Persistence Modules on Commutative Ladders: Auslander-Reiten Theory in Topological Data Analysis

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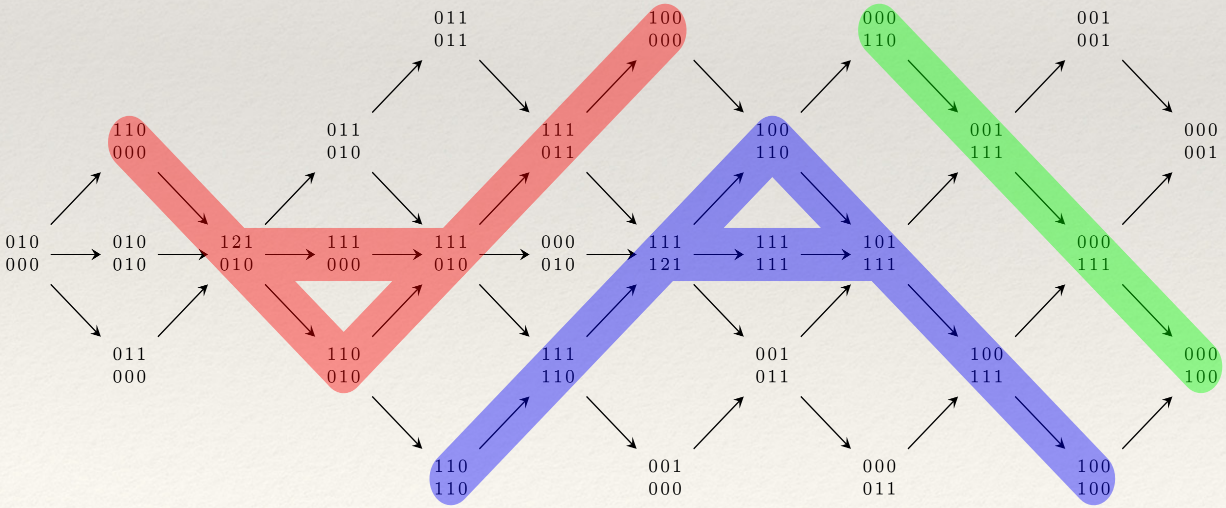
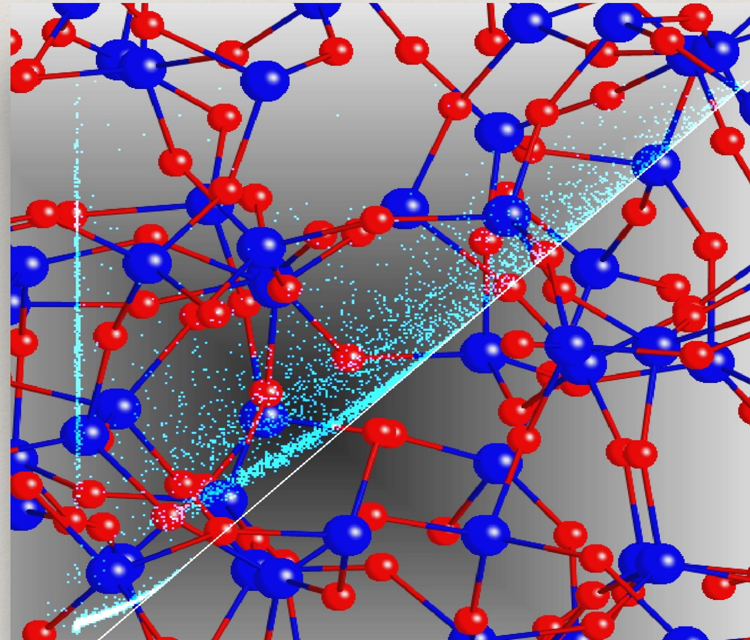
(Kyushu University)





Reference

Mathematical Part:

E. Escolar & Y.H.
Persistence Modules on Commutative Ladders of Finite Type.
arXiv:1404.7588

TDA on Glass:

T. Nakamura, Y.H., et al.
Description of Medium-Range Order in Amorphous Structures by Persistent Homology
preprint

Acknowledgement

AR Theory

D. Tamaki, H. Asashiba, H. Ochiai

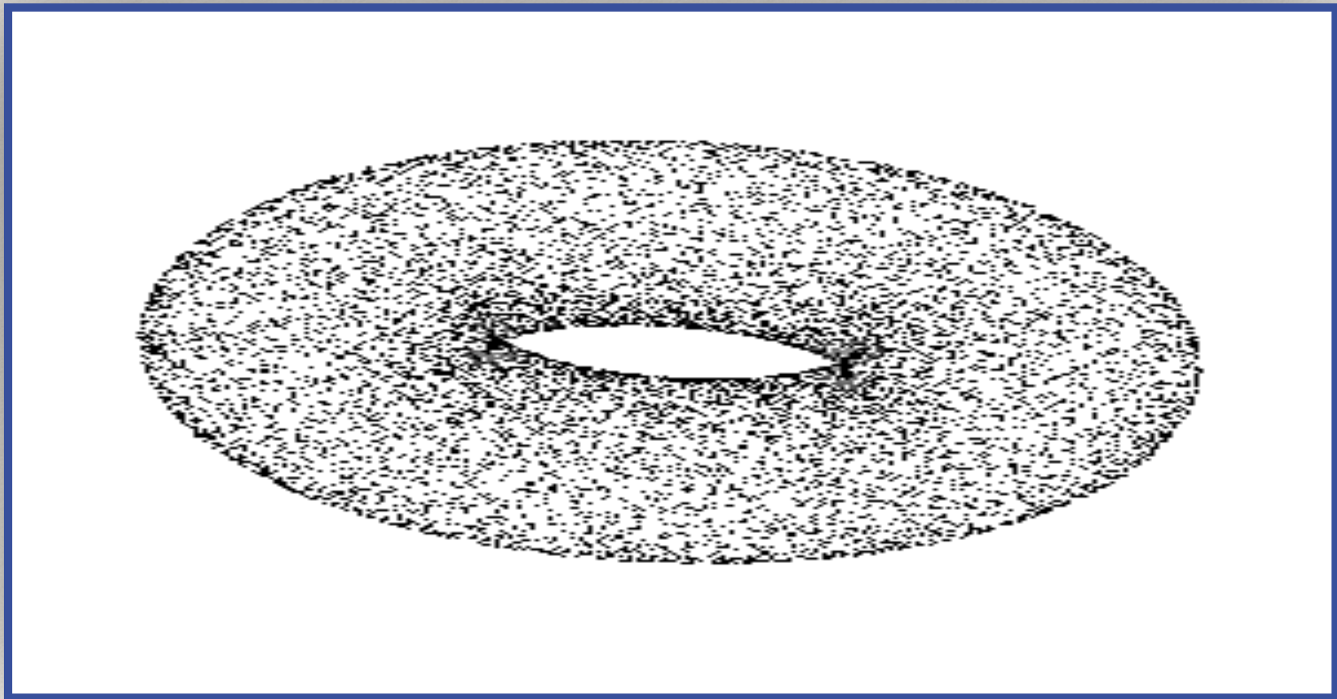
Materials Science

A. Hirata, K. Matsue, T. Nakamura, Y. Nishiura

Topological Data Analysis

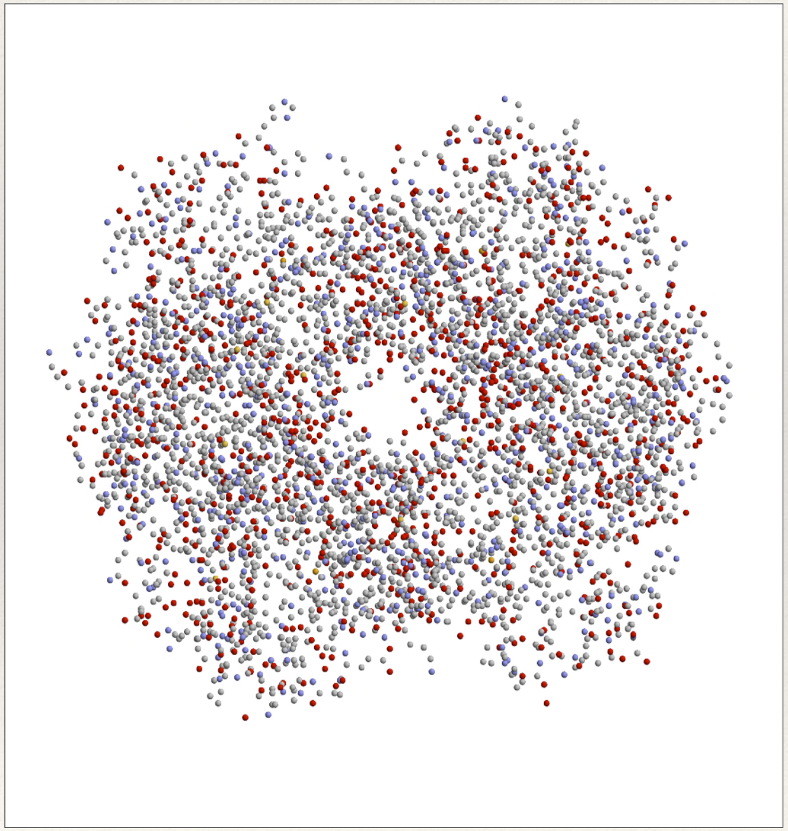
Topological characterizations of real data

- finite observations
- big
- error, noise

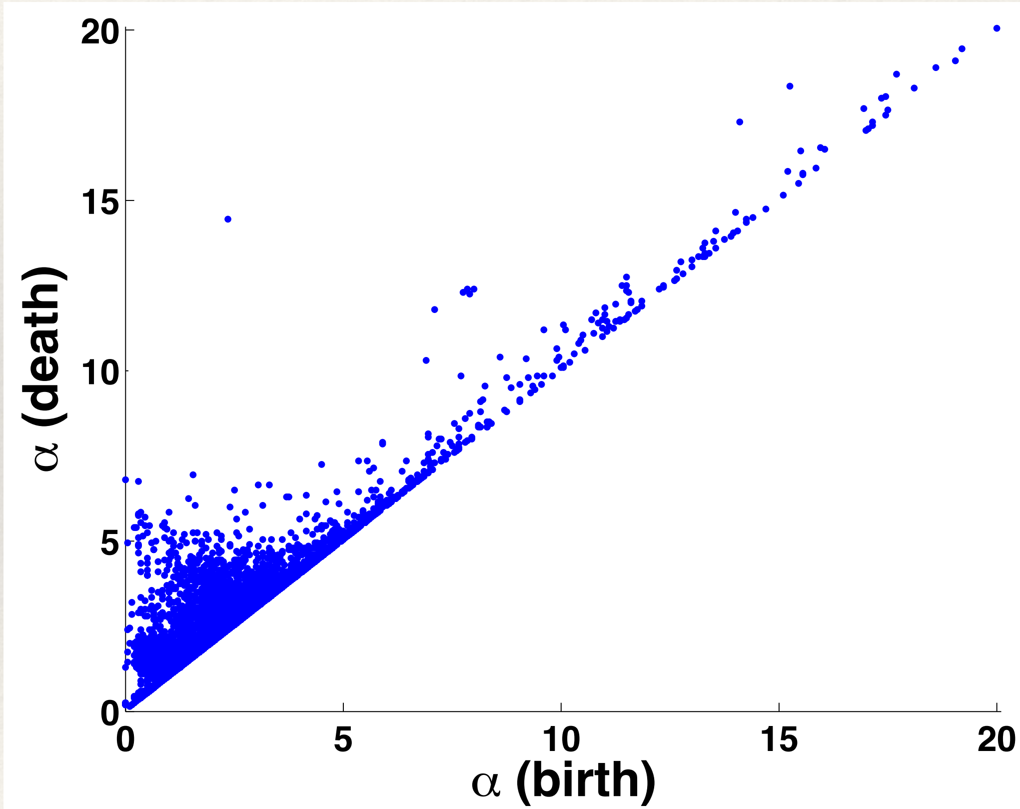


Persistent Homology

Characterize robust & noisy topological features in data



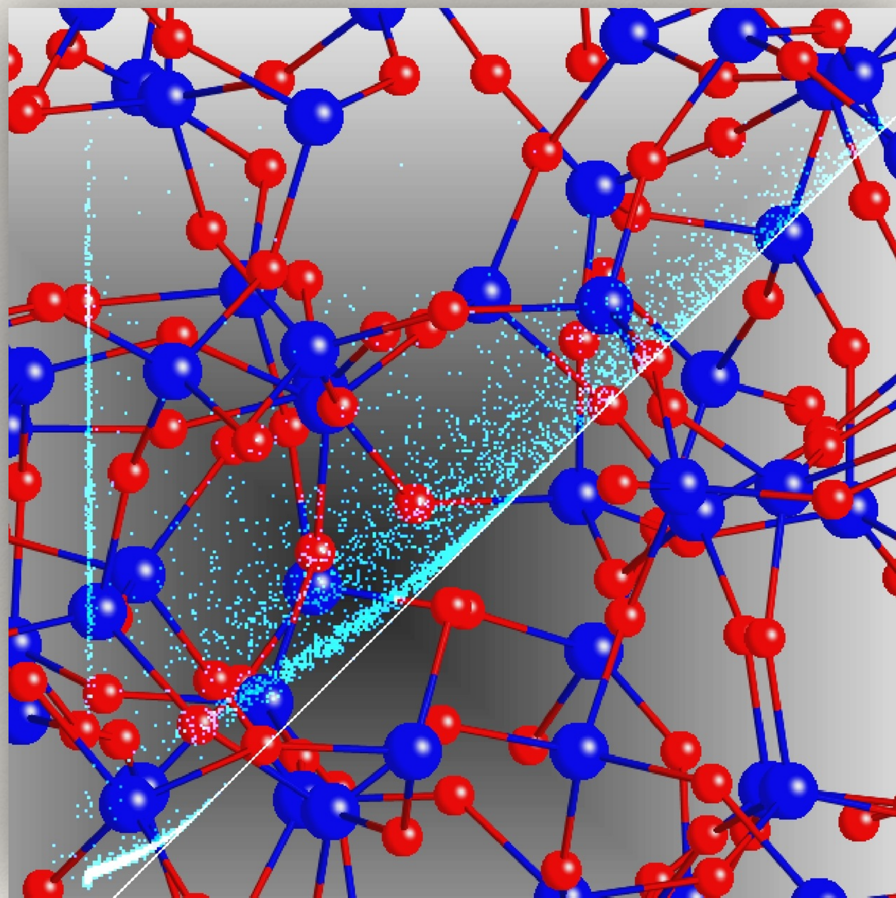
Hemoglobin



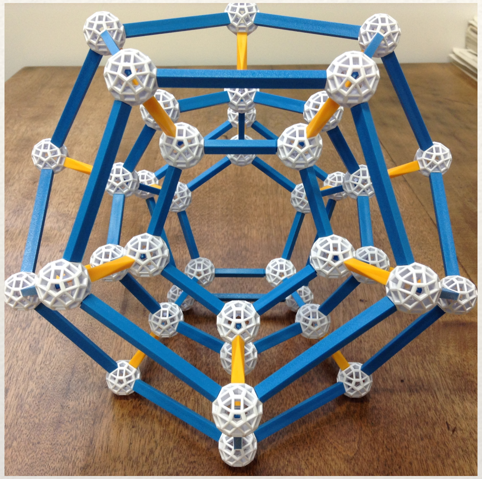
Persistence Diagram

Applications of Persistent Homology

1. AYASDI (company of TDA by G. Carlsson)
2. Image processing
3. Sensor networks
4. Statistics
5. Proteins
6. Materials Science (Glass, Grain, etc)

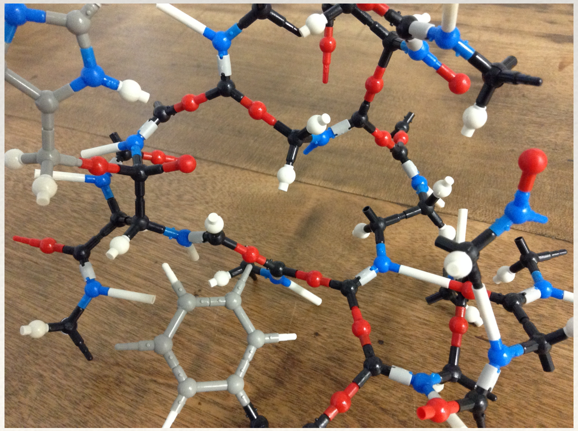


Atomic Location and Geometry



Crystal

- Group Theory
- Combinatorics
- Discrete Geometry, etc

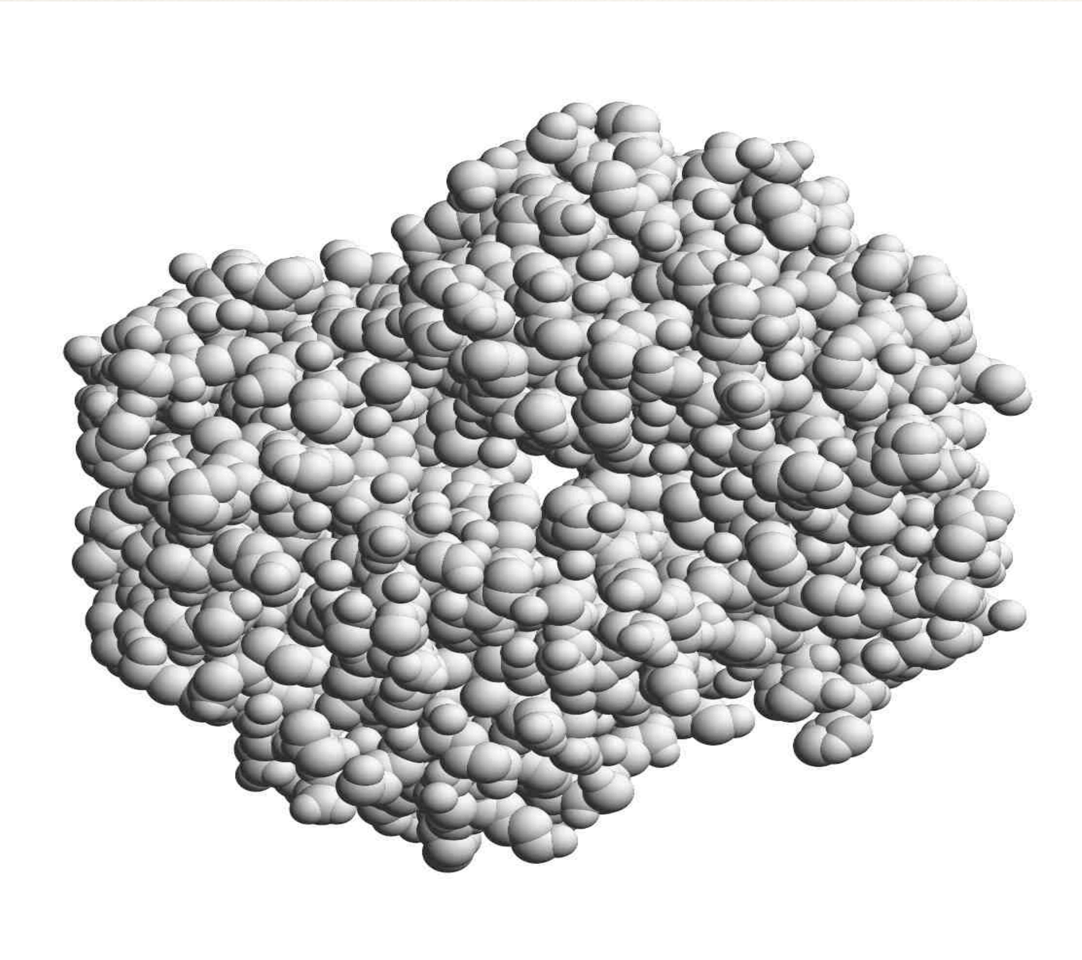


Amorphous (glass), Protein

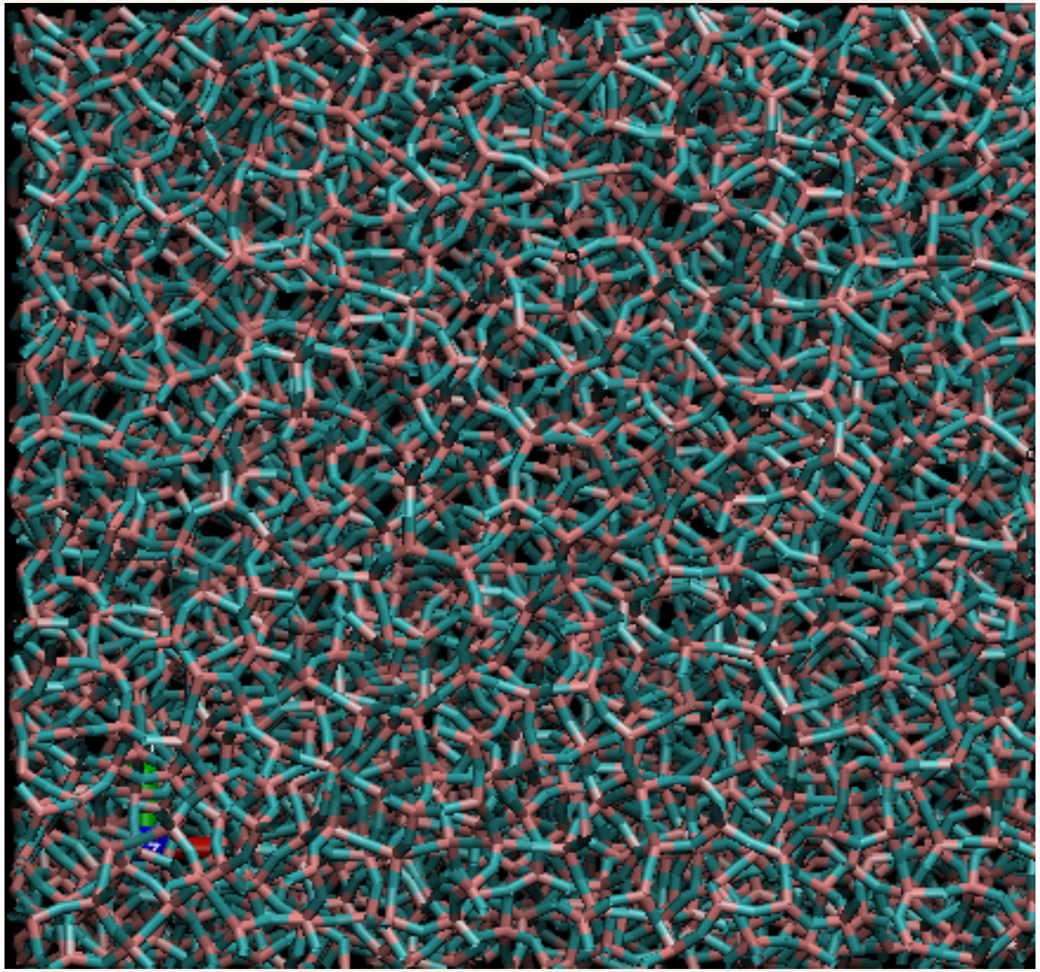
- Alpha shape
- Persistent Homology

Atomic Location and Geometry

Protein

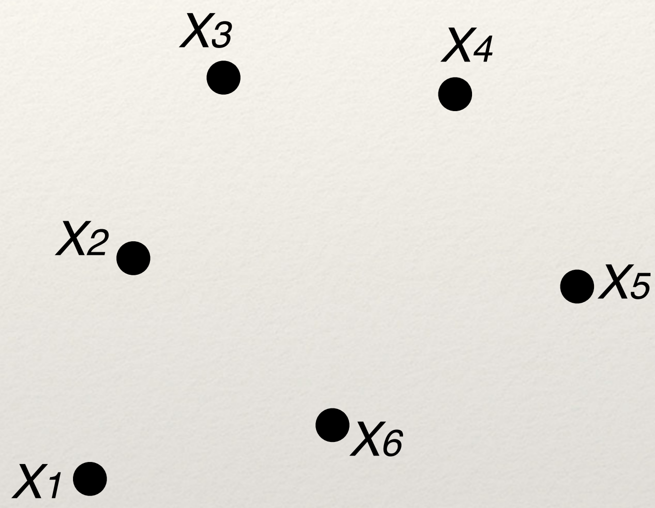


Glass



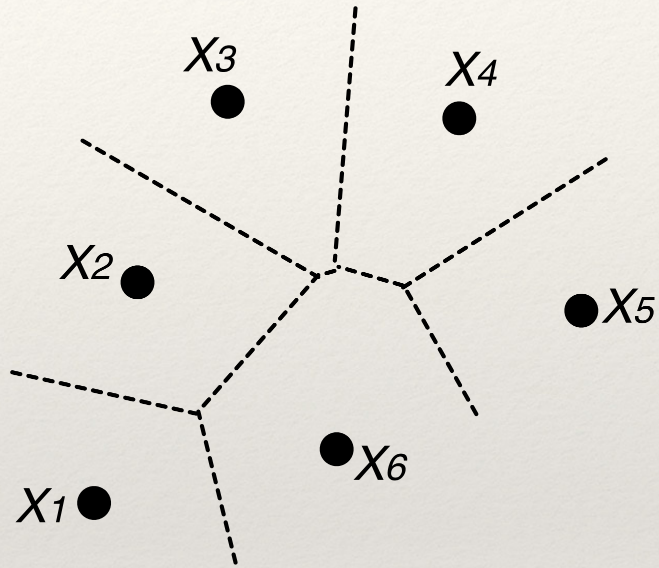
Alpha Shape

- $X = \{x_i \in \mathbf{R}^3 \mid i = i, \ldots, n\}$



Alpha Shape

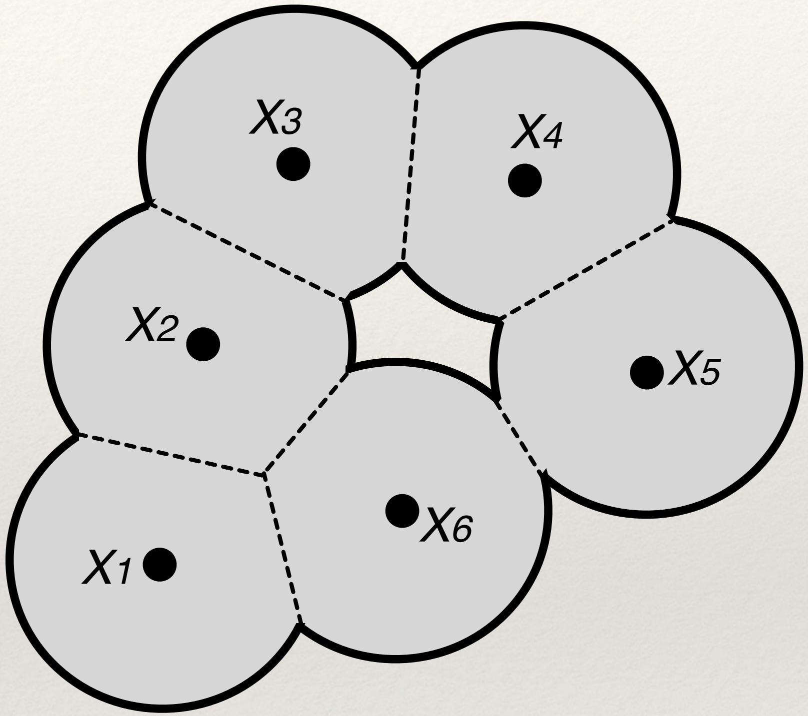
- $X = \{x_i \in \mathbf{R}^3 \mid i = i, \ldots, n\}$
- $\mathbf{R}^3 = \bigcup_{i=1}^{n} V_i$ **: Voronoi decomp.**



Alpha Shape

- $X = \{x_i \in \mathbf{R}^3 \mid i = i, \ldots, n\}$
- $\mathbf{R}^3 = \bigcup_{i=1}^{n} V_i$: **Voronoi decomp.**
- $\bigcup_{i=1}^{n} B_i(r) = \bigcup_{i=1}^{n} (B_i(r) \cap V_i)$

$$B_i(r) = \{x \in \mathbf{R}^3 \mid ||x - x_i|| \leq r\}$$



Alpha Shape

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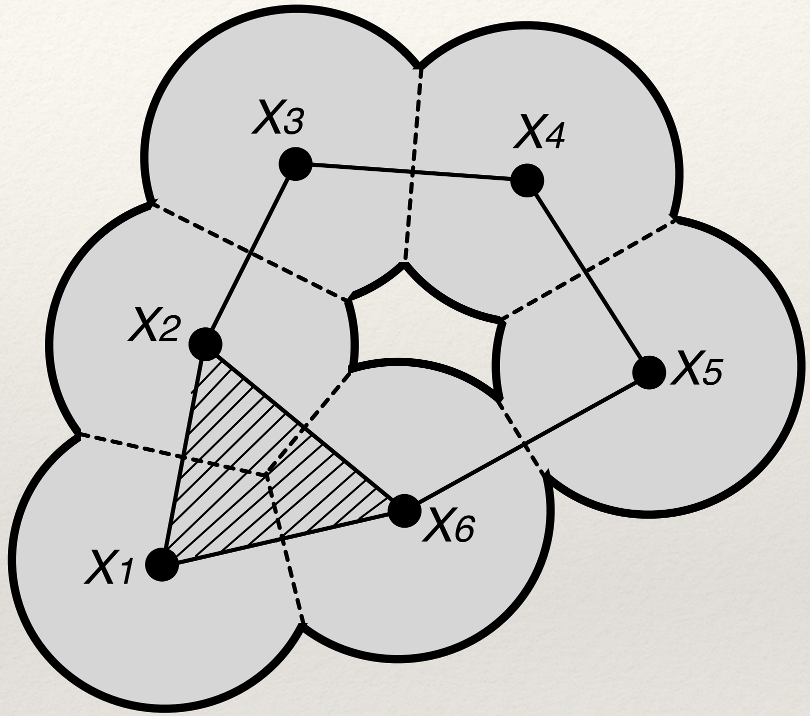
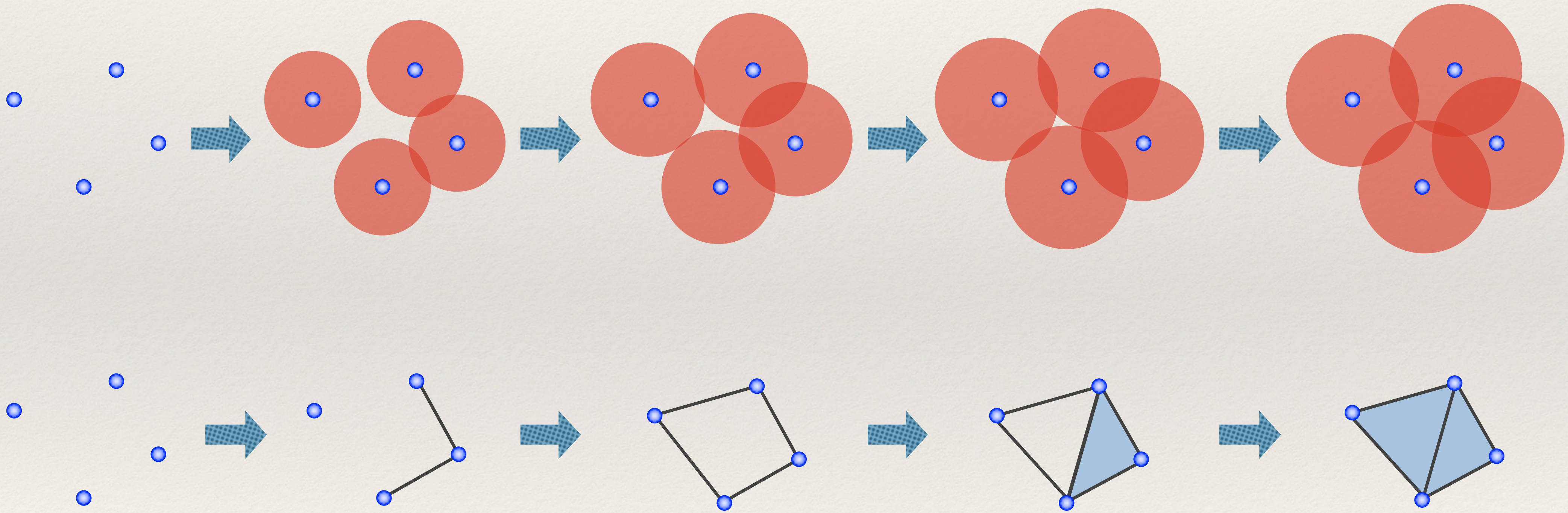


- **Alpha shape** $\mathcal{A}(X, r)$ **: dual of** $\{B_i(r) \cap V_i \mid i = 1, \ldots, n\}$

  (simplicial complex)

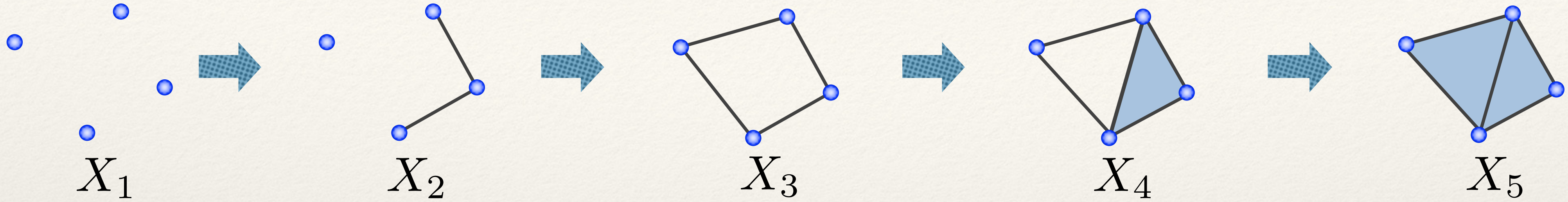
Alpha Filtration

- $\mathcal{A}(X, r) \subset \mathcal{A}(X, s)$ **for** $r < s$



Note: Alpha shape (filtration) can be computed by CGAL

Persistent Homology



- **filtration** $\mathcal{X} : X_1 \subset X_2 \subset \cdots \subset X_n$

$$PH_1(\mathcal{X}) \simeq I[3,4]$$

- **persistent homology**

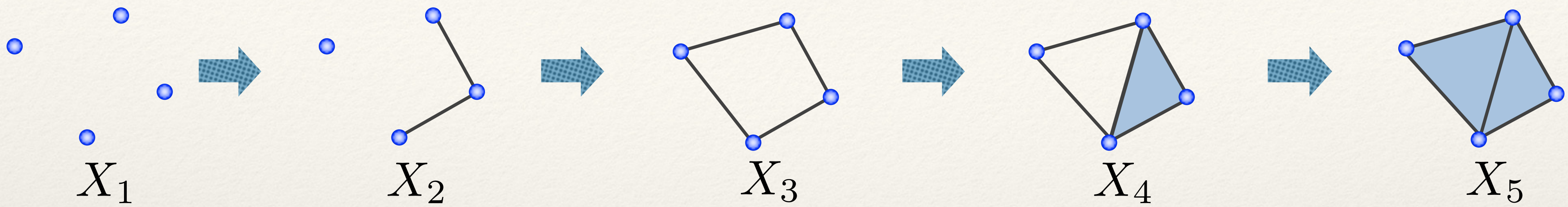
$$PH_\ell(\mathcal{X}) : H_\ell(X_1) \to H_\ell(X_2) \to \cdots \to H_\ell(X_n)$$

- **interval decomposition (Gabriel's Theorem)**

$$PH_\ell(\mathcal{X}) \simeq \bigoplus_{i=1}^{s} I[b_i, d_i]$$

$$I[b,d] : 0 \to \cdots \to 0 \to \underset{\textbf{at } X_b}{K} \to \cdots \to \underset{\textbf{at } X_d}{K} \to 0 \to \cdots \to 0$$

Persistence Diagram

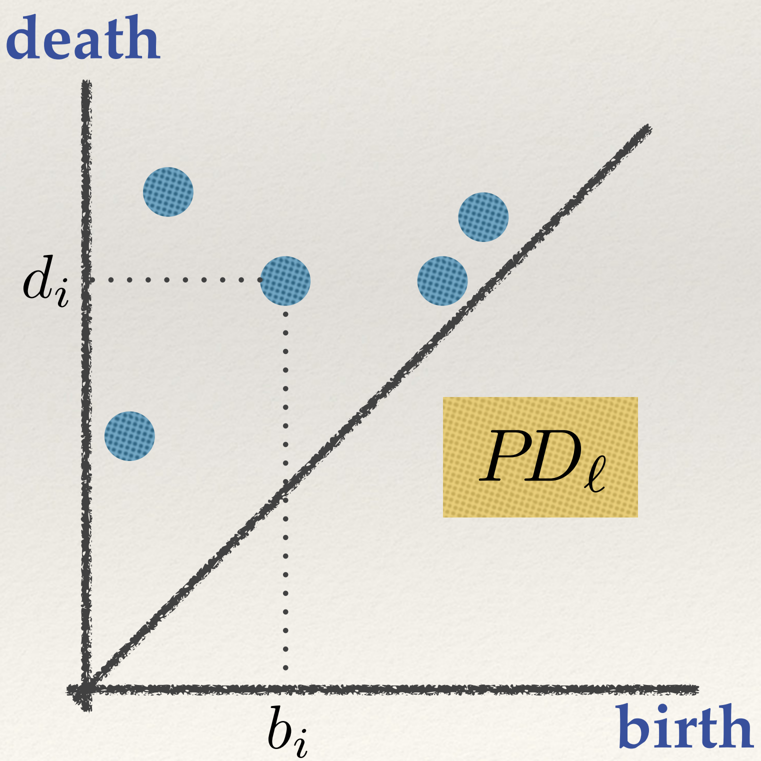


- **interval decomposition**

$$PH_\ell(\mathcal{X}) \simeq \bigoplus_{i=1}^{s} I[b_i, d_i]$$

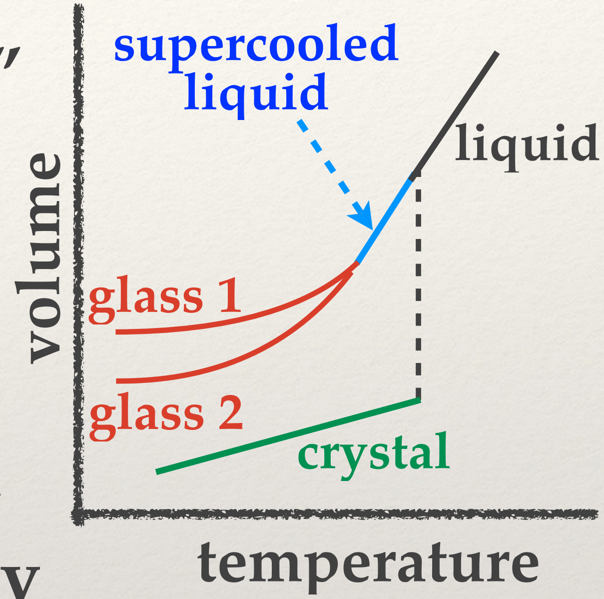
- **persistence diagram**

$$PD_\ell = \{(b_i, d_i) \in \mathbf{R}^2 \mid i = 1, \ldots, s\}$$

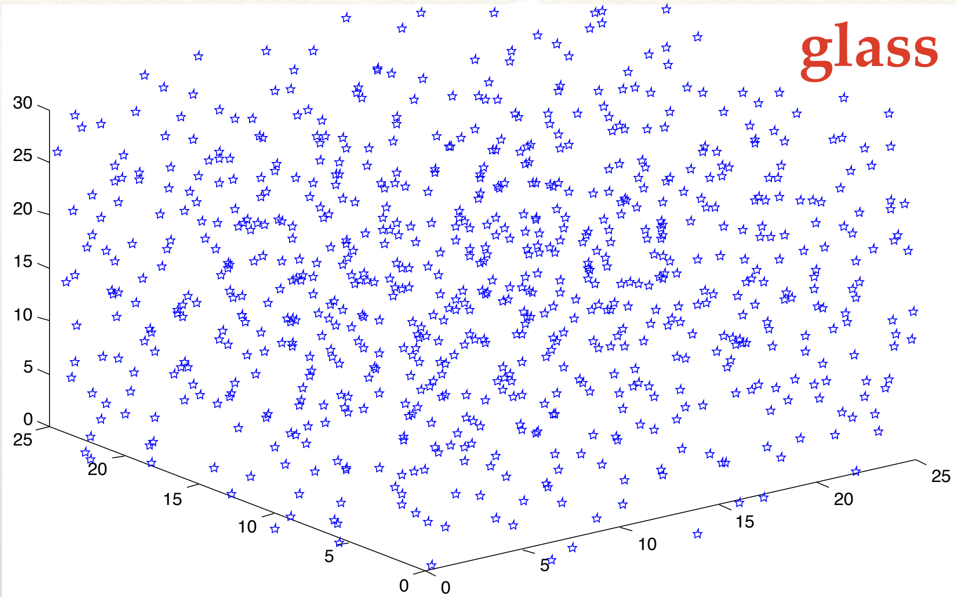


What is Glass?

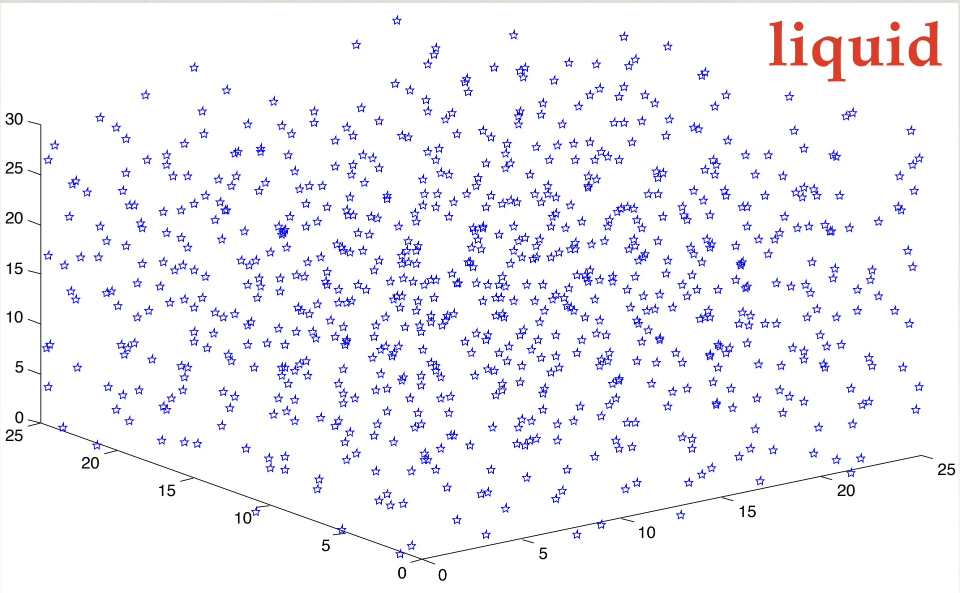
- Not yet fully answered to "what is glass?"
- Not liquid, not solid, but something in-between
- Molecules have disordered arrangements, but sufficient cohesion to maintain rigidity
- Further geometric understandings of atomic arrangements are required
- In applications, Solar Energy Glass, DVD, BD, etc.

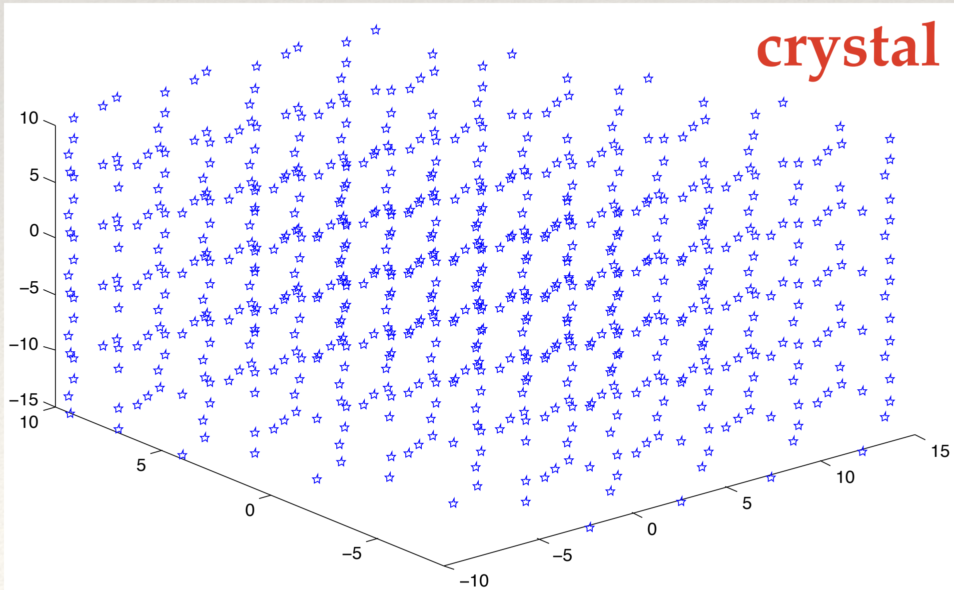


Atomic Arrangement of SiO_2

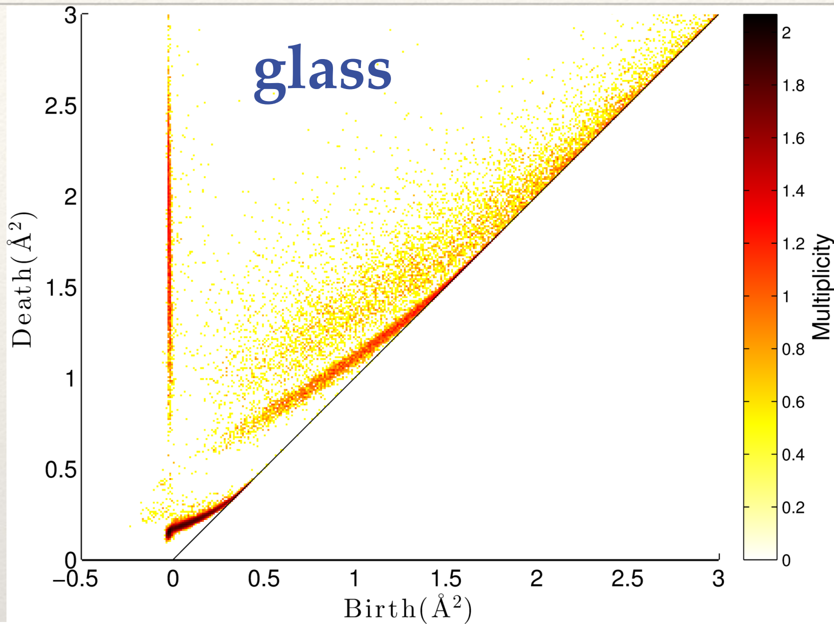


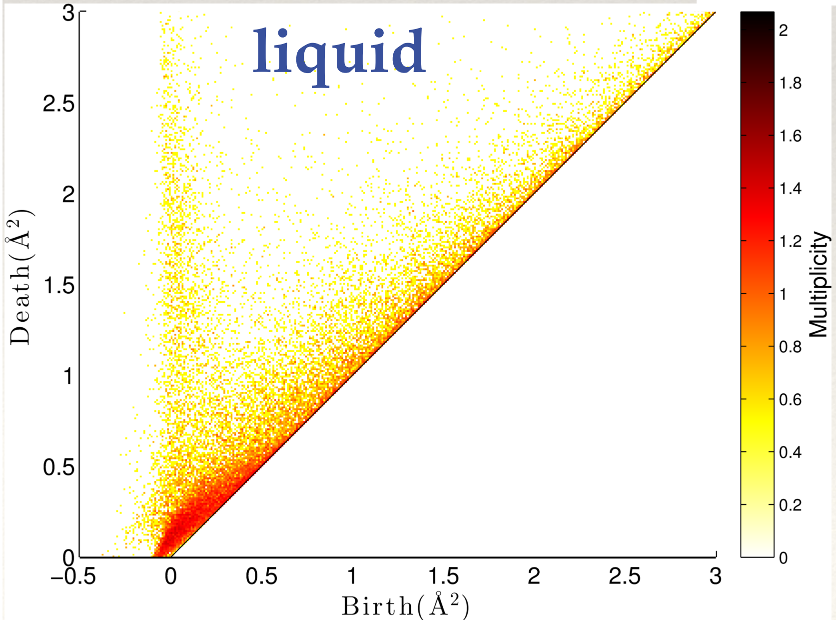
Note: they are obtained by MD simulations

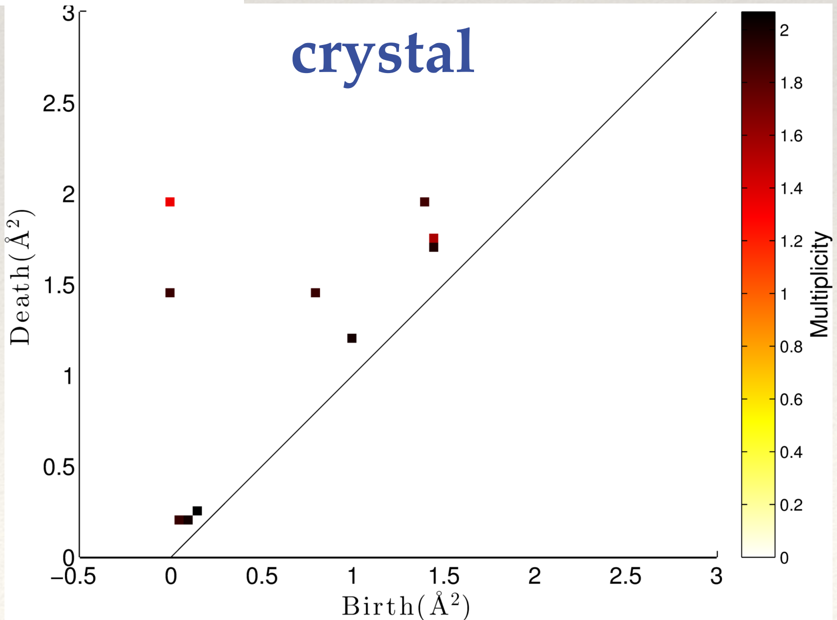




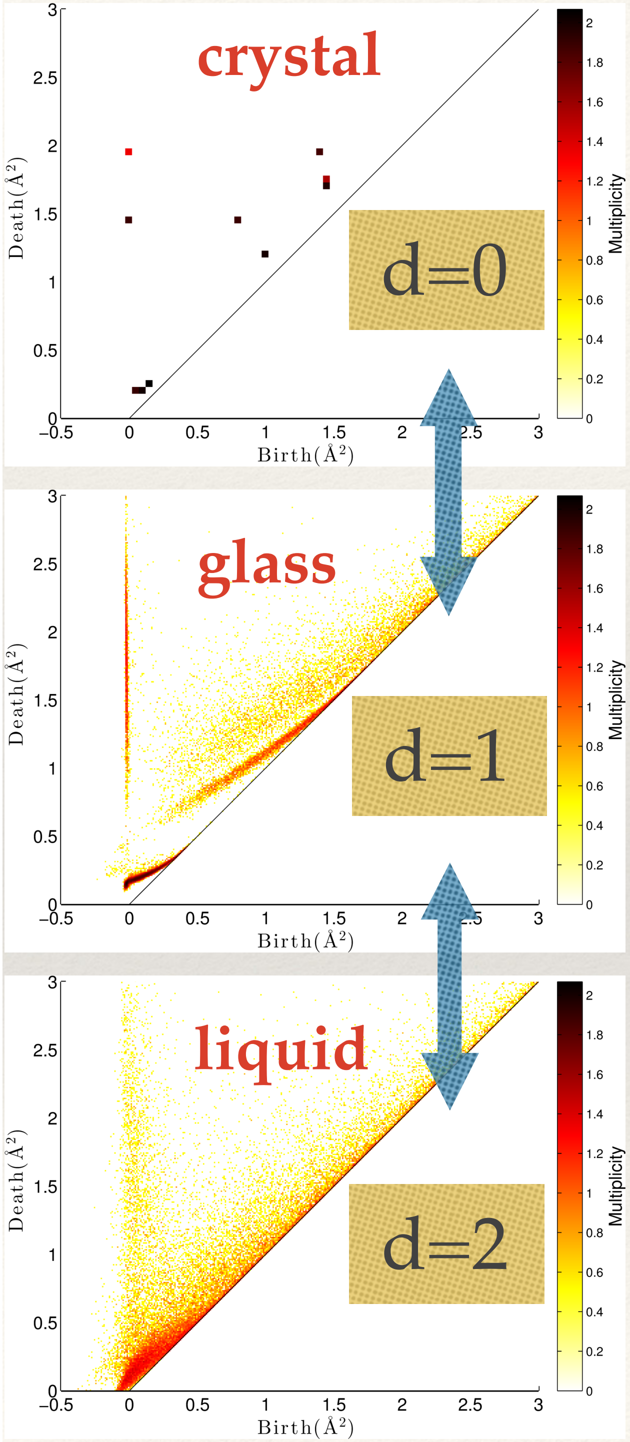
1-dim Persistence diagrams of SiO_2







Persistence Diagrams PD_1



0 dim support results from **regular** atomic locations of crystals

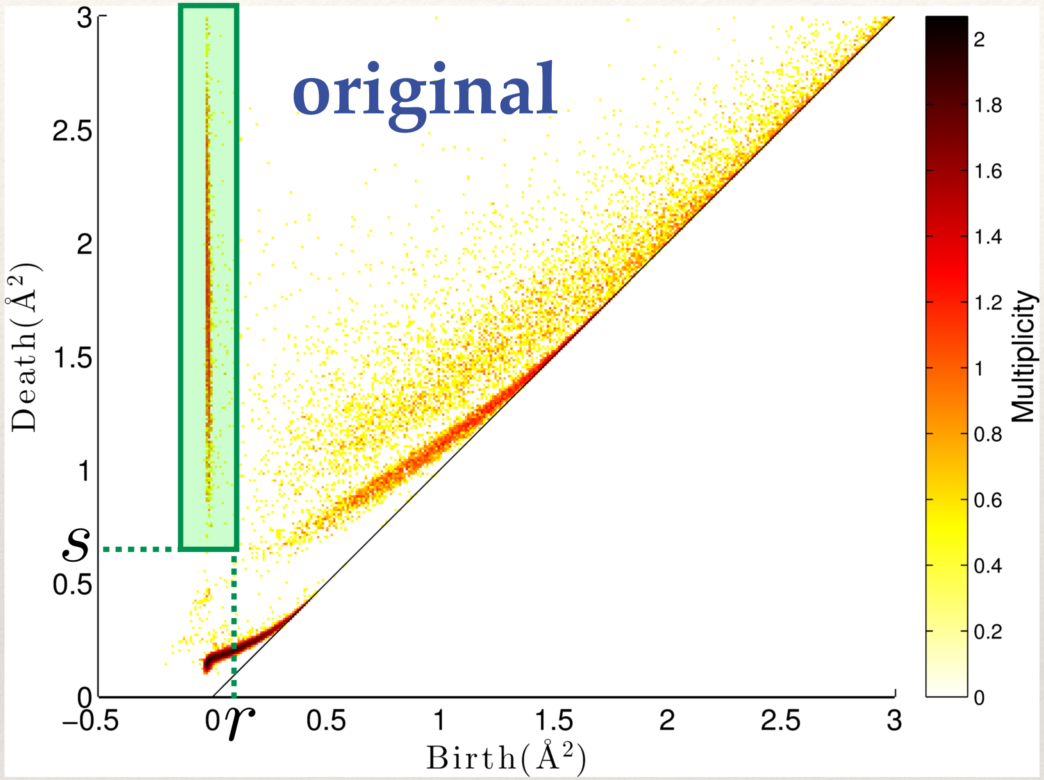
transition

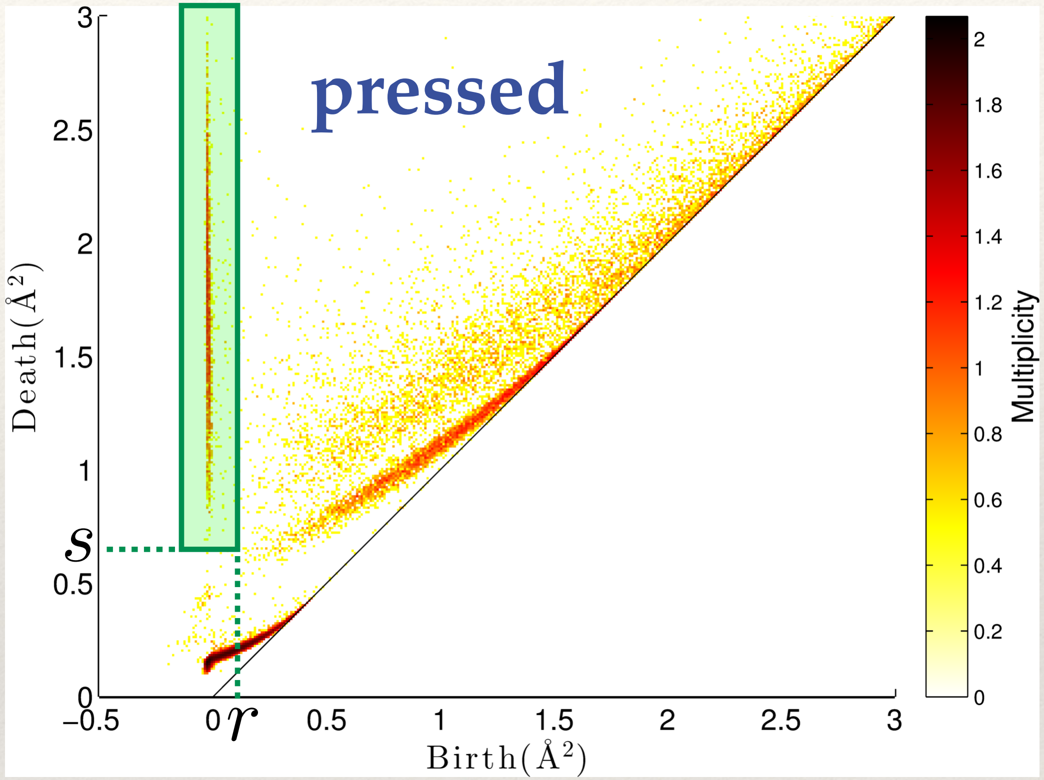
1 dim support (curves!) appears

transition

2 dim support results from **random** atomic locations of liquids

How robust under pressure?

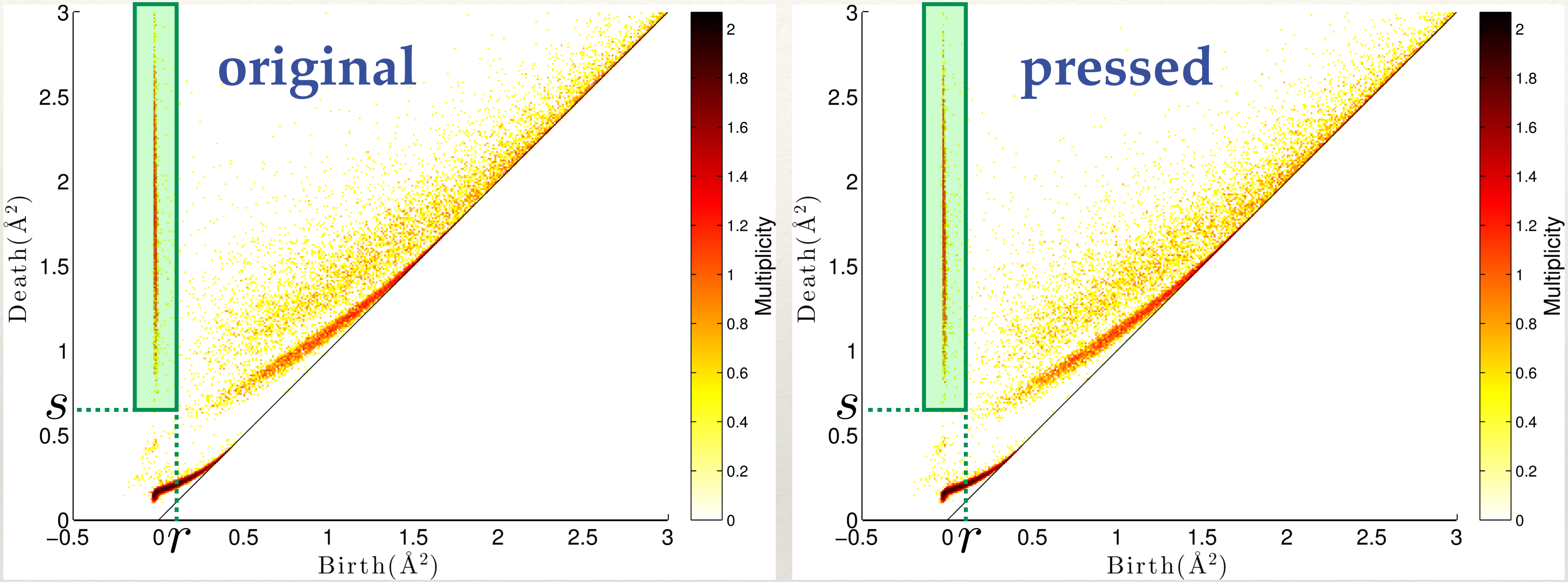




- corresponds to middle range rings
- characterized by birth time ≤ r and death time ≥ s
- how robust are these rings under pressurization?

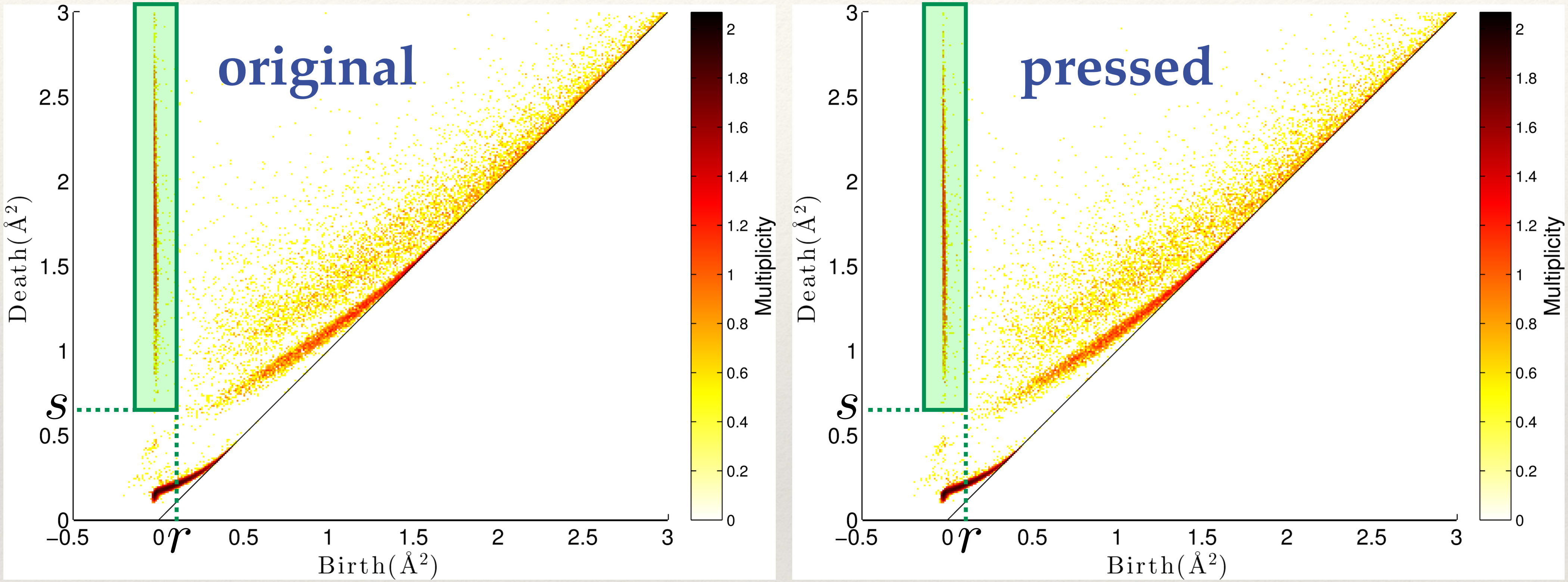
  X_α (or Y_α) denotes the rings subset of left (or right) with $\alpha = r, s$

How robust under pressure?



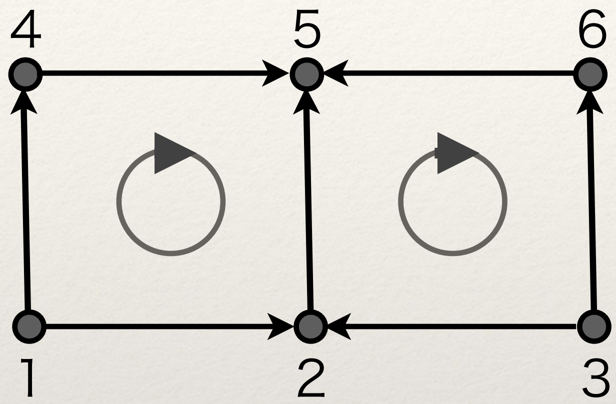
$$
\begin{array}{ccccc}
X_s & \subset & X_s \cup Y_s & \supset & Y_s \\
\cup & & \cup & & \cup \\
X_r & \subset & X_r \cup Y_r & \supset & Y_r
\end{array}
$$

How robust under pressure?



$$
\begin{bmatrix} K \\ \uparrow \\ K \end{bmatrix}^n \subset
\begin{array}{ccccc}
H_1(X_s) & \rightarrow & H_1(X_s \cup Y_s) & \leftarrow & H_1(Y_s) \\
\uparrow & & \uparrow & & \uparrow \\
H_1(X_r) & \rightarrow & H_1(X_r \cup Y_r) & \leftarrow & H_1(Y_r)
\end{array}
\supset \begin{bmatrix} K \\ \uparrow \\ K \end{bmatrix}^m
$$

Persistence on Commutative Ladder



$$\begin{array}{ccccc} X_s & \subset & X_s \cup Y_s & \supset & Y_s \\ \cup & & \cup & & \cup \\ X_r & \subset & X_r \cup Y_r & \supset & Y_r \end{array} \quad \xrightarrow{H_*(\bullet)} \quad \begin{array}{ccccc} H_*(X_s) & \rightarrow & H_*(X_s \cup Y_s) & \leftarrow & H_*(Y_s) \\ \uparrow & & \uparrow & & \uparrow \\ H_*(X_r) & \rightarrow & H_*(X_r \cup Y_r) & \leftarrow & H_*(Y_r) \end{array}$$

Persistence on Commutative Ladder

ex) TDA of Protein Foldings

P_t : **Atomic location at time** t **(** $t=1,2,\ldots,T$ **)**

$X_t = \mathcal{A}(P_t, s)$: **Alpha cplx with radius** s

time evolution

$$H_*(X_1) \longrightarrow H_*(X_1 \cup X_2) \longleftarrow H_*(X_2) \longrightarrow \ldots \longleftarrow H_*(X_T)$$

Persistence on Commutative Ladder

ex) TDA of Protein Foldings

P_t : **Atomic location at time** ***t*** **(** ***t*=1,2,…,*T*** **)**

$X_t = \mathcal{A}(P_t, s)$: **Alpha cplx with radius** ***s***

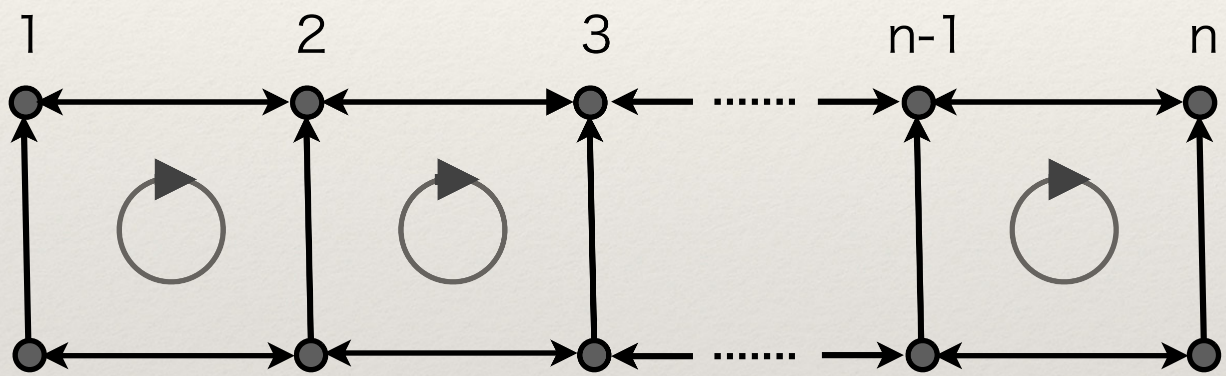
$Y_t = \mathcal{A}(P_t, r)$: **Alpha cplx with radius** ***r*** **(*r* < *s*)**

time evolution

robustness

$$
\begin{tikzcd}
H_*(X_1) \arrow[r] & H_*(X_1 \cup X_2) & H_*(X_2) \arrow[l] \arrow[r] & \dots & H_*(X_T) \arrow[l] \\
H_*(Y_1) \arrow[u] \arrow[r] & H_*(Y_1 \cup Y_2) \arrow[u] & H_*(Y_2) \arrow[u] \arrow[l] \arrow[r] & \dots & H_*(Y_T) \arrow[u] \arrow[l]
\end{tikzcd}
$$

Commutative Ladder



Quiver and Path Algebra

- A quiver $Q = (Q_0, Q_1)$ is a directed graph

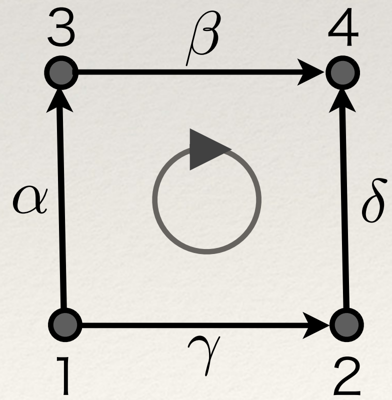
  Q_0 : a set of vertices $\qquad$ Q_1 : a set of directed edges

- A path algebra KQ : K-vector space spanned by all paths.

  The product of two paths is the composed path.

- Relations of paths generate an ideal $I \subset KQ$

- $A = KQ/I$ is an associative algebra



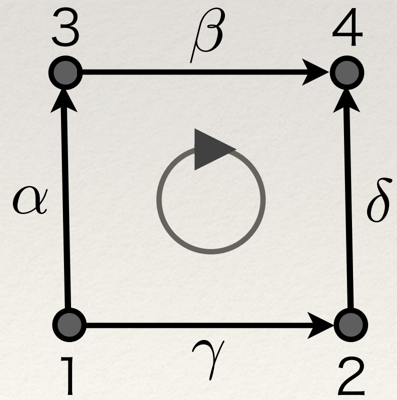
$I = \langle \alpha\beta - \gamma\delta \rangle$

Representation and Module

- A representation M on Q
  - A vector space M_a for each vertex a
  - A linear map $\varphi_\alpha : M_a \to M_b$ for each edge $\alpha : a \to b$

- A representation M on $A = KQ/I$

$$\varphi_\rho = 0 \quad \text{for each relation } \rho \in I$$



$$I = \langle \alpha\beta - \gamma\delta \rangle$$

$$\varphi_\beta\varphi_\alpha - \varphi_\delta\varphi_\gamma = 0$$

- Equivalence of category

$$\text{mod } A \simeq \text{rep } (A)$$

Krull-Schmidt Theorem

- A submodule $W \subset (M, \varphi)$
  - $W_a \subset M_a$ for each vertex a
  - $\varphi_\alpha(W_a) \subset W_b$ for each edge $\alpha : a \to b$

- An indecomposable module M

$$M \simeq W \oplus W' \Longrightarrow W = 0 \text{ or } W' = 0$$

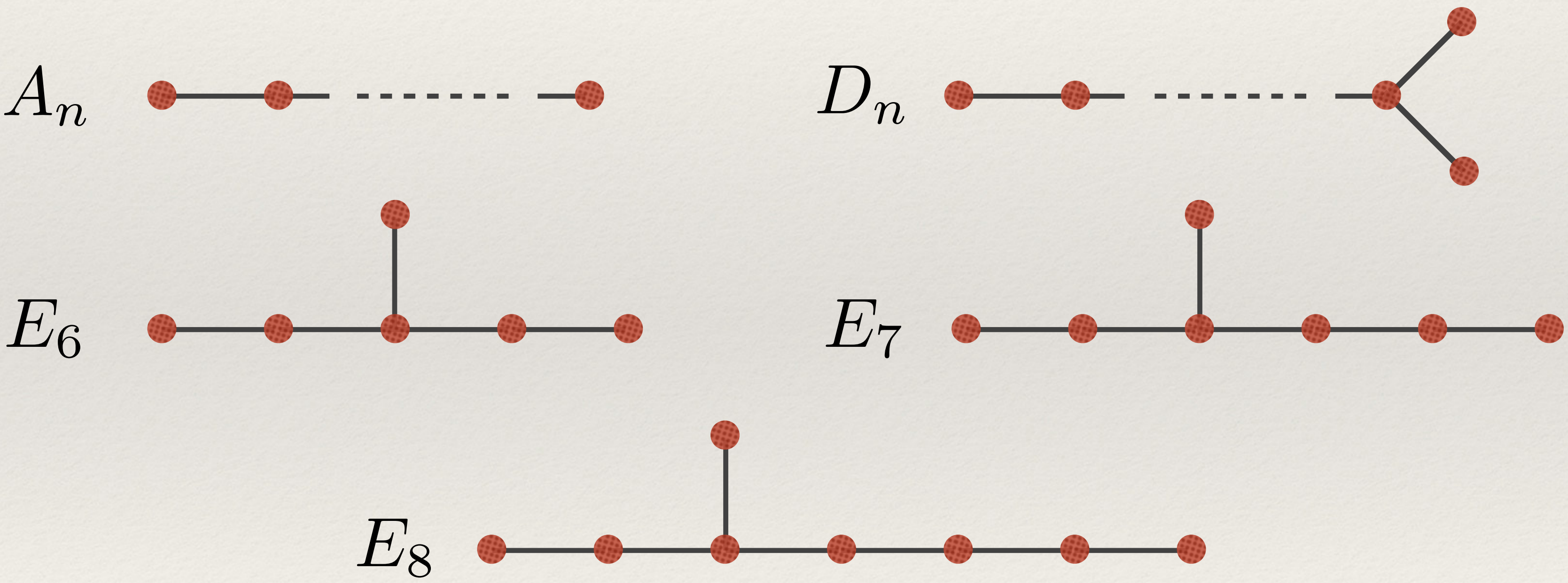
- Unique decomposition into indecomposables

$$M \simeq W^{(1)} \oplus \cdots \oplus W^{(\ell)}$$

Gabriel's Theorem

- A quiver Q is representation-finite

  $\Longleftrightarrow$ Q is a Dynkin diagram (A_n, D_n, E_6, E_7, E_8)



- Note that this is NOT a theorem for $A = KQ/I$

Persistence Module and Diagram

Representations on A_n

Carlsson & de Silva

- Persistence Module

$$H_*(X_1) \to H_*(X_2) \to \cdots \to H_*(X_n)$$

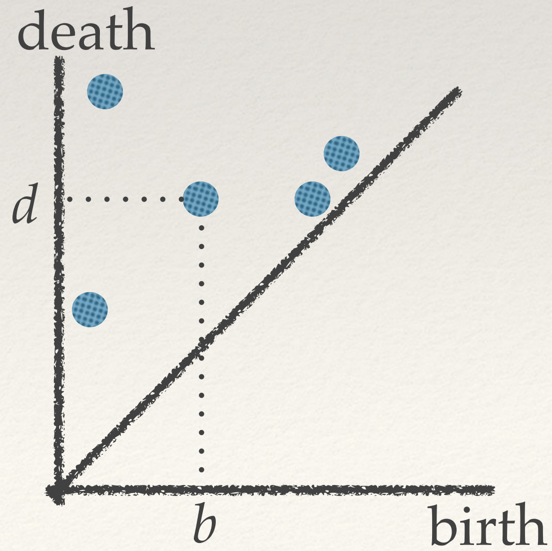
- Zigzag Persistence Module

$$H_*(X_1) \leftrightarrow H_*(X_2) \leftrightarrow \cdots \leftrightarrow H_*(X_n)$$

- Indecomposable Decomposition

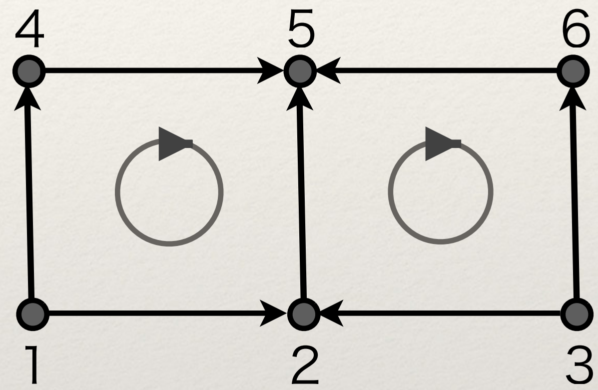
$$M \simeq \bigoplus_k I[b_k, d_k]$$

- Persistence Diagram



Finite or Infinite Type?

- Commutative ladder is NOT Gabriel types



- Commutativity is assigned
- Commutative ladder is finite type or not?
- What are counterparts of p-intervals and p-diagrams?

Auslander-Reiten Quiver

The AR-quiver $\Gamma(A)$ of A is defined as follows:

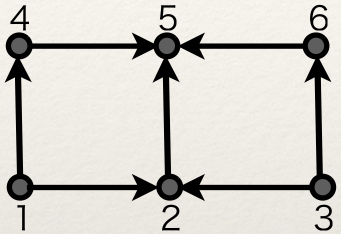
- The vertices are the indecomposable isomorphism classes $[X]$ in $\mathrm{mod}\ A$

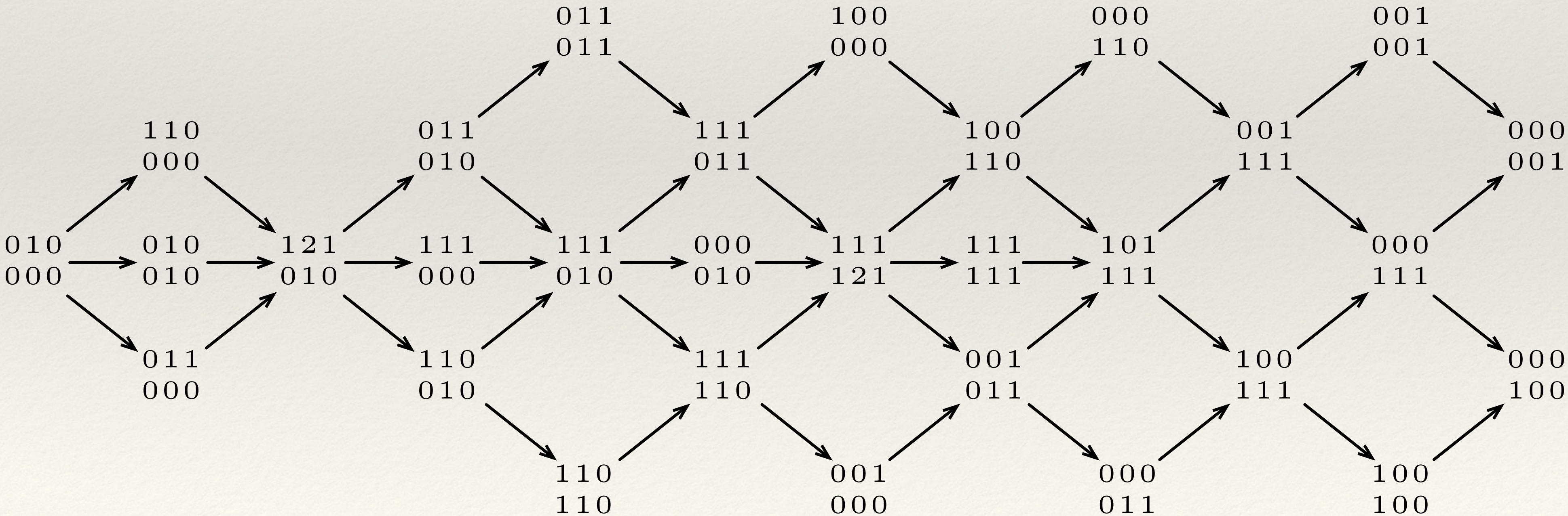
  (e.g., p-intervals $I[b,d]$ in standerd persistence)

- The arrow $[X] \to [Y]$ exists iff $\exists$irr. morphism $X \to Y$

  (e.g., $I[b,d] \to I[b-1,d]$, $I[b,d] \to I[b,d-1]$)

Main Theorem

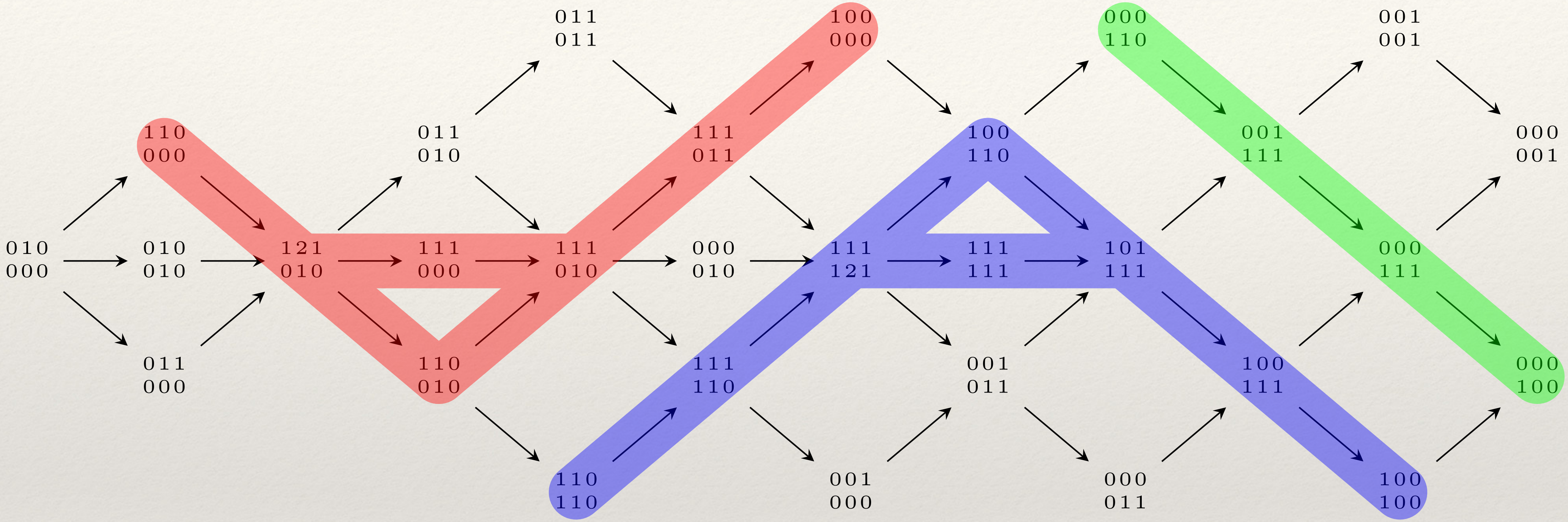
- The commutative ladders of length less than 5 is representation-finite (independently of orientations)
- The AR quiver of  is given as follows



Proof: AR theory (inductive applications of AR translations).

Further Decomposition of 2-Step Persistence

$$H_*(X_r) \to H_*(X_s) \simeq \mathbf{I}[r,r]^\ell \oplus \mathbf{I}[s,s]^m \oplus \mathbf{I}[r,s]^n$$

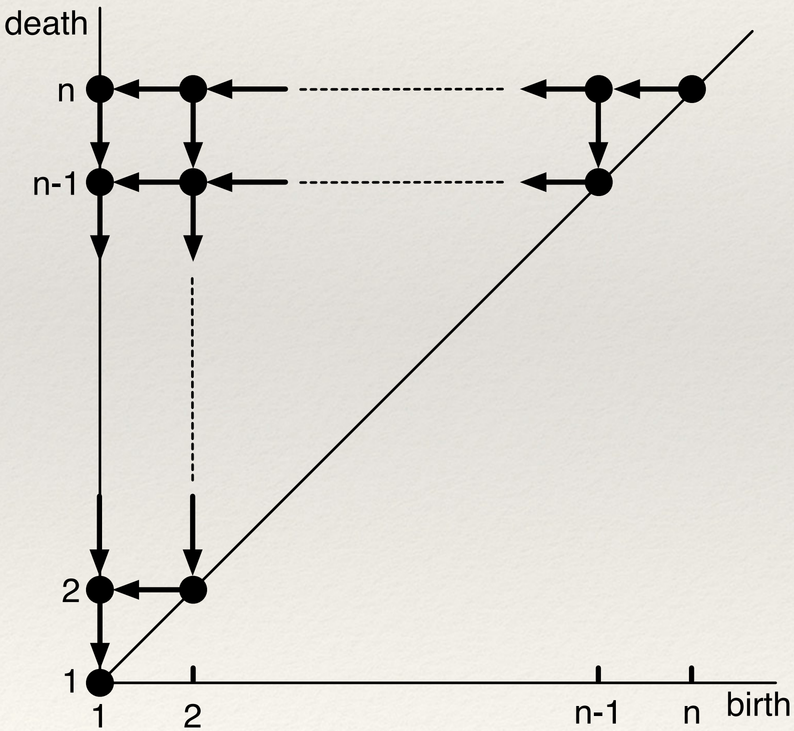


$$\begin{array}{ccccc} H_*(X_s) & \to & H_*(X_s \cup Y_s) & \leftarrow & H_*(Y_s) \\ \uparrow & & \uparrow & & \uparrow \\ H_*(X_r) & \to & H_*(X_r \cup Y_r) & \leftarrow & H_*(Y_r) \end{array}$$

- Decompositions of zigzag persistence are similar

Persistence Diagram and AR quiver

- AR quiver $\Gamma = (\Gamma_0, \Gamma_1)$ of $\mathbf{A}_n$ type is the support of persistence diagram



persistence module

$$M \simeq \bigoplus_{[I]\in\Gamma_0} I^{k_{[I]}} \qquad k_{[I]} \in \mathbf{N}_0$$

persistence diagram

$$D_M : \Gamma_0 \to \mathbf{N}_0$$
$$[I] \mapsto k_{[I]}$$

Persistence Diagram and AR quiver

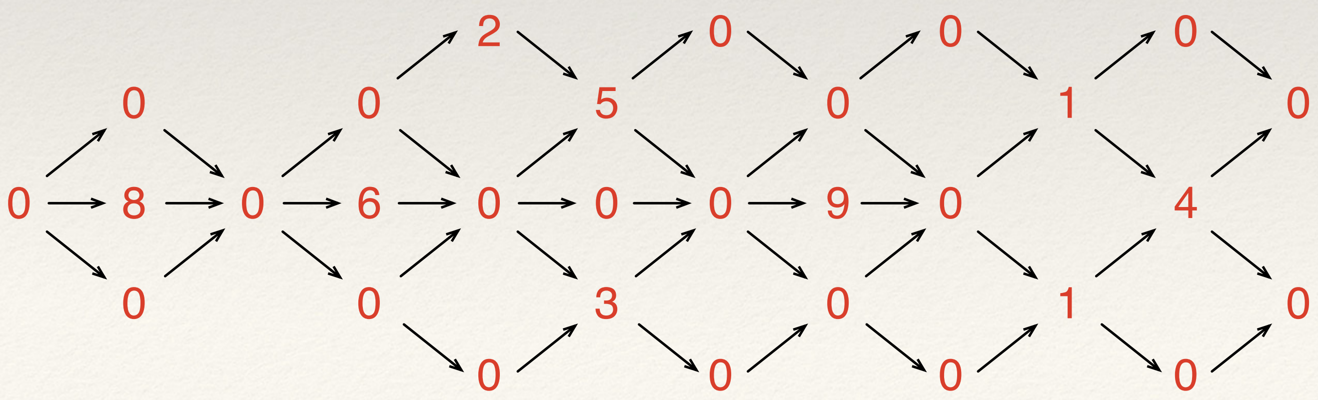
- Persistence diagram of persistence module

$$M \simeq \bigoplus_{[I]\in\Gamma_0} I^{k_{[I]}}$$

is given by a function (equivalently mulitiset)

$$D_M : \Gamma_0 \to \mathbf{N}_0 \qquad [I] \mapsto k_{[I]}$$

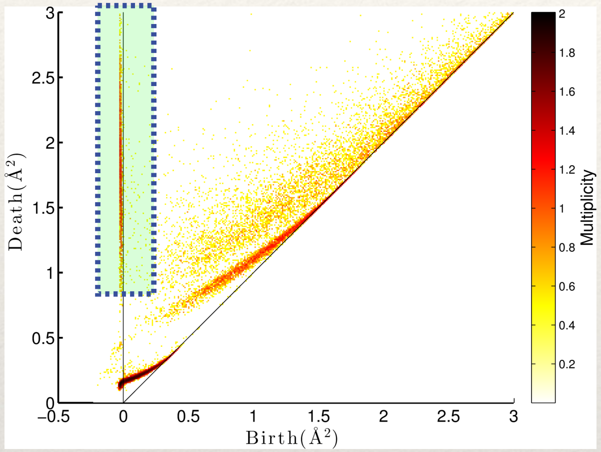
on AR quiver $\Gamma = (\Gamma_0, \Gamma_1)$



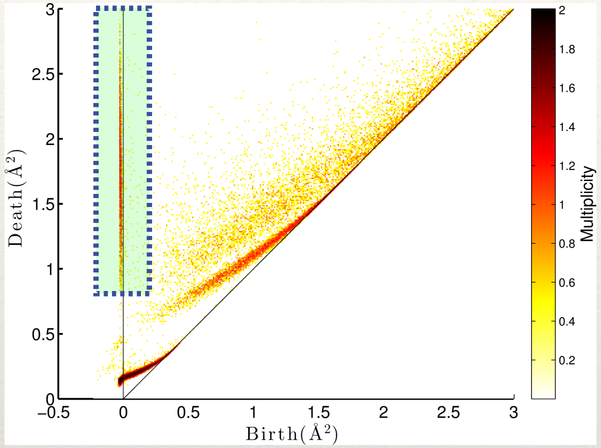
example of PD in C.T.L.

Pressurization and C.L.

X : original

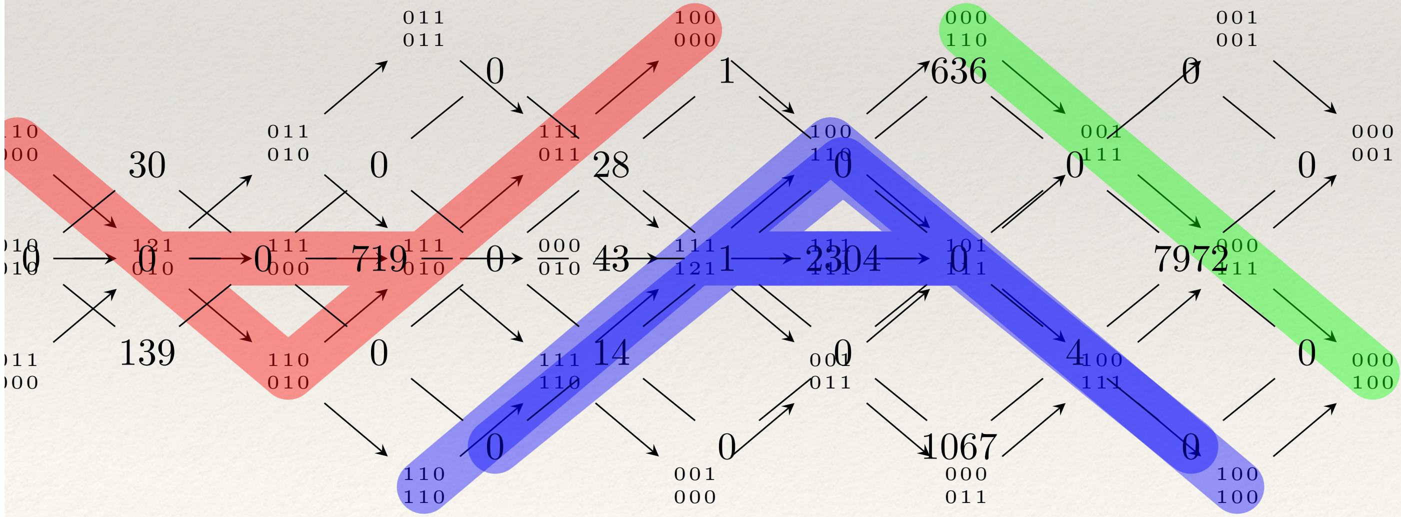


Y : pressured



$$
\begin{tikzcd}
H_*(X_s) \arrow[r] & H_*(X_s \cup Y_s) & H_*(Y_s) \arrow[l] \\
H_*(X_r) \arrow[r] \arrow[u] & H_*(X_r \cup Y_r) \arrow[u] & H_*(Y_r) \arrow[l] \arrow[u]
\end{tikzcd}
$$

$$
\begin{tikzcd}
\boxed{K} \arrow[r] & \boxed{?} & \boxed{K} \arrow[l] \\
\boxed{K} \arrow[r] \arrow[u] & \boxed{?} \arrow[u] & \boxed{K} \arrow[l] \arrow[u]
\end{tikzcd}
$$



99.18%(~2304/2323) generators persist under pressurization!

persistence diagram

Computations

- The Auslander-Reiten quiver provides a flowchart of the algorithm to compute persistence diagrams
- Discrete Morse reduction can be applied to C.L.

#	$\lvert X \rvert$	$\lvert A \rvert$	t	t
1	15,341	2,777	903.31	39.53
2	17,626	7,164	3497.55	143.41
3	32,540	7,834	5162.12	42.34

Thank you very much