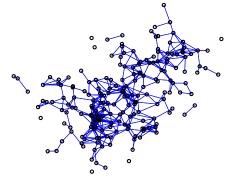
Model

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Graph properties:

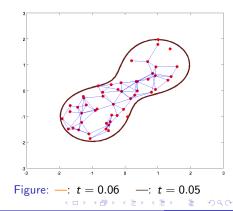
- Homophily
- Transitivity

• Sparsity:
$$\zeta_n = \frac{2}{n(n-1)} \sum_{1 \le i,j \le n} X_{ij}$$

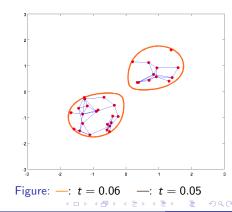
$$\mathbb{E}(\zeta_n)\sim_{h_n\to 0} h_n^d \int_{\mathbb{R}^d} f^2(z)dz$$

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- Find a graph \widehat{X} covering $\mathcal{L}(t)$ to make a link between clusters of $\mathcal{L}(t)$ and connected components of the graph \widehat{X} : Biau, Cadre, Pelletier (2007).
- Extract \widehat{X} from X by removing low degree nodes.
- nh_n^d -normalized degrees : $T_i^{h_n} = \frac{D_i}{nh_n^d}$



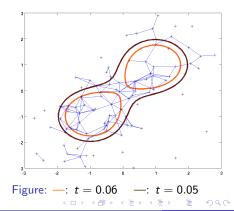
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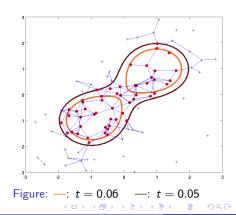
Algorithm

Compute nh^d_n-normalized degrees



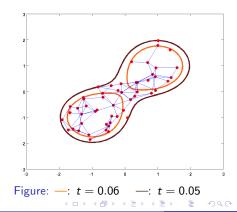
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- Compute nh^d_n-normalized degrees
- Sind the set Ĵ_n(t) of nodes i such that T^{h_n}_i ≥ t



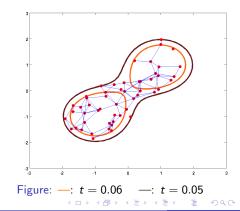
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- Compute nh^d_n-normalized degrees
- Solution Find the set $\widehat{J}_n(t)$ of nodes i such that $T_i^{h_n} \ge t$
- 8 Remove other nodes from X



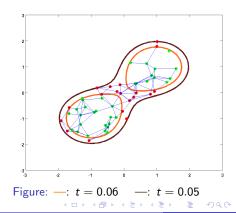
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- Compute nh^d_n-normalized degrees
- Solution $\widehat{J}_n(t)$ of nodes i such that $T_i^{h_n} \ge t$
- 8 Remove other nodes from X
- Count the number $\widehat{Q_n}(t)$ of connected components of the graph $\widehat{X} = X_{\widehat{J_n}(t)}$ with DFS (linear)



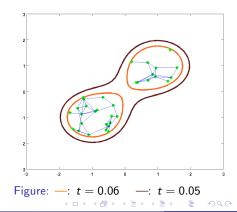
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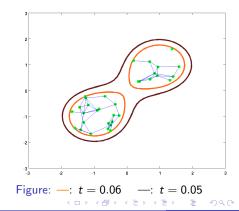


Counting the *t*-clusters with a covering graph

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Algorithm

- Compute nh^d_n-normalized degrees
- Solution $\widehat{J}_n(t)$ of nodes *i* such that $T_i^{h_n} \ge t$
- 8 Remove other nodes from X
- Count the number $\widehat{Q_n}(t)$ of connected components of the graph $\widehat{X} = X_{\widehat{J_n}(t)}$ with DFS (linear)



Biau, Cadre, Pelletier (2007)

Model X is deterministic w.r.t. Z: $k(x) = \mathbb{1}_{||x|| \le 1}$

Generalization

Model k is a kernel function with support in the unit ball

Biau, Cadre, Pelletier (2007)

Model X is deterministic w.r.t. Z: $k(x) = \mathbb{1}_{||x|| \le 1}$ Context not latent, positions Z are observed

Generalization

Model k is a kernel function with support in the unit ball Context latent, positions Z are not observed

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Model X is deterministic w.r.t. Z: $k(x) = \mathbb{1}_{||x|| \le 1}$

Context not latent, positions Z are observed

Estimator of the density at the node positions $\hat{f}_n(Z_i)$, with a kernel estimator:

$$\widehat{f}_n(z) = \frac{1}{nh_n^d} \sum_{i=1}^n K\left(\frac{z-Z_i}{h_n}\right)$$
 where K is a kernel function

Generalization

Model k is a kernel function with support in the unit ball

Context latent, positions Z are not observed

Estimator of the density at the node positions, nh_n^d -normalized degrees of X:

$$T_i^{h_n} = \frac{1}{nh_n^d} \sum_{i=1}^n X_{ij}$$

Algorithm

Biau, Cadre, Pelletier (2007)

Model X is deterministic w.r.t. Z: $k(x) = \mathbb{1}_{||x|| < 1}$

Context not latent, positions Z are observed

Estimator of the density at the node positions $\hat{f}_n(Z_i)$, with a kernel estimator:

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Estimator of the density at the node positions, nh_n^d -normalized degrees of X:

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Proposition:
$$\mathbb{E}\left(T_{i}^{h_{n}}|Z\right) = \widehat{f}_{n}(Z_{i})$$
 where $\widehat{f}_{n}(z) = \frac{1}{nh_{n}^{d}}\sum_{j=1}^{n}k\left(\frac{z-Z_{j}}{h_{n}}\right)$

Hypotheses and result (article to be submitted)

- f uniformly continuous and of class C^1 on the neighborhood of $\{f = t\}$.
- $df \neq 0$ on $\{f = t\}$.

•
$$h_n$$
 small enough and $\frac{nh_n^d}{\ln n} \xrightarrow[n \to \infty]{} +\infty$

Theorem

Non-underestimation $\widehat{Q_n}(t)$ =number of connected components of $X_{\widehat{J_n}(t)}$. For some ε_n , h_n small enough:

$$P\left(\widehat{Q_n}(t) < Q(t)\right) \leq 3n \exp\left(-K_0 \varepsilon_n^2 n h_n^d\right)$$

Non-overestimation $J_n(t)$ set of the nodes *i* such that $f(Z_i) \ge t$. $\widetilde{Q}_n(t)$ is the number of connected components of $X_{J_n(t)}$. For h_n small enough:

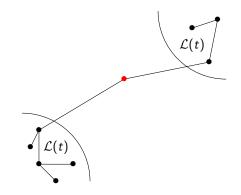
$$P\left(\widetilde{Q}_n(t) > Q(t)\right) \leq K_1 n \exp(-K_2 n h_n^d)$$

 $\mathcal{L}(t)$



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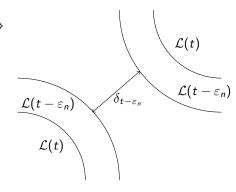
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• On the event $\left\{\sup_{i\in[n]} |T_i^{h_n} - f(Z_i)| \le \varepsilon_n\right\}$ with $\varepsilon_n > 0$

$$T_i^{h_n} \geq t \Rightarrow Z_i \in \mathcal{L}(t - \varepsilon_n)$$



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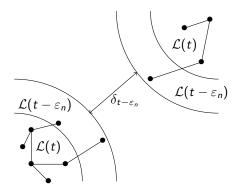
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• δ_t = distance between two *t*-clusters.

$$h_n < \delta_{t-\varepsilon_n}$$

No connection between distinct clusters.



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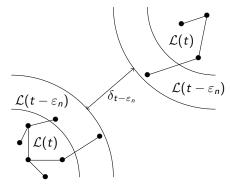
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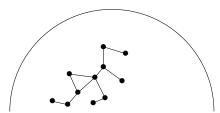
Concentration inequality (Bernstein):

$$P\left(\sup_{i\in[n]}|T_i^{h_n}-f(Z_i)|>\varepsilon_n\mid Z_i\right)\leq 2n\exp(-K_3\varepsilon_n^2nh_n^d)$$



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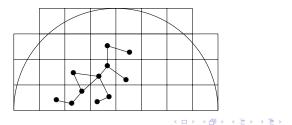
Connectivity of the subgraph induced by each cluster:



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Connectivity of the subgraph induced by each cluster:

• Cover of each cluster with hypercubes of side $h_n/2$

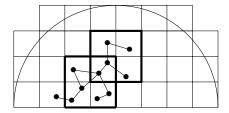


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Connectivity of the subgraph induced by each cluster:

- Cover of each cluster with hypercubes of side $h_n/2$
- Local connectivity:
 - In hypercubes of side h_n , any two nodes can be connected
 - Comparison to Erdős-Rényi. Let C be one hypercube of the cover:

 $P(X_C \text{ is connected}) \geq P(\mathcal{ER} \text{ is connected})$



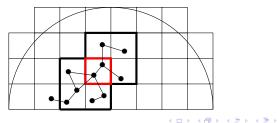
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Connectivity of the subgraph induced by each cluster:

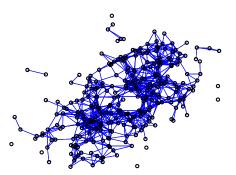
- Cover of each cluster with hypercubes of side $h_n/2$
- Local connectivity:
 - In hypercubes of side h_n , any two nodes can be connected
 - Comparison to Erdős-Rényi. Let C be one hypercube of the cover:

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P(X_C \text{ is connected}) \geq P(\mathcal{ER} \text{ is connected})
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- From local to global connectivity:
 - Filling of the hypercubes



Classification



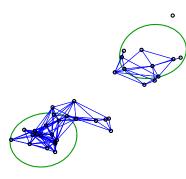
Two kinds of error controlled in the theorems :

• support error (thresholding error)

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classification error

Classification



Two kinds of error controlled in the theorems :

• support error (thresholding error)

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classification error

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Simulation study

Simulation design

- $R_i \sim 0.15 \mathcal{N}(0, 1) + 0.85 \mathcal{N}(5, 1)$
- $\theta_i \sim \mathcal{U}([0, 2\pi])$
- k Epanechnikov kernel
- $h_n = h = 1$
- t = 0.005
- 300 graphs drawn

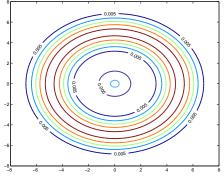


Figure: Isolines of the density

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Illustration of the consistency of $\widehat{Q_n}(t)$

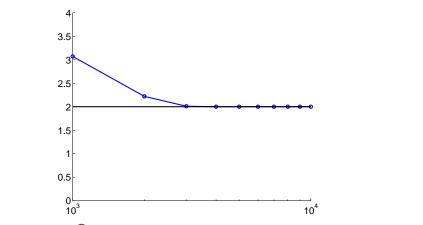
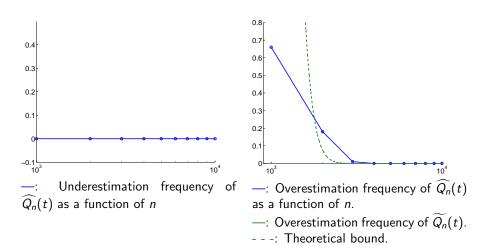


Figure: —: Estimator $\widehat{Q}_n(t)$ as a function of *n* (averaged over 300 graphs); —: Objective

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Under- and overestimation frequency



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Clustering profile: a practical implementation

Invariance under similarity transformations of the latent space

If *R* is a similarity transformation of \mathbb{R}^d with scale factor λ :

- $Z_i \longrightarrow Z'_i = R(Z_i)$
- $h_n \longrightarrow \lambda h_n$

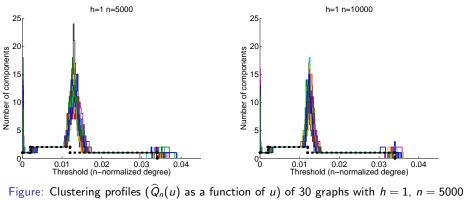
$$P(X_{ij} = 1 \mid Z'_i, Z'_j) = k\left(\frac{\|R(Z_i) - R(Z_j)\|}{\lambda h_n}\right) = k\left(\frac{\|Z_i - Z_j\|}{h_n}\right)$$

Practical algorithm

- Compute *n*-normalized degrees: $T_i = \frac{D_i}{n}$. (threshold: $u = th_n^d$)
- Sort (T_i) without ex-aequo values $\longrightarrow (T_{(k)})_{k \in [m]}$
- Run the algorithm: remove nodes *i* such that $T_i \ge u = T_{(k)}$ for each *k*
- Plot $\widehat{Q}_n(u)$ as a function of u.

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Clustering profile: simulation



and n = 10000

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Clustering profile: simulation

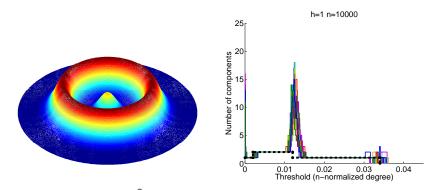


Figure: Clustering profiles ($\hat{Q}_n(u)$ as a function of u) of 30 graphs with h = 1, n = 5000and n = 10000

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Conclusions and perspectives

Conclusions

- No likelihood-based strategy
- Behaviour of the degree distribution of the graph model
- Fast algorithm, able to process large graphs
- Theoretical guarantees: consistency proof

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Conclusions and perspectives

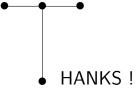
Conclusions

- No likelihood-based strategy
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- Fast algorithm, able to process large graphs
- Theoretical guarantees: consistency proof

Perspectives

- Application to real-world networks
- Complete consistency of $\widehat{Q}_n(t)$
- Statistical properties of clustering profiles
- Robustness: small components filtering and theoretical arguments
- First step to test " latent distribution clustered" vs. "not clustered"

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