Random walks on simplicial complexes

Working group 'Machine learning and optimization'

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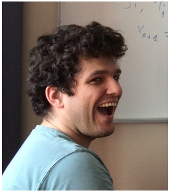
With...



Random graph

★ Static non oriented random graph $\mathcal{G} = (V, E)$ with $V = \{1, \dots n\}$.

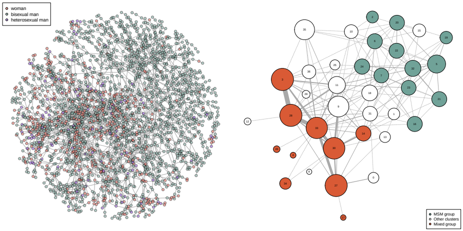
Edges of the graph are non-oriented pairs $\{u, v\}$, but if we want to orient them, $[u, v]$ we will call u the ego of the edge and v the alter.

★ The adjacency matrix is a matrix $G = (G_{uv})_{u,v \in V} \in \mathcal{M}_{V \times V}(\mathbb{R})$.

The degree of a vertex $u \in V$ is $D_u = \sum_{v \in V} G_{uv}$.

Clustering of a graph

★ Connected components or almost disconnected components?



★ Laplacian of the graph:

$$Lf(u) = \sum_{v \sim u} f(v) - f(u) = (G - D) f(u), \qquad \text{for } f : V \to \mathbb{R}.$$

The number of connected components $= \dim(\ker L)$.

If we have k small eigenvalues in L, the graph contains k 'dense' compts.

★ L is the generator of a random walk on the graph $\rightarrow$ random walks reveal information on the topology of the graph.

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1. Clémençon, De Arazoza, Rossi, Tran, *Soc. Netw. Anal. Min.*, 2015
2. Luxburg, *Statistics and Computing*, 2007

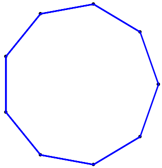
Homology and Betti numbers

Cycle random walks

Rescaling of a geometric cycle random walk

Can we go further?

★ Most existing algorithms study the connectivity of the graph, can we go further?



★ For example, this graph has a very particular structure -it is a circle- which is hard to detect using graph Laplacians or random walks.

★ The homology of a topological space can be viewed as the number of 'holes' in the space.

Simplicial complexes

★ A k-simplex is a set $\{v_0, \dots v_{k-1}\}$.

There are two orientations for a k-simplex: $[v_0, \dots v_{k-1}]$ and $-[v_0, \dots v_{k-1}]$.

★ The faces of $[v_0, \dots v_{k-1}]$ are the $k-1$-simplices

$$[v_0, \dots v_{j-1}, v_{j+1}, \dots v_{k-1}]$$

and the cofaces are the $k+1$-simplices that admits $[v_0, \dots v_{k-1}]$ as face.

1. e.g. Armstrong, *Basic Topology*, Springer, 1983.

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★ **Simplicial complex $\mathcal{C}$ = vertices + edges + triangles + tetrahedra...+ k-simplex + ...**

with the constraint that is $[v_0, \dots v_{k-1}] \subset \mathcal{C}$, its faces are all in $\mathcal{C}$ etc.

The set of k-simplices of $\mathcal{C}$ are $\mathcal{S}_k(\mathcal{C})$.

1. e.g. Armstrong, *Basic Topology*, Springer, 1983.

Examples of simplicial complices

★ Cech complex, Čech(V, R) for $R > 0$, points have a position x_i.

$\mathcal{S}_0 = V$ and $[v_{i_0}, v_{i_1}, \cdots, v_{i_{k-1}}] \in \mathcal{S}_k$ if

$$\bigcap_{m=0}^{k} B(x_{i_m}, R) \neq \emptyset.$$

★ Rips-Vietoris complex, Rips(V,R).

Same vertices V and edges as the Čech complex, but for $k \geq 3$, $[v_{i_0}, \cdots, v_{i_{k-1}}] \in \mathcal{S}_k$ if all the possible pairs made by choosing two points among $\{v_{i_0}, \cdots, v_{i_{k-1}}\}$ belong to the set $\mathcal{S}_1$.

$$\text{Rips}(V, R) \subset \text{Čech}(V, R) \subset \text{Rips}(V, 2R).$$

1. Boissonnat, 2018.

Chains and co-chains

★ $\mathcal{C}_k = \text{span}(\mathcal{S}_k)$: a chain τ can then be written as

$$\tau = \sum_{s_i n \mathcal{S}_k^+} \lambda_s(\tau)\, s,$$

with the $\lambda_s(\tau) \in \mathbb{R}$.

★ Defining

$$\|\tau\|^2_{\mathcal{C}_k} = \|\sum_{s \in \mathcal{S}_k^+} \lambda_s(\tau)\, s\|^2_{\mathcal{C}_k} = \sum_{s \in \mathcal{S}_k^+} |\lambda_s(\tau)|^2,$$

we put a Hilbert structure on $\mathcal{C}_k$.

★ Co-chains:

$$\mathcal{C}^k = \{f \;:\; \mathcal{C}_k \to \mathbb{R}\}.$$

is the dual of $\mathcal{C}_k$.

★ $\mathcal{C}_k$ and $\mathcal{C}^k$ are isomorphic.

Boundary maps

★ Boundary map:

$$\begin{array}{rcccc} \partial_k & : & \mathcal{C}_k & \to & \mathcal{C}_{k-1} \\ & & [v_0, \ldots v_{k-1}] & \mapsto & \sum_{i=0}^{k} (-1)^i [v_0, \ldots, v_{i-1}, v_{i+1}, \ldots, v_{k-1}], \end{array}$$

with the convention that $\partial_0 \equiv 0$.

It can be checked that $\partial_k \circ \partial_{k+1} = 0$.

★ Thus, $\mathrm{Im}(\partial_{k+1}) \subset \mathrm{Ker}(\partial_k)$ and

$$H_k = \ker(\partial_k) / \operatorname{im}(\partial_{k+1})$$

is the k-th homology vector space.

★ k-th Betti number:

$$\beta_k = \dim(H_k) = \dim(\ker \partial_k) - \dim(\operatorname{im} \partial_{k+1}).$$

Links with 'usual' random walks?

★ Recall $\beta_k = \dim(H_k)$.

★ $H_0 = \text{span}(V)/\text{span}\{u - v,\ [u, v] \in \mathcal{S}_1\}$

$\beta_0 =$ number of connected components
'Usual' random walks are connected with β_0: V is the state space, $\text{im}\,\partial_1$ is the space of transitions.

★ Are there a 'random walks' that bring information on β_k ? For example:

- $\beta_1 =$ number of holes,
- $\beta_2 =$ number of cavities...

Homology and Betti numbers

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Rescaling of a geometric cycle random walk

Co-boundary maps and combinatorial Laplacian

★ Co-boundary:

$$\begin{array}{cccc} \partial_k^* & : & \mathcal{C}^k & \to & \mathcal{C}^{k+1} \\ & & f & \mapsto & \partial_k^* f, \end{array}$$

where

$$\partial_k^* f[v_0, \ldots v_k] \mapsto \sum_{i=0}^{k+1} (-1)^i \langle f, [v_0, \ldots, v_{i-1}, v_{i+1}, \ldots, v_{k-1}] \rangle_{\mathcal{C}^k, \mathcal{C}_k}.$$

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★ Definition:

$$\begin{array}{rccc} L_k & : & \mathcal{C}_k & \rightarrow & \mathcal{C}_k \\ & & \tau & \mapsto & (L_k^{\uparrow} + L_k^{\downarrow})(\tau), \end{array}$$

where

$$L_k^{\uparrow} = \partial_{k+1} \circ \partial_k^*, \qquad \text{and} \qquad L_k^{\downarrow} = \partial_{k-1}^* \circ \partial_k.$$

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★ Combinatorial Hodge theorem:

$$\mathcal{C}_k = \operatorname{im} \partial_{k+1} \oplus \operatorname{im} \partial_k^* \oplus \ker L_k,$$

implying that

$$\ker L_k \simeq H_k \qquad \text{and} \qquad \beta_k = \dim(\ker L_k).$$

Case of the graph Laplacian

★ For $k = 0$, $L_0 = \partial_1 \partial_1^* = GG^T$:

$$(L_0)_{uv} = \begin{cases} \deg(v) & \text{if } u = v \\ -1 & \text{if } u \sim v \\ 0 & \text{otherwise.} \end{cases}$$

Hence,

$$\begin{aligned} L_0 \ : \ & \mathcal{C}^0 \longrightarrow \mathcal{C}^0 \\ & u^* \longmapsto -\sum_{v \in V : [uv] \in \mathcal{S}_2} (v^* - u^*) = \sum_{v \in V : [uv] \in \mathcal{S}_2} \partial_1 [uv]. \end{aligned}$$

and for $f = \sum_{v \in V} \lambda_v v^*$:

$$\begin{aligned} -L_0 f(u) &= \sum_{v \in V} \lambda_v L_0 v^*(u) = \sum_{v \in V} \lambda_v \sum_{w \sim v} (w^* - v^*)(u) \\ &= \sum_{v \sim u} \lambda_v - \lambda_u \mathrm{Card}(w \sim u) = \sum_{v \sim u} \left(f(v) - f(u) \right). \end{aligned}$$

More random walks

★ Upper and lower-adjacency.

★ If D_k is the diagonal with the upper degrees of the k-simplices and

$$A_k^{\uparrow/\downarrow}(u,v) = \begin{cases} 1 & \text{if } u \text{ and } v \text{ are upper/lower adjacent and similarly oriented,} \\ -1 & \text{if } u \text{ and } v \text{ are upper/lower adjacent and dissimilarly oriented,} \\ 0 & \text{otherwise.} \end{cases}$$

$$L_k = L_k^{\uparrow} + L_k^{\downarrow} = \left(D_k - A_k^{\uparrow}\right) + \left((k+1)\mathrm{Id} + A_k^{\downarrow}\right)$$

The map $L_k^{\uparrow}$ has the feature of a random walk, but not $L_k^{\downarrow}$

$\rightarrow$ If we consider a r.w. valued in $\ker \partial_k$, the part with $L_k^{\downarrow}$ disappear.

1. Mukherjee, Steenbergen, *Random Str. and Alg.*, 2016
2. Parzanchevski, Rosenthal, *Random Str. and Alg.*, 2017
3. With Bonis, Decreusefond and Zhang, in progress.

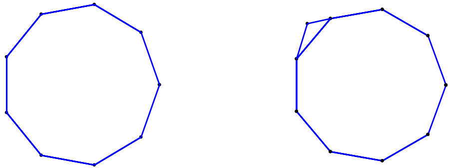
Cycle-random walk

- Generator of a 'usual random walk' on the graph:

$$Lf(x) = \sum_{y \sim x} f(y) - f(x) = \sum_{y \in V / [x,y] \in \mathcal{S}_2} f\big(x + \partial_1[x,y]\big) - f(x).$$

- For $\sigma \in \ker \partial_k$ and $f \ : \ \ker \partial_k \to \mathbb{R}$:

$$-L_k f(\sigma) = \sum_{\sigma' \in \mathcal{S}_k / \sigma' \subset \sigma} \ \sum_{y \in V / [\sigma', y] \in \mathcal{S}_{k+1}} f\big(\sigma + \partial_{k+1}[\sigma', y]\big) - f(\sigma).$$



- It can be proved that:

$$-L_k f(\sigma) = \sum_{\sigma' \in \ker \partial_k} \big(f(\sigma') - f(\sigma)\big) K(\sigma, \sigma'),$$

where $K(\sigma, \sigma') = \langle \sigma, \sigma - \sigma' \rangle_+$ counts the number of faces that they have in common.

Some properties of the cycle-random walk $(X_t)_{t\geq 0}$

★ The chain X_t remains in the same homology class as X_0 by construction.

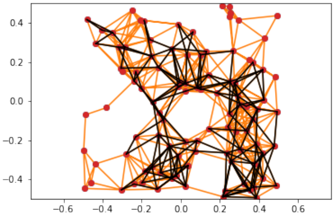
★ A chain is simple if the weights of the k-simplices in its support are -1 or 1.

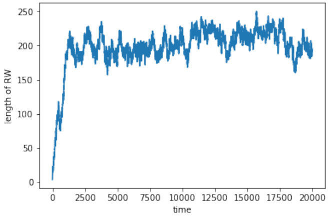
When $\mathrm{Card}(V) < +\infty$, if X_0 is simple, then X_t is simple for any $t > 0$ and so the states space of the chain is finite.

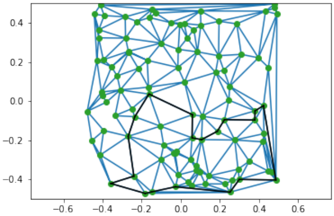
★ Let $\omega(t) = \mathbb{P}\big(\langle X(t),\, \tau\rangle_{\mathcal{C}^k,\mathcal{C}_k} = 1 \,|\, X(0)\big)$, it satisfies

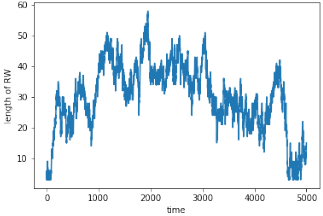
$$\frac{d}{dt}\omega(t) = -L_k^{\uparrow}\omega(t).$$

Simulations









Cycle random walk on the triangular lattice

★ Consider the flat torus $\mathbb{T}_2 := \mathbb{R}^2/\mathbb{Z}^2$ with the triangular lattice of mesh $\varepsilon_n = 1/(2n)$. V_n is the corresponding set of vertices.

★ Our cycle $\sigma \in \mathcal{C}_1(V_n)$ is now embedded in the torus, and we can consider it as a path from $[0, 1]$ to $\mathbb{T}_2$ (piecewise differentiable).

★ Natural test functions in this context are of the form:

$$\sigma \in \ker \partial_k \mapsto \Phi\Big(\int_\sigma \phi\Big)$$

where Φ is a smooth function from $\mathbb{R}$ to $\mathbb{R}$ and where ϕ is a 1-differential form: $\phi = \phi^1 dx_1 + \phi^2 dx_2$.

Convergence of generators

★ **Prop:** For a twice differentiable 1-form ϕ, and $v \in \mathcal{S}_1(V_n)$,

$$\sup_n \sup_{v \in \mathcal{S}_1(V_n)} \epsilon_n^{-2} \left| \epsilon_n^{-2} A_n \left(\int_v \phi \right) - \int_v \mathcal{L}^{\uparrow} \phi \right| < \infty. \qquad (1)$$

where $\mathcal{L}^{\uparrow}$ is the Laplace-Beltrami operator:

$$\mathcal{L}^{\uparrow}\left(\phi^1\, dx_1 + \phi^2\, dx_2\right) = \left(\phi^1_{22} - \phi^2_{12}\right) dx_1 + \left(\phi^2_{11} - \phi^1_{12}\right) dx_2$$

1. Simulation by Marc Glisse

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Thanks for listening!

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