

Consistency of Modularity Clustering on Random Geometric Graphs

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Outline

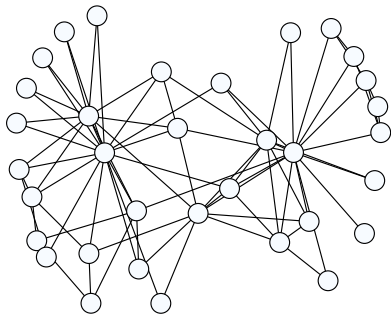
Introduction to Modularity Clustering

Pointwise Convergence

Convergence of Optimal Partitions

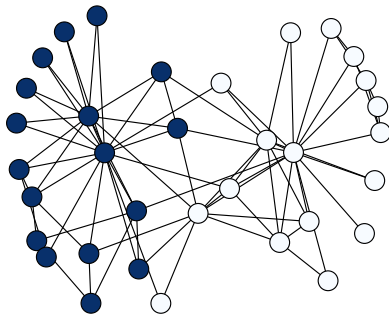
Graph Clustering

$$G = (X, W)$$



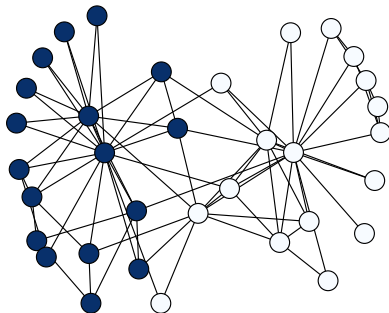
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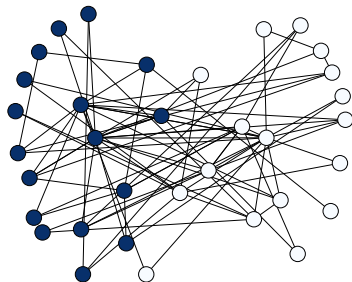
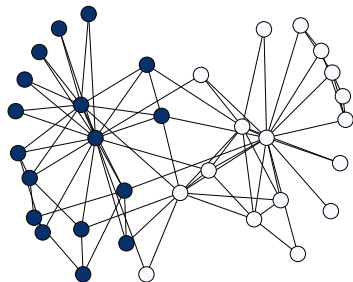


$$\frac{1}{2m} \sum_{i,j} W_{ij} \delta(c_i, c_j) \text{ where } m = \frac{1}{2} \sum_{i,j} W_{ij}.$$

Modularity (Newman & Girvan '04)

$$Q(\mathcal{U}) = \frac{1}{2m} \sum_{i,j} W_{ij} \delta(c_i, c_j) - \frac{1}{2m} \sum_{i,j} \frac{d_i d_j}{2m} \delta(c_i, c_j)$$

where $d_i = \sum_j W_{ij}$, \mathcal{U} a clustering.



Modularity Clustering

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More generally (α -modularity):

$$Q(\mathcal{U}) = \frac{1}{2m} \sum_{i,j} W_{ij} \delta(c_i, c_j) - \frac{1}{S^2} \sum_{i,j} d_i^\alpha d_j^\alpha \delta(c_i, c_j)$$

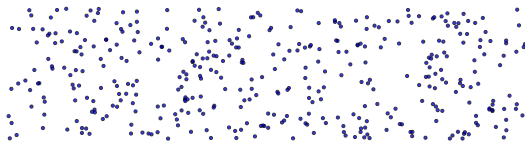
where $S = \sum_i d_i^\alpha$.

Random Geometric Graphs

Fix open $D \subset \mathbb{R}^d$ with Lipschitz boundary, $\nu = \rho(x) dx$ probability measure on D .

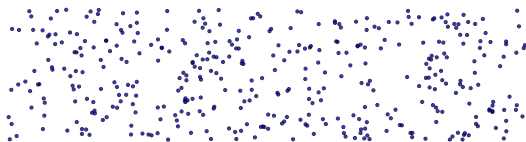
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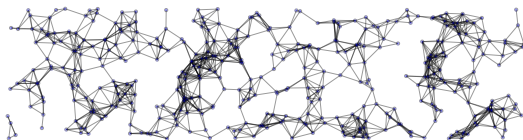
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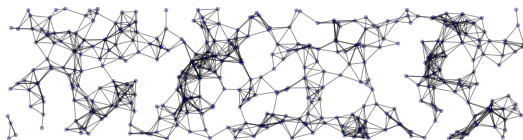


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Graph $\mathcal{G}_n = (\mathcal{X}_n, W)$.

Questions

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Consistency: Subject to certain technical assumptions, $\mathcal{U}_n^* \rightarrow \mathcal{U}^*$ where \mathcal{U}^* is a partition of D characterized as the solution to a (deterministic) continuum optimization problem.

Consistency of Clustering Methods

- ▶ K-Means (Pollard 1981)
- ▶ Spectral Clustering (von Luxburg, Belkin, & Bosquet 2008)
- ▶ Modularity (Bickel & Chen 2009, Zhao, Levina, & Zhu 2012)
- ▶ Cheeger Cut (García-Trillos, Slepčev, von Brecht, Laurent, & Bresson 2014)

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Convergence of Optimal Partitions

Key Identity

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Then

$$1 - 1/K - Q_n(\mathcal{U}_n) = \frac{1}{S^2} \sum_{k=1}^K \left(\sum_i d_i^\alpha [u_{n,k}(X_i) - 1/K] \right)^2 \\ + \epsilon_n \frac{n^2}{4m} \sum_{k=1}^K GTV_n(u_{n,k}),$$

where

$$GTV_n(u) := \frac{1}{\epsilon_n} \frac{1}{n^2} \sum_{i,j} \eta_{\epsilon_n}(X_i - X_j) |u(X_i) - u(X_j)|.$$

Continuum Partitioning

Domain $D \subset \mathbb{R}^d$, fixed $K \geq 1$, and partition $\mathcal{U} = \{U_k\}_{k=1}^K$ of D .

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- ▶ \mathcal{U} is *balanced* with respect to μ if $\mu(U_k) = 1/K$ for $k = 1, \dots, K$.
- ▶ The *perimeter* of U_k in D , with respect to a weight ρ^2 , is

$$\text{Per}(U_k; \rho^2) = \int_{\partial U_k} \rho^2(x) d\mathcal{H}^{d-1}(x).$$

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More generally,

$$\text{Per}(U_k; \rho^2) = TV(\mathbb{1}_{U_k}; \rho^2) := \sup_{\substack{\Phi \in C_c^1(D; \mathbb{R}^d) \\ |\Phi(x)| \leq \rho^2(x)}} \int_D \mathbb{1}_{U_k}(x) \text{div } \Phi(x) dx.$$

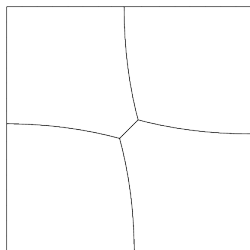
Remark: When f smooth, $TV(f; \rho^2) = \int_D |\nabla f| \rho^2(x) dx$.

Continuum Partitioning

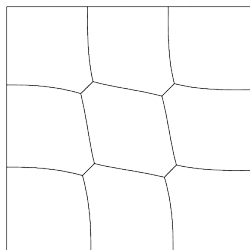
$$\mathcal{U}^* = \arg \min_{\substack{|\mathcal{U}|=K \\ \mu(U_k)=1/K}} \sum_{k=1}^K \text{Per}(U_k; \rho^2).$$

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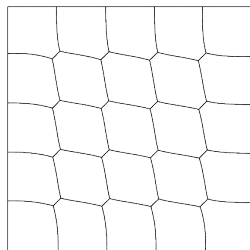
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(a) $K = 4$



(b) $K = 9$.



(c) $K = 25$.

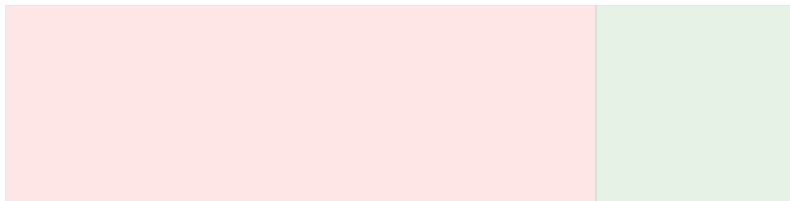
Figure: Local minimizers on $D = (0, 1)^2$, with $\rho(x) = 1$, $d\mu = dx$, produced using *The Surface Evolver*.

“Pointwise” Convergence

A (finite perimeter) partition \mathcal{U} of D induces a partition \mathcal{U}_n of $\mathcal{X}_n \subset D$.

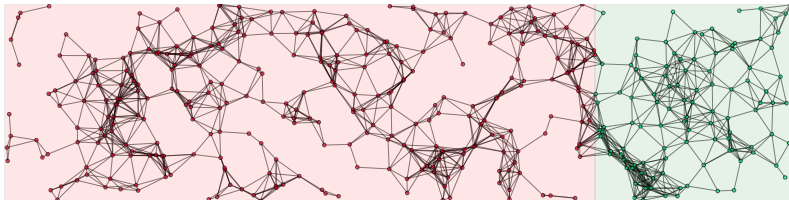
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Theorem (Asymptotics)

Let \mathcal{U} be a finite perimeter partition. Suppose $\{\epsilon_n\}$ satisfies $\sum_{n=1}^{\infty} \exp(-n\epsilon_n^{(d+1)/2}) < \infty$ when $\alpha = 0, 1$ and $\sum_{n=1}^{\infty} \exp(-n\epsilon_n^d) < \infty$ otherwise.

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$$\frac{1 - 1/K - Q_n(\mathcal{U}_n)}{\epsilon_n} \xrightarrow{a.s.} \begin{cases} C_{\eta, \rho} \sum_{k=1}^K \text{Per}(U_k; \rho^2) & \text{if } \sum_{k=1}^K \left(\mu(U_k) - 1/K \right)^2 = 0, \\ \infty & \text{otherwise,} \end{cases}$$

where

$$d\mu(x) = \frac{\rho^{1+\alpha}(x) dx}{\int_D \rho^{1+\alpha}(x) dx} \quad \text{and} \quad C_{\eta, \rho} = \frac{\int_{\mathbb{R}^n} \eta(x) |x_1| dx}{2 \int_D \rho^2(x) dx}.$$

Sketch of Proof: Convergence of Graph Total Variation

Recall

$$GTV_n(u) = \frac{1}{\epsilon_n} \frac{1}{n^2} \sum_{i,j} \eta_{\epsilon_n}(X_i - X_j) |u(X_i) - u(X_j)|.$$

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Proposition

Fix $u = \mathbb{1}_U$, and let $\{\epsilon_n\}_{n \in \mathbb{N}}$ be a sequence converging to zero such that

$$\sum_{n=1}^{\infty} \exp(-n\epsilon_n^{(d+1)/2}) < +\infty.$$

Then

$$GTV_n(u) \xrightarrow{\text{a.s.}} \sigma_\eta TV(u; \rho^2).$$

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Ingredients:

- ▶ Nonlocal TV (Ponce '04)
- ▶ Exponential bounds for U -statistics (Giné, Latała, & Zinn '00)

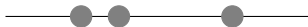
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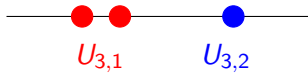
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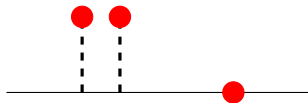
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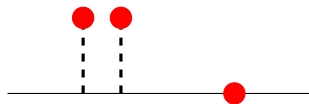


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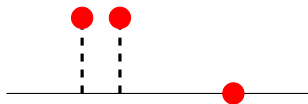
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$$\gamma_1 \in \mathcal{P}(D \times \{0, 1\})$$

Convergence of Partitions

Given partition $\mathcal{U}_n = \{U_{n,k}\}_{k=1}^K$ of \mathcal{X}_n , we associate the measures $\gamma_{n,k} \in \mathcal{P}(D \times \{0, 1\})$, for $k = 1, \dots, K$, by

$$\gamma_{n,k} = \frac{1}{n} \sum_{i=1}^n \delta_{(X_i, \mathbb{1}_{U_{n,k}}(X_i))} = (Id \times \mathbb{1}_{U_{n,k}})_{\#} \nu_n.$$

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Given partition $\mathcal{U} = \{U_k\}_{k=1}^K$ of D , we similarly define

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We say that $\mathcal{U}_n \xrightarrow{w} \mathcal{U}$ if there exists a sequence $\{\pi_n\}_{n \in \mathbb{N}}$ of permutations of $\{1, \dots, K\}$ such that

$$\gamma_{n, \pi_n k} \xrightarrow{w} \gamma_k, \quad \text{for } k = 1, \dots, K.$$

Convergence of Optimal Partitions

Theorem (Convergence of Optimal Partitions)

Suppose $\{\epsilon_n\}_{n \in \mathbb{N}}$ satisfies suitable conditions. For $n \geq 1$, let

$\mathcal{U}_n^* \in \arg \max_{|\mathcal{U}| \leq K} Q_n(\mathcal{U})$ be an optimal partition.

If \mathcal{U}^* is the unique solution (up to relabeling of its constituent sets) to the problem

$$\underset{\substack{|\mathcal{U}|=K \\ \mu(U_k)=1/K}}{\text{minimize}} \sum_{k=1}^K \text{Per}(U_k; \rho^2) \quad (\text{P})$$

with $d\mu(x) = \rho^{1+\alpha}(x) dx / \int_D \rho^{1+\alpha}(x) dx$, then $\mathcal{U}_n^* \xrightarrow{\text{a.s.}} \mathcal{U}^*$.

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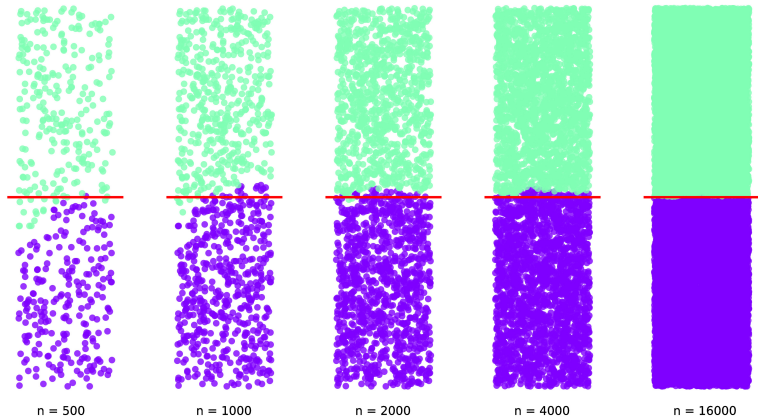
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$$\begin{aligned} & \underset{\substack{|\mathcal{U}|=K \\ \mu(U_k)=1/K}}{\text{minimize}} \sum_{k=1}^K \text{Per}(U_k; \rho^2) \end{aligned} \quad (\text{P})$$

with $d\mu(x) = \rho^{1+\alpha}(x) dx / \int_D \rho^{1+\alpha}(x) dx$, then $\mathcal{U}_n^* \xrightarrow{\text{a.s.}} \mathcal{U}^*$. If there is more than one solution to (P), then almost surely i) $\{\mathcal{U}_n^*\}_{n \in \mathbb{N}}$ has at least one cluster point, and ii) every cluster point is a solution to (P).

Example



Remarks on Theorem

- ▶ Weak convergence of measures via Wasserstein metric.

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- ▶ Weak convergence of measures via Wasserstein metric.
- ▶ Useful tool: transport maps relating empirical measures ν_n to ν , with bound on ∞ -transport cost (García-Trillos, Slepčev).
- ▶ Because modularity clusterings are optimizers of discrete energies, we use Γ -convergence to prove that their limit is the optimizer of a continuum energy.
- ▶ Balance constraint in the continuum problem presents a technical difficulty.
- ▶ We modified the notion of Γ -convergence for random functionals to allow the use of our pointwise convergence result.

Existence of Transport Maps

Let $D \subset \mathbb{R}^d$ be open, connected with Lipschitz boundary. Assume $\nu = \rho(x) dx$ with ρ continuous and bounded above/below by positive constants.

Proposition (García-Trillos, Slepčev '14)

There is a constant $C > 0$ such that, with probability one, there exists a sequence of transportation maps $\{T_n\}_{n \in \mathbb{N}}$, $T_{n\sharp} \nu = \nu_n$ with

$$\limsup_{n \rightarrow \infty} \frac{n^{1/2} \|Id - T_n\|_{\infty}}{(2 \log \log n)^{1/2}} \leq C \quad (d = 1),$$

$$\limsup_{n \rightarrow \infty} \frac{n^{1/d} \|Id - T_n\|_{\infty}}{(\log n)^{3/4}} \leq C \quad (d = 2),$$

$$\limsup_{n \rightarrow \infty} \frac{n^{1/d} \|Id - T_n\|_{\infty}}{(\log n)^{1/d}} \leq C \quad (d \geq 3).$$

Assumption on ϵ_n

Assume $\{\epsilon_n\}_{n \in \mathbb{N}}$ is such that $\epsilon_n > 0$ and $\epsilon_n \rightarrow 0$. For $\alpha = 0, 1$, assume that

$$\lim_{n \rightarrow \infty} \frac{\sqrt{2 \log \log n}}{\sqrt{n}} \frac{1}{\epsilon_n} = 0, \quad \text{if } d = 1$$

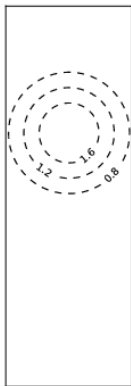
$$\lim_{n \rightarrow \infty} \frac{(\log n)^{3/4}}{n^{1/2}} \frac{1}{\epsilon_n} = 0 \quad \text{if } d = 2$$

$$\lim_{n \rightarrow \infty} \frac{(\log n)^{1/d}}{n^{1/d}} \frac{1}{\epsilon_n} = 0 \quad \text{if } d \geq 3.$$

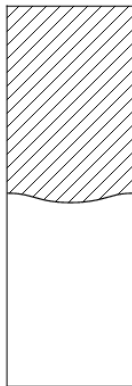
For $\alpha \neq 0, 1$, assume that

$$\sum_{n=1}^{\infty} n \exp(-n \epsilon_n^{d+1}) < \infty.$$

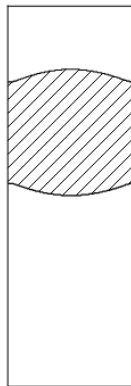
The role of α



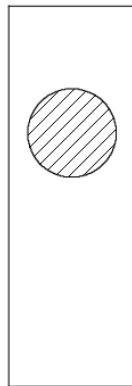
(a) Level sets



(b) $\alpha = -1$



(c) $\alpha = 0$



(d) $\alpha = 1$

$$d\mu(x) \propto \rho(x)^{1+\alpha}, \quad \rho(x) \propto \min(2 \exp(-4\|x - x_0\|^2), 1/2).$$

Thanks for coming!