

Optimal cuts of random geometric graphs

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Random geometric graphs (Penrose 2003)

Let D be a bounded region in \mathbb{R}^d (or more generally, a d -dimensional Riemannian manifold) with $d \geq 2$.

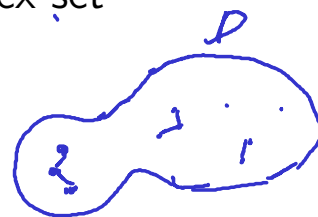
Let X_1, X_2, \dots, X_n be points sampled randomly uniformly from D .

Aim: Learn about D from the sample, via the following graph.

Given $r > 0$, let $G(n, r)$ be the weighted graph on vertex set

$V_n := \{X_1, \dots, X_n\}$ with weights

$$W_{xy} := \phi\left(\frac{|x - y|}{r}\right)$$



where $\phi(t) = \mathbf{1}_{[0,1]}(t)$, $t \geq 0$, and $|\cdot|$ is Euclidean.

i.e., connect any two points of V_n at Euclidean distance at most r_n .

[Could also consider non-uniform samples,

and other weight functions ϕ such as $\phi(t) = \exp(-t^2)$]

Isolated vertices of $G(n, r)$

Assume $D \subset \mathbb{R}^d$ open and connected. Also assume D has unit volume and a *Lipschitz boundary* ∂D [this holds e.g. if ∂D is smooth or D is a cube].

Assume we have access to a large sample and can choose $r = r_n, r_n \rightarrow 0$. Then asymptotic (large- n) properties of $G(n, r_n)$ may be relevant.

Let $I(G)$ denotes the number of isolated vertices of G ,

$\mathbb{E}[I(G(n, r_n))] \sim \underline{n \exp(-n\omega_d r_n^d)}$ as $n \rightarrow \infty$. [$\omega_d :=$ volume of unit ball]

So if $\underline{\omega_d n r_n^d} = a \log n$ then

av. degree

$$\lim_{n \rightarrow \infty} \mathbb{E}[I(G(n, r_n))] = \begin{cases} \infty & \text{if } a < 1 \\ 0 & \text{if } a > 1. \end{cases}$$



Connectivity of $G(n, r)$

From above: if $\omega_d n r_n^d = a \log n$ [i.e., $r_n = (a \log n / (n \omega_d))^{1/d}$] then

$$\lim_{n \rightarrow \infty} \mathbb{E}[I(G(n, r_n))] = \begin{cases} \infty & \text{if } a < 1 \\ 0 & \text{if } a > 1. \end{cases}$$

In fact it turns out that

$$\lim_{n \rightarrow \infty} \mathbb{P}[G(n, r_n) \text{ is connected}] = \begin{cases} 0 & \text{if } a < 1 \\ 1 & \text{if } a > 1 \end{cases}$$



If $\omega_d n r_n^d \geq (1 + \varepsilon) \log n$, $G(n, r_n)$ is likely to be connected for large n .

Conversely, if D is *not* connected and $r_n \rightarrow 0$, then $G(n, r_n)$ will *not* be connected for large n .

i.e. we can learn about connectivity of D from that of $G(n, r_n)$.

[In preparation with Xiaochuan Yang, exact limit of $\mathbb{P}[G(n, r_n) \text{ connected}]$.]

Optimal cuts of a (weighted) graph $G = (V, W)$

For $U \subset V$, set $\partial_G(U) := \sum_{v \in U} \sum_{w \in V \setminus U} W_{vw}$ and $\text{vol}_G(U) := \frac{\#(U)}{\#(V)}$. The **minimum bisection cost** and **cheeger constant (conductance)** of G are

$$\text{MBIS}(G) := \min_{U \subset V: |U| = \lfloor |V|/2 \rfloor} \partial_G(U)$$

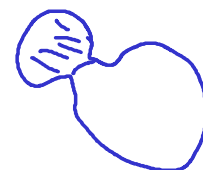
$$\text{CHE}(G) = \min \left\{ \frac{\partial_G(U)}{\text{vol}_G(U)} : U \subset V, 0 < \text{vol}_G(U) \leq 1/2 \right\}$$

The denominator penalizes unbalanced cuts. [Alternatively could define $\text{vol}(U)$ by counting edges rather than vertices]

Uses: bounds on mixing times of random walk on graph, bounds on graph laplacian; reasonable criteria for optimal cut.

Question: Do these quantities for $G(n, r_n)$ converge to analogous quantities of interest for D ?

Optimal cuts of a bounded domain $D \subset \mathbb{R}^d$



Define the **minimal bisection** and **Cheeger constant** of D by

$$\text{MBIS}(D) := \inf\{|\partial_D A| : A \subset D, |A| = 1/2\}$$

$$\text{CHE}(D) := \inf \left\{ \frac{|\partial_D A|}{|A|} : A \subset D, 0 < |A| \leq |D|/2 \right\},$$

$|A|$ denotes the volume of A , $|\partial_D A|$ denotes the perimeter of A within D , i.e. the surface measure of $\overline{A} \cap \overline{D} \setminus \overline{A}$ (where \overline{A} means closure of A).

[Cheeger's inequality: $\lambda_1 \geq \frac{(\text{CHE}(D))^2}{4}$, where λ_1 is the first non-zero eigenvalue of $-\Delta$ on D .]

Can we learn about D from the sample V_n ?

In particular, about $\text{CHE}(D)$ from $\text{CHE}(G(n, r_n))$, given $(r_n)_{n \geq 1}$?

Given $U \subset V_n$, we'll use notation

$$\begin{aligned}\partial_n(U) &:= \partial_{G(n, r_n)}(U), \\ \text{vol}_n(U) &:= \text{vol}_{G(n, r_n)}(U) = \#(U)/n.\end{aligned}$$

Also, assume that $r_n \ll 1$ and (unless stated otherwise) that

$$nr_n^d \gg \log n,$$

where $a_n \ll b_n$ or $b_n \gg a_n$ means $(a_n/b_n) \rightarrow 0$ as $n \rightarrow \infty$.

Note: $\exists c > 0$: if $nr_n^d \leq c \log n$ then G is not connected so $\text{CHE}(G) = 0$.
Need at least $nr_n^d \geq c \log n$ to have any chance of learning anything from $\text{CHE}(G(n, r_n))$. But want r_n small for computational reasons.

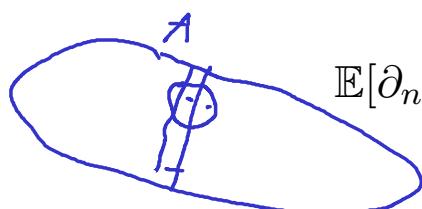



Asymptotic upper bound for $\text{CHE}(G)$

$$\text{CHE}(G(n, r_n)) = \min \left\{ \frac{\partial_n(U)}{\text{vol}_n(U)} : U \subset V_n, 0 < \text{vol}_n(U) \leq 1/2 \right\}$$

Choose $A \subset D$ to minimize $|\partial_D A|/|A|$ subject to $0 < |A| \leq \frac{1}{2}$.

Let $U_n = V_n \cap A$. By the Law of Large Numbers, $\text{vol}_n(U_n) \rightarrow |A|$. Also,



$$\begin{aligned} \mathbb{E}[\partial_n(U_n)] &= n^2 \int_A \int_{D \setminus A} \mathbf{1}_{[0, r_n]}(|y-x|) dy dx \\ &\sim |\partial_D A| \sigma n^2 r_n^{d+1}, \end{aligned}$$


with $\sigma := (1/2) \int_{\mathbb{R}^d} x_1 \mathbf{1}_{[0,1]}(|x|) dx$. ['Surface tension' of $\phi = \mathbf{1}_{[0,1]}$].

So assuming $\partial_n(U_n) \sim \mathbb{E}[\partial_n(U_n)]$, as $n \rightarrow \infty$

$$\begin{aligned} \limsup n^{-2} r_n^{-d-1} \text{CHE}(G(n, r_n)) &\leq \limsup n^{-2} r_n^{-d-1} \left(\frac{\partial_n(U_n)}{\text{vol}_n(U_n)} \right) \\ &= \frac{\sigma |\partial_D A|}{|A|} = \sigma \text{CHE}(D) \end{aligned}$$

Theorem (García Trillos et al. '16; Müller/P. '20)

[Recall $\text{CHE}(D) := \inf \left\{ \frac{|\partial_D A|}{|A|} : A \subset D, 0 < |A| \leq |D|/2 \right\}$
 $\text{CHE}(G) = \min \left\{ \frac{\partial_G(U)}{\text{vol}_G(U)} : U \subset V(G), 0 < \text{vol}_G(U) \leq 1/2 \right\}$]

Under our conditions ($|D| = 1$, ∂D Lipschitz, $r_n \rightarrow 0$, $nr_n^d \gg \log n$), a.s.:

- $n^{-2}r_n^{-d-1}\text{CHE}(G(n, r_n)) \rightarrow \sigma\text{CHE}(D)$. [already shown \leq]
- If $A \subset D$ is the (essentially) unique Cheeger minimizer, i.e. $|A| < 1/2$ and $\frac{|\partial_D A|}{|A|} < \frac{|\partial_D A'|}{|A'|}$ for all $A' \subset D$ with $|A' \Delta A| \neq 0$, then

$\forall A_n$ minimizing in $\text{CHE}(G(n, r_n))$

$$n^{-1} \sum_{x \in A_n} \delta_x \rightarrow \text{Leb}_d|_A \quad \text{weakly.}$$

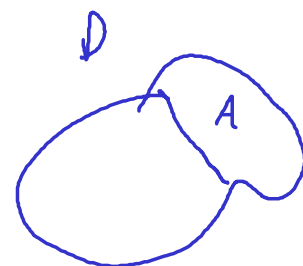


- If A is not unique, we still have convergence on a subsequence.
- Also $n^{-2}r_n^{-d-1}\text{MBIS}(G(n, r_n)) \rightarrow \sigma\text{MBIS}(D)$,

G. Trillos et al. needed the additional condition $nr_n^2 \gg (\log n)^{3/2}$ if $d = 2$.

Sketch proof of lower bound

- Let $U_n \subset V_n, n \geq 1$ be any sequence of Cheeger minimisers in $G(n, r_n)$. Label points of U_n 'red', points of $V_n \setminus U_n$ 'green'.
- Divide D into cubes (boxes) of side $\gamma_n r_n$, where γ_n is a sequence of constants with $1 \gg \gamma_n$ and $n(\gamma_n r_n)^d \gg \log n$.
- WHP, each box contains about $n(\gamma_n r_n)^d$ points of V_n .
- All the boxes must be 'mostly red' or 'mostly green'.
- Let U_n^* be the union of 'mostly red' boxes. Then



$$n^{-2} r_n^{-d-1} \partial_n(U_n) \approx r_n^{-d-1} \int_D \int_D \phi\left(\frac{|x-y|}{r_n}\right) |\mathbf{1}_{U_n^*}(y) - \mathbf{1}_{U_n^*}(x)| dy dx$$

$=: F_n(\mathbf{1}_{U_n^*})$, where $F_n(\mathbf{1}_B)$ is a smoothed measure of $|\partial B|$, $B \subset D$.

- Homogeneity: $F_n(af) = aF_n(f)$ for all $f \in L^1(D)$ and $a > 0$.

Continuing, recall U_n is a Cheeger minimiser in $G(n, r_n) =: G_n$.

$$n^2 r_n^{-d-1} \text{CHE}(G_n) = n^2 r_n^{-d-1} \frac{\partial_n(U_n)}{\text{vol}_n(U_n)} \approx F_n(g_n)$$

where we define $g_n := |U_n^*|^{-1} \mathbf{1}_{U_n^*} \in L^1(D)$ and for $g \in L^1(D)$ we define

$$F_n(g) := r_n^{-d-1} \int_D \int_D \phi\left(\frac{|y-x|}{r_n}\right) |g(y) - g(x)| dy dx.$$

The g_n are bounded in L^1 , and by a compactness result of Garcia Trillos and Slepčev (2016), there exist $g \in L^1(D)$ and a subsequence of \mathbb{N} with $g_n \rightarrow g$ in L^1 as n goes to infinity along the subsequence. Then by a Gamma-convergence result (also GT&S 2016),

$$\liminf F_n(g_n) \geq F(g)$$

where $F : L^1(D) \rightarrow \mathbb{R}$ is homogeneous and for $A \subset D$, we have

$$F(\mathbf{1}_A) = \sigma |\partial_D A|.$$

But $g = \mathbf{1}_A/|A|$ for some A so $F(g) = |\partial_D A|/|A| \geq \text{CHE}(F)$. \square

The largest component of $G_n := G(n, r_n)$

Let $L(G)$ be the number of vertices in the largest component of G .

The asymptotic behaviour of $L(G_n)$ is governed by that of nr_n^d
[note the average degree $\sim nr_n^d \omega_d$, where $\omega_d = \text{vol. of unit ball}$]

If $\lim_{n \rightarrow \infty} nr_n^d < \lambda_c(d)$ then $n^{-1}L(G_n) \xrightarrow{P} 0$ as $n \rightarrow \infty$.

If $nr_n^d = \lambda > \lambda_c(d)$ then $n^{-1}L(G_n) \xrightarrow{P} \theta(\lambda) \in (0, \infty)$.

($\lambda_c(d)$ is a percolation threshold, not known explicitly.)

This is called a **giant component** phenomenon.

If $nr_n^d \rightarrow \infty$ but $nr_n^d/(\log n) \rightarrow 0$, then $n - L(n) = I(G_n)$ to first order.
[P. and Yang, in preparation]

Open problems (now $G_n := G(n, r_n)$)

We know $a_n \text{CHE}(G_n) \rightarrow \text{CHE}(D)$ and $a_n \text{MBIS}(G_n) \rightarrow \text{MBIS}(D)$ when $1 \gg r_n \gg ((\log n)/n)^{1/d}$.

Can we extend this to when $r_n = c((\log n)/n)^{1/d}$, large c ?

Or even to when $r_n \gg n^{-1/d}$, at least for MBIS?

(If $n^{-1/d} \ll r_n \ll ((\log n)/n)^{1/d}$ then $1 \ll (n - L(G_n)) \ll n$, where $L(G)$ is the order of the largest component of G .)

Or to the k -nearest-neighbour graph on V_n where $k = k(n) \gg \log n$?
(connect each vertex by an undirected edge to its k nearest neighbours).

Or to other point processes on D , e.g. a regular grid?

References

- García Trillos, N. and Slepčev, D. (2016) Continuum limit of total variation on point clouds. *Arch. Ration. Mech. Anal.* **220**, 193-241.
- García Trillos, N., Slepčev, D., von Brecht, J., Laurent, T. and Bresson, X. (2016) Consistency of Cheeger and ratio cuts. *Journal of Machine Learning Research.*
- Müller, T. and Penrose, M.D. (2020) Optimal Cheeger cuts and bisections of random geometric graphs. *Annals of Applied Probability.*
- Penrose, M. (2003) *Random Geometric Graphs*. Oxford Uni. Press