Random Topology, Minimum Spanning Acycle, and Persistent Homology

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Random Topology, Minimum Spanning Acycle, and Persistent Homology

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Joint work with
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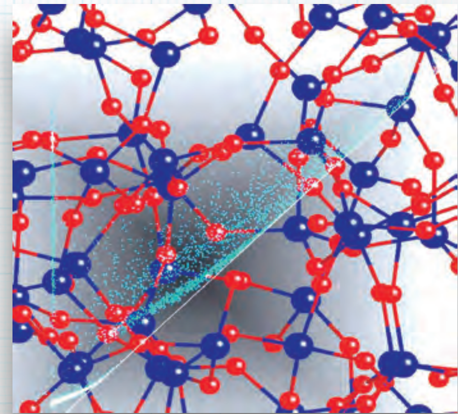


Content

1. Motivation: Materials Science

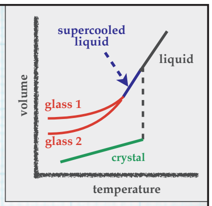
2. From Random Graph to Random Topology

3. Persistent Homology

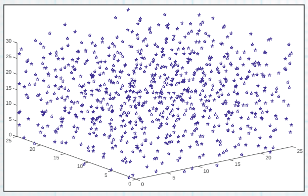
4. Main Result: Generalization of
   Frieze's zeta(3)-Limit Theorem

1. Motivation: Materials Science

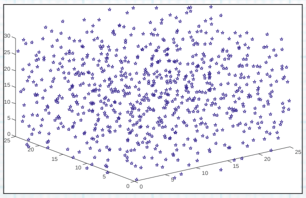
Liquid, Glass or Crystal?



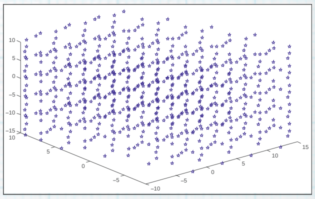
liquid



glass



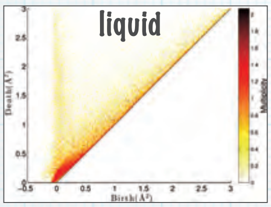
crystal

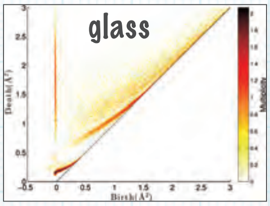


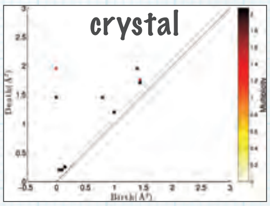
- Atomic configurations of crystal, glass, and liquid states of SiO2
- Geometric properties of glass are not well-understood
- Industrially important (solar energy panel, DVD, BD, etc)
- Can we distinguish between crystal and glass?

1. Motivation: Materials Science arXiv:1501.003611, arXiv:1502.07445

Persistence Diagram (PD)

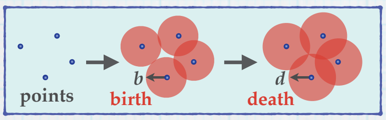




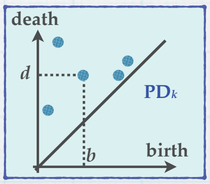


- 1st Persistence Diagrams (PDs) distinguish three states (info. of persistent ring)
- Inverse problem from PDs to atomic configurations clarifies new geometric characterizations of glass
- What are the topological properties in liquid (random) state?

Brief Sketch of PDs for points data



blow up balls and detect appearance and disappearance of topological features



Content

Erdös-Rényi Random Graph

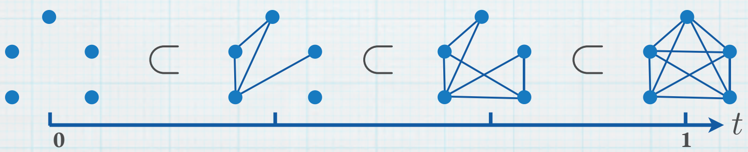
- $K_n = V_n \sqcup E_n$ **: complete graph with** n **vertices**

  $$V_n = \{1, \dots, n\}, \ E_n = \{|ij| \ : \ i < j\}$$

- $t_e \in [0, 1]$**: i.i.d. uniform random variable for** $e \in E_n$

Erdös–Rényi Random Graph (Process)

$$K_n(t) = V_n \sqcup \{e \in E_n \ : \ t_e \leq t\}$$



Erdös-Rényi Random Graph

Thm(Erdös-Rényi): For $t = (\log n + \omega(n))/n$,

$\omega(n) \to \infty \Longrightarrow K_n(t)$ **is a.s. connected as** $n \to \infty$

$\omega(n) \to -\infty \Longrightarrow K_n(t)$ **is a.s. disconnected as** $n \to \infty$

- **rewriting by reduced homology**

$$\omega(n) \to \infty \Longrightarrow \tilde{H}_0(K_n(t)) = 0$$

$$\omega(n) \to -\infty \Longrightarrow \tilde{H}_0(K_n(t)) \neq 0$$

Random Graph G → $H_0(G)$, $H_1(G)$ (connectivity, cycle)

In this talk, we study

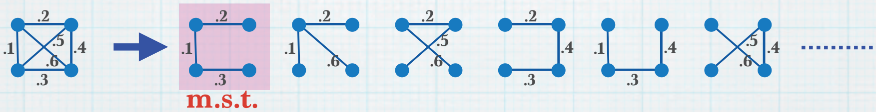
Random Simplicial Complex X → $H_k(X)$ (higher topological features)

Frieze's zeta(3)-Limit Theorem

- $K_n(t)$: **ER random graph**
- $K_n = K_n(1)$: **complete graph**
- $T \subset K_n$ **is a spanning tree if** T **is a tree containing all vertices**
- $\mathcal{S}^{(1)}$**: the set of spanning trees in** K_n

Cayley's formula: $|\mathcal{S}^{(1)}| = n^{n-2}$

- $T \in \mathcal{S}^{(1)}$ **is the minimum spanning tree if the weight** $\mathrm{wt}(T) = \sum_{e \in T} t_e$ **is minimum in** $\mathcal{S}^{(1)}$

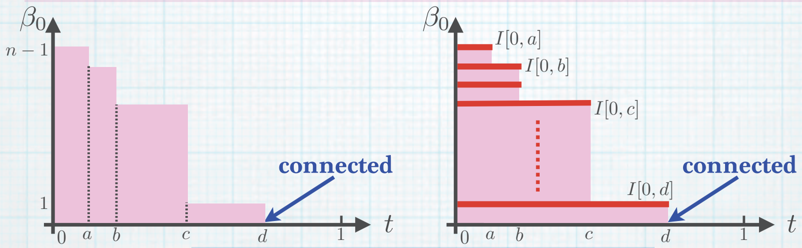


Frieze's zeta(3)-limit thm:

$$\mathbb{E}[\min_{T \in \mathcal{S}^{(1)}} \mathrm{wt}(T)] \to \zeta(3) = 1.202\cdots \quad \text{as } n \to \infty$$

Persistence and Frieze's Thm

Key observation: $\min_{T \in \mathcal{S}^{(1)}} \mathrm{wt}(T) = \int_0^1 \beta_0(t)dt$ ★



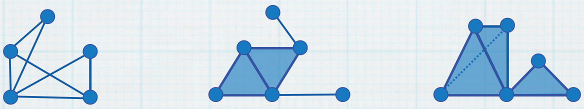
$\int_0^1 \beta_0(t)dt =$ **lifetime sum**

Generalization of Frieze's Thm

- **random graph** → **random simplicial complex**
- **spanning tree** → **spanning acycle**
- ★ → **identity using persistent homology**

Simplicial Complex

- **Simplicial Complex** X **on the vertices** $\{1, \dots, n\}$**:**
  - **a collection of nonempty subsets**
  - $\{i\} \in X, \quad \forall i \in \{1, \dots, n\}$
  - $\sigma \in X, \ \tau \subset \sigma \Longrightarrow \tau \in X$
- $\sigma = \{i_0, \dots, i_k\}$ **:** k**-simplex,** $\quad \dim \sigma = k$
- $\dim X = \max_{\sigma \in X} \dim \sigma$
- $X_k = \{\sigma \in X : \dim \sigma = k\}, \ X^{(k)} = \sqcup_{i=0}^k X_i$ ← **k-dim skeleton**
- **graph = 1 dim simplicial complex**



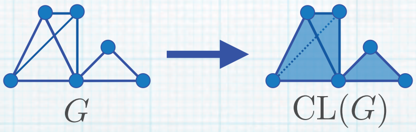
dim = 1 **dim = 2** **dim = 3**

Random Simplicial Complex 1

- **Random Clique Complex** $\mathrm{CL}(G)$

  $\mathrm{CL}(G)$ **: clique of a graph** G

  $\mathrm{CL}(G) \ni \{i_1, \dots, i_k\} \iff \{i_s i_t\} \in G, \ \forall s, t \in \{1, \dots, k\}$



Take ER random graph $G = K_n(t)$ **, then**

Kahle (2009): For random clique complex $\mathrm{CL}(K_n(t))$**,**

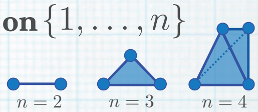
$$t = \left(\frac{(2k+1)\log n + \omega(n)}{n} \right)^{1/(2k+1)} \implies H_i(\mathrm{CL}(K_n(t))) = 0$$

$\omega(n) \to \infty$ $\qquad i = 0, \dots, k$

$k = 0$ **recovers one-side of the ER theorem**

Random Simplicial Complex 2

- Δ_{n-1} : $(n-1)$**-dim maximal simpl cplex on** $\{1, \dots, n\}$



- $t_\sigma \in [0, 1]$ **: i.i.d. uniform random variable for** $\sigma \in (\Delta_{n-1})_d$

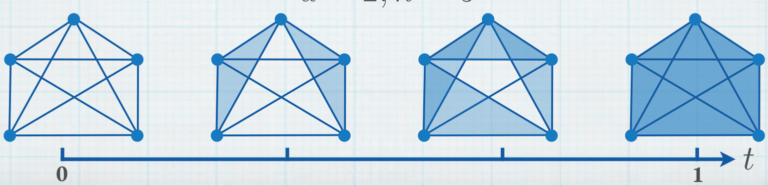
Linial-Meshulam Process

$$\mathcal{K}^{(d)}(t) = \Delta_{n-1}^{(d-1)} \sqcup \{\sigma \in (\Delta_{n-1})_d : t_\sigma \leq t\}$$

- $d = 1$ **gives ER random graph**

higher dim generalization of ER graph process

$d = 2, n = 5$



Spanning Acycle

Remark on simplicial homology

we use
- integer coefficient
- reduced homology

- X : simplicial complex
- For a set of k-splexs $S \subset X_k$, define $X_S = S \sqcup X^{(k-1)}$

S is called a **k-spanning acycle** if

(a) $H_k(X_S) = 0$ (b) $|H_{k-1}(X_S)| < \infty$

$\mathcal{S}^{(k)}$: the set of k-spanning acycles

- For $k=1$, the graph X_S has (a) no cycles and is (b) connected, meaning a spanning tree.
- This definition is originally introduced by Kalai. (also relating to simplicial spanning tree, k-bases, etc)
- Set $\gamma_k(X) = |X_k^{(k)}| - \beta_k(X^{(k)}) + \beta_{k-1}(X^{(k)})$

Any two of (a), (b), and (c) $|S| = \gamma_k(X)$ imply the third.

Minimum Spanning Acycle

- $\{X(t)\}_t$: random filtration of simpl. cplx. (e.g., clique ER process, LM process)
- t_σ : birth time of the simplex, i.e.,

$$t_\sigma = \min\{t : \sigma \in X(t)\}$$

- $S \in \mathcal{S}^{(k)}$ is a **minimum spanning acycle**

if the weight $\mathrm{wt}(S) = \sum_{\sigma \in S} t_\sigma$ is minimum in $\mathcal{S}^{(k)}$

Content

(Persistent) Homology 1

Quick review of simplicial homology

- X : **simplicial complex**
- **chain complex in $\mathbb{Z}$-coefficient**

$$\cdots \longrightarrow C_{k+1}(X) \xrightarrow{\partial_{k+1}} C_k(X) \xrightarrow{\partial_k} C_{k-1}(X) \longrightarrow \cdots$$

remove

$$\partial_k \langle v_0 \cdots v_k \rangle = \sum_i (-1)^i \langle v_0 \cdots \widehat{v_i} \cdots v_k \rangle$$ **: boundary map** $(\partial_k \circ \partial_{k+1} = 0)$

- $Z_k(X) = \ker\partial_k$ **: k-cycle,** $B_k(X) = \mathrm{im}\partial_{k+1}$ **: k-boundary**

betti number

- $H_k(X) = Z_k(X)/B_k(X) \simeq \mathbb{Z}^{\beta_k} \oplus T_k$ **($\mathbb{Z}$-module)**

Homology to Persistent Homology

Replace $\mathbb{Z}$-module with graded $K[\mathbb{R}_{\geq 0}]$-module using filtration

Persistent Homology 2

- $\mathcal{X} = \{X(t) : t \in \mathbb{R}_{\geq 0}\}$: **(right cont.) filtration of a simpl. cplex** X

$$(X(t) \subset X(s) \subset X,\ t \leq s, \quad X(t) = \textstyle\bigcap_{t<s} X(s))$$

Assume there exists a saturation time T **s.t.** $X(T) = X$

- t_σ **: birth time of the simplex** σ**, i.e.,** $t_\sigma = \min\{t : \sigma \in X(t)\}$
- K **: field with** $\mathrm{char}(K) = 0$

  $K[\mathbb{R}_{\geq 0}]$ **: monoid ring, i.e., the set of formal polynomials with**

$$az^t \cdot bz^s = abz^{t+s}, \quad a, b \in K,\ t, s \in \mathbb{R}_{\geq 0}$$

- $C_k(X(t))$ **:** K**-vector space spanned by** k**-simplices in** $X(t)$
- **graded** $K[\mathbb{R}_{\geq 0}]$**-module**

$$C_k(\mathcal{X}) = \textstyle\bigoplus_{t \in \mathbb{R}_{\geq 0}} C_k(X(t)) = \{(c_t) : c_t \in C_k(X(t)),\ t \in \mathbb{R}_{\geq 0}\}$$

$$z^s \cdot (c_t) = (c'_t), \quad c'_t = \begin{cases} c_{t-s}, & t \geq s \\ 0, & t < s \end{cases}$$

Persistent Homology 3

- **For oriented simplex** $\langle\sigma\rangle$**, define** $\langle\langle\sigma\rangle\rangle = (c_t), \quad c_t = \begin{cases} \langle\sigma\rangle, & t = t_\sigma \\ 0, & t \neq t_\sigma \end{cases}$

  → $\Xi_k = \{\langle\langle\sigma\rangle\rangle : \sigma \in X_k\}$ **forms a basis of** $C_k(\mathcal{X})$

- **boundary map:** $\delta_k \langle\langle\sigma\rangle\rangle = \sum_{j=0}^{k} (-1)^j z^{t_\sigma - t_{\sigma_j}} \langle\langle\sigma_j\rangle\rangle$

$$\langle\sigma\rangle = \langle v_0 \cdots v_k \rangle, \quad \sigma_j = \sigma \setminus \{v_j\}$$

$$B_k(\mathcal{X}) = \mathrm{im}\delta_{k+1} \subset Z_k(\mathcal{X}) = \ker\delta_k$$

- **persistent homology:** $H_k(\mathcal{X}) = Z_k(\mathcal{X}) / B_k(\mathcal{X})$ **(graded** $K[\mathbb{R}_{\geq 0}]$**-module)**
- **structure thm of PID module (with saturation) implies**

$$H_k(\mathcal{X}) \simeq \textstyle\bigoplus_{i=1}^{p} I[b_i, d_i]$$

$I[b_i, d_i] = (z^{b_i})/(z^{d_i})$ **: interval representation**

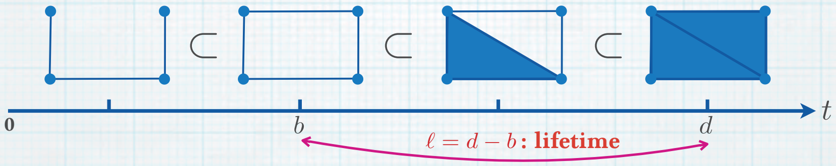
$(z^a) = \{z^a f(z) : f(z) \in K[\mathbb{R}_{\geq 0}]\}$ **: ideal generated by** z^a

Persistence Diagram 1

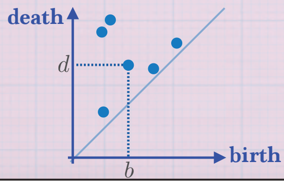
Interval decomp: $H_k(\mathcal{X}) \simeq \bigoplus_{i=1}^{p} I[b_i, d_i]$

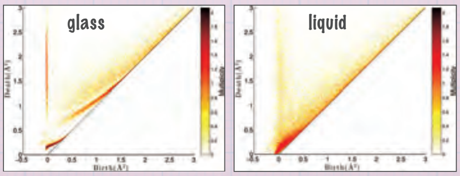
- $I[b, d]$ **represents appearance and disappearance of a topological feature at** $t = b, d$ **in** $\mathcal{X} = \{X(t)\}_t$

birth time　death time



- $D_k(\mathcal{X}) = \{(b_i, d_i) \in \mathbb{R}^2_{\geq 0} : i = 1, \ldots, p\}$ **: persistence diagram**





Persistence Diagram 2

- **persistence diagram (multiset):**

$$D_k(\mathcal{X}) = \{(b_i, d_i) \in \mathbb{R}^2_{\geq 0} : i = 1, \ldots, p\}$$

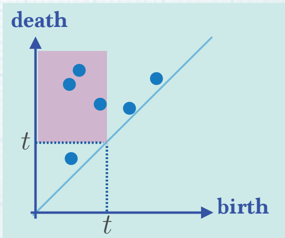
- **persistence diagram (counting measure):**

$$\xi_k = \sum_{0 \leq x < y < \infty} m_{(x,y)} \delta_{(x,y)}$$

where $\delta_{(x,y)}$ **is the delta measure and**

$$m_{(x,y)} = |\{1 \leq i \leq p \mid (b_i, d_i) = (x, y)\}|$$

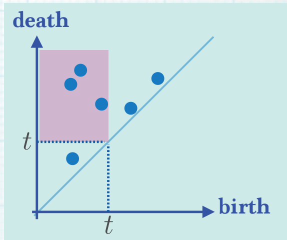
- $\beta_k(t) = \beta_k(X(t)) = \xi_k([0, t] \times [t, \infty))$



Persistence Diagram 2

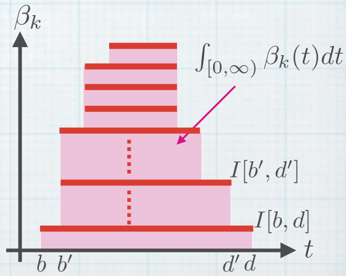
- **Let** $L_k = \sum_i (d_i - b_i)$ **be the lifetime sum**

→ $L_k = \int_{[0,\infty)} \beta_k(t)dt$



pf) By Fubini,

$$\begin{aligned} L_k &= \int_\Delta (y-x)\xi_k(dxdy) \\ &= \int_\Delta \xi_k(dxdy) \int_{[0,\infty]} I(0 \le x \le t \le y \le \infty)dt \\ &= \int_{[0,\infty]} dt \int_\Delta I_{[0,t]}(x) I_{[t,\infty]}(y) \xi_k(dxdy) \\ &= \int_{[0,\infty]} \beta_k(t)dt. \quad \blacksquare \end{aligned}$$



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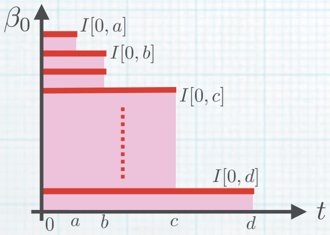
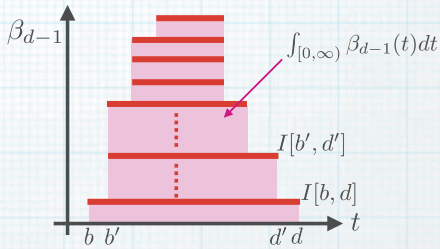
4. Main Result: Generalization of Frieze's zeta(3)-Limit Theorem

Algebraic Formula of L_{d-1}

key observation of ER graph process:

$L_0 = \min_{T \in \mathcal{S}^{(1)}} \mathrm{wt}(T) = \int_0^\infty \beta_0(t)dt$ ★





Theorem: Let X be a simpl. cplx $(1 \le d \le \dim X)$ with

$$\beta_{d-1}(X^{(d)}) = \beta_{d-2}(X^{(d-1)}) = 0$$

and $\mathcal{X} = \{X(t) : t \in \mathbb{R}_{\ge 0}\}$ be a filtration of X. Then,

$$L_{d-1} = \min_{T \in \mathcal{S}^{(d)}} \mathrm{wt}(T) - \max_{S \in \mathcal{S}^{(d-1)}} \mathrm{wt}(X_{d-1} \setminus S) = \int_0^\infty \beta_{d-1}(t)dt$$

Remark: d=1 recovers ★

Sketch of Proof: Algebraic Formula of L_{d-1}

M **: matrix form of the d-boundary map of P.H. under standard bases (entries are $\pm z^t$)**

$D = M|_{z=1}$ **: matrix form of the d-boundary map of H**

For $K \subset X_{d-1}, S \subset X_d$, M_K, D_{KS} (etc) mean the restriction to K, S

Prop: For $|K| = \gamma_d(X)$, $\det M_K M_K^t = z^{2e(K)} \sum_{S \in \mathcal{S}^{(d)}} (\det D_{KS})^2 z^{2\tau(S)}$
(|d-S.A.|)
where $\tau(S) = \mathrm{wt}(S) - \min_{S \in \mathcal{S}^{(d)}} \mathrm{wt}(S)$, $e(K) = \min_{S \in \mathcal{S}^{(d)}} \mathrm{wt}(S) - \mathrm{wt}(K)$

Pf) Binet-Cauchy. ■

Prop: For the elementary divisors $d_1 = z^{e_1}, \dots, d_r = z^{e_r}$ of M,

$$\min_{K \in \mathcal{S}_c^{(d-1)}} e(K) = e_1 + \cdots + e_r,$$

where $\mathcal{S}_c^{(d-1)} = \{X_{d-1} \setminus L : L \in \mathcal{S}^{(d-1)}\}$

Pf) Use $d_1 \cdots d_r = \Delta_r(M)$ (deteminantal divisor) and

$$D_{KS} \neq 0 \Longleftrightarrow S \in \mathcal{S}^{(d)}, K \in \mathcal{S}_c^{(d-1)} \quad ■$$

➡ $L_{d-1} = e_1 + \cdots + e_r$ **leads to**

$$L_{d-1} = \min_{T \in \mathcal{S}^{(d)}} \mathrm{wt}(T) - \max_{S \in \mathcal{S}^{(d-1)}} \mathrm{wt}(X_{d-1} \setminus S) \quad ■$$

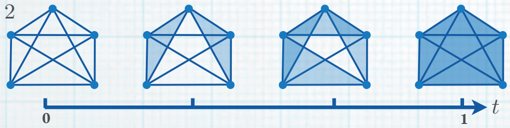
Main Result

Frieze's zeta(3)-limit thm:

$$\mathbb{E}[L_0] = \mathbb{E}[\min_{T \in \mathcal{S}^{(1)}} \mathrm{wt}(T)] \to \zeta(3) = 1.202\cdots \quad \text{as } n \to \infty$$

d-Linial-Meshulam Process: $\mathcal{K}^{(d)}(t) = \Delta_{n-1}^{(d-1)} \sqcup \{\sigma \in (\Delta_{n-1})_d : t_\sigma \le t\}$

$d = 2$



iid uniform on [0,1]

higher dim generalization of ER graph process (d = 1)

Theorem: For d-LM process, $\mathbb{E}[L_{d-1}] = O(n^{d-1})$, as $n \to \infty$

Clique Complex Process: $\Delta_{n-1}^{(0)} = \mathcal{C}(0) \subset \mathcal{C}(t) \subset \mathcal{C}(1) = \Delta_{n-1}$

(clique of ER process) **where** $\mathcal{C}(t) = \mathrm{Cl}(\mathcal{K}^{(1)}(t)), \quad 0 \le t \le 1$

Theorem: For clique complex process,

$$cn^{d-1} \le \mathbb{E}[L_{d-1}] \le Cn^{d-1} \log n \quad (d = 1, 2)$$

$$cn^{\frac{(d+2)(d-1)}{2d}} \le \mathbb{E}[L_{d-1}] \le Cn^{d-1} \quad (d \ge 3)$$

Sketch of Proof: d-LM process

Prove: $\mathbb{E}[L_{d-1}] = O(n^{d-1})$, as $n \to \infty$

$$L_{d-1} = \min_{T \in \mathcal{S}^{(d)}} \mathrm{wt}(T) - \max_{S \in \mathcal{S}^{(d-1)}} \mathrm{wt}(X_{d-1} \setminus S) = \int_0^1 \beta_{d-1}(t)dt$$

Let $Y_t = \mathcal{K}^{(d)}(t)$.

- **For a lower bound, use** ▢ **(with complete (d-1)-skeleton)**

$$L_{d-1} = \mathrm{wt}(T) \ge \sum_{i=1}^{|T|} u_i \qquad N = \binom{n}{d+1}$$

T **: minimum spanning acycle**

$u_1 \le u_2 \le \cdots \le u_N$ **: rearrangement of** $\{t_\sigma : \sigma \in (\Delta_{n-1})_d\}$

$$\Rightarrow \mathbb{E}[L_{d-1}] \ge \sum_{i=1}^{|T|} \mathbb{E}[u_i] = \sum_{i=1}^{|T|} \frac{i}{N+1} \sim \frac{d+1}{2d!} n^{d-1}$$

lemma: $|T| = \binom{n-1}{d}$

- **For an upper bound, use** ▢

$$\mathbb{E}[L_{d-1}] = \int_0^1 \mathbb{E}[\beta_{d-1}(t)]dt \le \frac{d+1}{n} \int_0^1 \mathbb{E}|\mathcal{R}_d(Y_t)|dt \le 8\frac{d+1}{n}\binom{n}{d} \sim \frac{8(d+1)}{d!} n^{d-1}$$

Sketch of Proof: d-LM process

- **For an upper bound, use** □

$$\mathbb{E}[L_{d-1}] = \int_0^1 \mathbb{E}[\beta_{d-1}(t)]dt \leq \frac{d+1}{n} \int_0^1 \mathbb{E}|\mathcal{R}_d(Y_t)|dt \leq 8\frac{d+1}{n}\binom{n}{d} \sim \frac{8(d+1)}{d!} n^{d-1}$$

$\leq$ $\mathcal{R}_d(Y) = \{\sigma \in (\Delta_{n-1})_d : \beta_{d-1}(Y \cup \sigma) = \beta_{d-1}(Y) - 1\}$

$\mathcal{S}_d(Y) = \{\sigma \in (\Delta_{n-1})_d : \beta_{d-1}(Y \cup \sigma) = \beta_{d-1}(Y)\}$

Lemma: $\beta_{d-1}(Y) \leq \frac{d+1}{n}|\mathcal{R}_d(Y)|$

pf) $\overline{Y} := Y \cup \mathcal{S}_d(Y)$ **. Then,**

$$\beta_{d-1}(Y) = \beta_{d-1}(\overline{Y}) = \binom{n-1}{d} - \text{rank}\partial_{\overline{Y},d} \leq \binom{n-1}{d} - \frac{d+1}{n}|\overline{Y}_d|$$

Linial, et al
$\text{rank}\partial_{Y,d} \geq \frac{d+1}{n}|Y_d|$

$\leq$ $\mathcal{C}_n^{(d)}$**: the set of** d**-dim simpl. cplx on** n **vertices with** $(d-1)$**-complete skeleton**

$\mathcal{C}_{n,m}^{(d)} = \{Y \in \mathcal{C}_n^{(d)} : |Y_d| = m\}$ $\quad Y^{(d)}(n,m)$**: uniform dist on** $\mathcal{C}_{n,m}^{(d)}$

First, we show $\int_0^1 \mathbb{E}|\mathcal{R}_d(Y_t)|dt \leq \frac{m}{1-\rho_{n,m}}, \ 1 \leq \forall m \leq N$

where $\rho_{n,m} = \mathbb{P}(\sigma \in \mathcal{R}_d(Z)), \quad Z \sim Y^{(d)}(n,m)$

Sketch of Proof: d-LM process

Let us set $m_c(n) = \min\{m \leq N : \rho_{n,m} \leq c\}$.

Hoffman-Kahle-Paquette
$m_{1/2}(n) \leq 4\binom{n}{d}$

By setting $c = 1/2$

$$\int_0^1 \mathbb{E}|\mathcal{R}_d(Y_t)|dt \leq \frac{m}{1-\rho_{n,m}} \leq 2m_{1/2}(n) \leq 8\binom{n}{d}.$$

Hence, we have

$$\mathbb{E}[L_{d-1}] = \int_0^1 \mathbb{E}[\beta_{d-1}(t)]dt \leq \frac{d+1}{n} \int_0^1 \mathbb{E}|\mathcal{R}_d(Y_t)|dt \leq 8\frac{d+1}{n}\binom{n}{d} \sim \frac{8(d+1)}{d!} n^{d-1}$$

■

Sketch of Proof: Clique complex process

Prove: $cn^{d-1} \le \mathbb{E}[L_{d-1}] \le Cn^{d-1}\log n \quad (d=1,2)$

$$cn^{\frac{(d+2)(d-1)}{2d}} \le \mathbb{E}[L_{d-1}] \le Cn^{d-1} \quad (d \ge 3)$$

$$L_{d-1} = \min_{T\in\mathcal{S}^{(d)}} \mathrm{wt}(T) - \max_{S\in\mathcal{S}^{(d-1)}} \mathrm{wt}(X_{d-1}\setminus S) = \int_0^1 \beta_{d-1}(t)dt$$

For both upper & lower bounds, use ▢ with the Morse inequality

$$-f_{d-2}(t) + f_{d-1}(t) - f_d(t) \le \beta_{d-1}(t) \le f_{d-1}(t)$$

where $\beta_i(t) = \beta_i(\mathcal{C}(t))$ **and** $f_i(t) = |\mathcal{C}(t)_i|$

- **Lower bound:** $\mathbb{E}[f_j(t)] = \binom{n}{j+1} t^{\binom{j+1}{2}}$ **and straightforward cal.**
- **Upper bound: Discrete Morse Theory, i.e.,**
  reduce $f_{d-1}(t)$ **by critical cells defined by**
  a lex-order Morse function

■

Further Discussions

- **Limiting constant of d-LM process**

$$I_{d-1} = \lim_{n\to\infty} \frac{1}{n^{d-1}} \mathbb{E}[L_{d-1}]$$

- **Central limit theorem of** L_{d-1} **in d-LM process**
- **Limit theorem of persistence diagram**
- **Order in the clique complex process**
- **Asymptotics of** ℓ^2**-norm and persistence landscape**
- **Wilson's algorithm for "uniform" spanning acycles**

Thank you very much