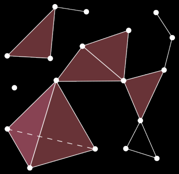


Universal dynamics in quantum many-body systems via persistent homology

Daniel Spitz

Cold Quantum Coffee

April 13, 2021

This talk is based on

DS, Berges, Oberthaler, Wienhard: *Finding universal structures in quantum many-body dynamics via persistent homology*, arXiv:2001.02616,

DS, Wienhard: *The self-similar evolution of stationary point processes via persistent homology*, arXiv:2012.05751.

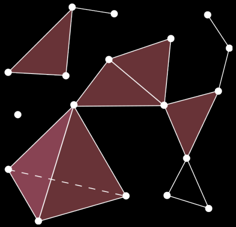
Topological data analysis (TDA)

General TDA pipeline:

(i) acquire point cloud data,

(ii) construct simplicial complexes,

(iii) infer topological properties via tools from algebraic topology.



Topological data analysis

TDA toolbox made up from

- Mapper algorithm for partial clustering (e.g. Singh, Memoli, Carlsson, Eurographics Symposium on Point-Based Graphics, 2007),
- Persistent homology.

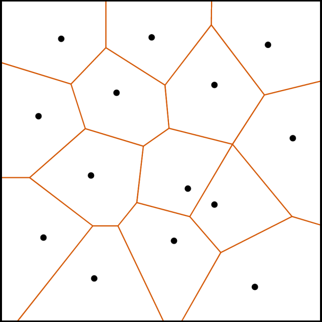
More information: STRUCTURES EP Math and Data, https://wiki.structures.mathi.uni-heidelberg.de/index.php/Main_Page

Contents

Delaunay complex

Point cloud $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$. Its Voronoi diagram consists of Voronoi cells for all $x \in X$:

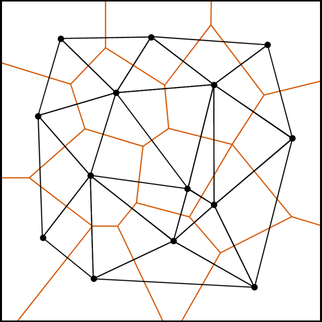
$$\mathrm{Vor}(x, X) = \left\{ y \in \mathbb{R}^d \,\middle|\, |y - x| \leq |y - p| \,\forall\, p \in X \right\}$$



Delaunay complex

Delaunay triangulation constructed as dual of Voronoi diagram:

$$\mathrm{Del}(X) = \{\sigma \subset X \,|\, \bigcap_{x \in \sigma} \mathrm{Vor}(x, X) \neq \emptyset\}$$



Alpha complexes

A simplex is the generalization of a triangle or tetrahedron to arbitrary dimensions.

Introduce radius function $\mathrm{Rad} : \mathrm{Del}(X) \to \mathbb{R}$, mapping a simplex $\sigma \in \mathrm{Del}(X)$ to the radius of its circumsphere.

Alpha complexes:

$$\mathrm{Alpha}_r(X) := \mathrm{Rad}^{-1}[0, r]$$

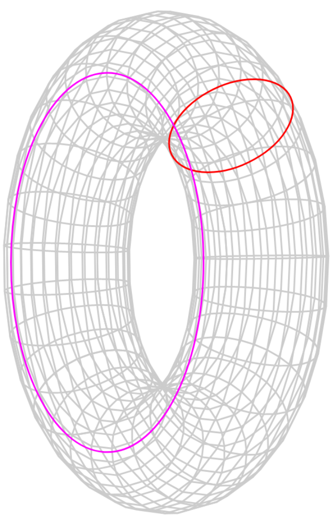
$\Longrightarrow$ *Encodes scale-dependent information on the point cloud* X*.*

Homology: Betti numbers

β_0 counts components - 1

β_1 counts tunnels

β_2 counts enclosed voids



Source: Wikimedia

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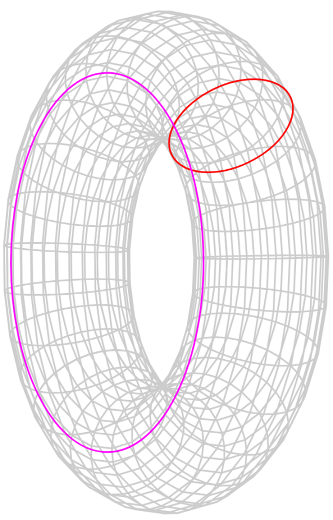
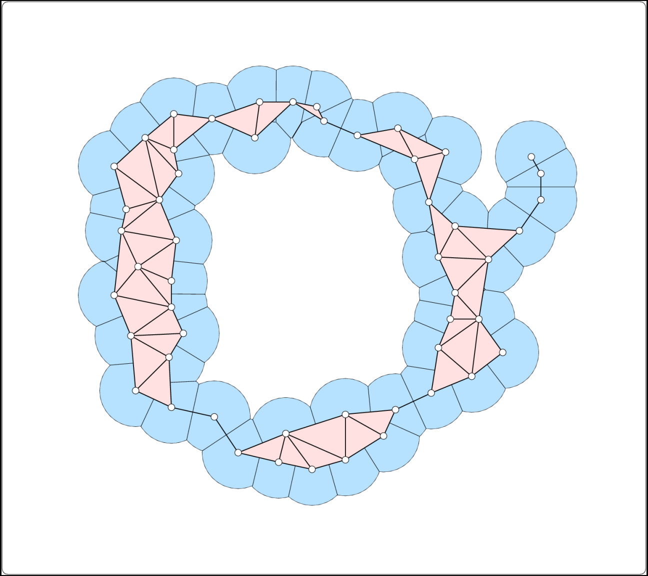


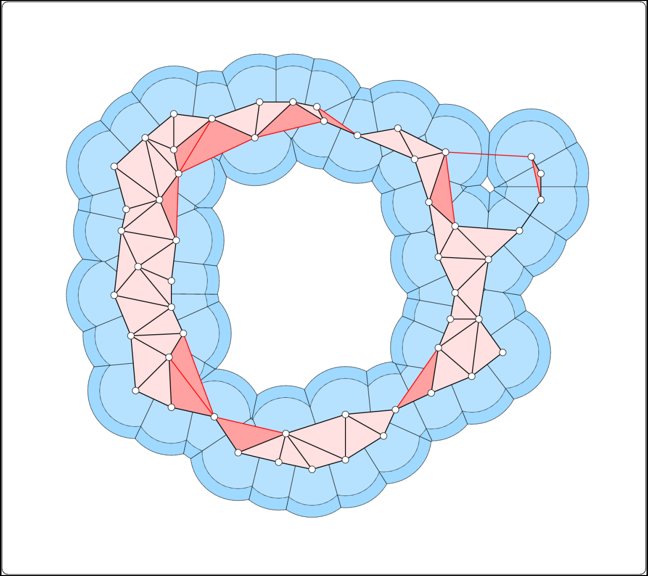
$\beta_0 = 0$, $\beta_1 = 2$, $\beta_2 = 1$.

Persistent homology



From a talk by H. Edelsbrunner

Persistent homology



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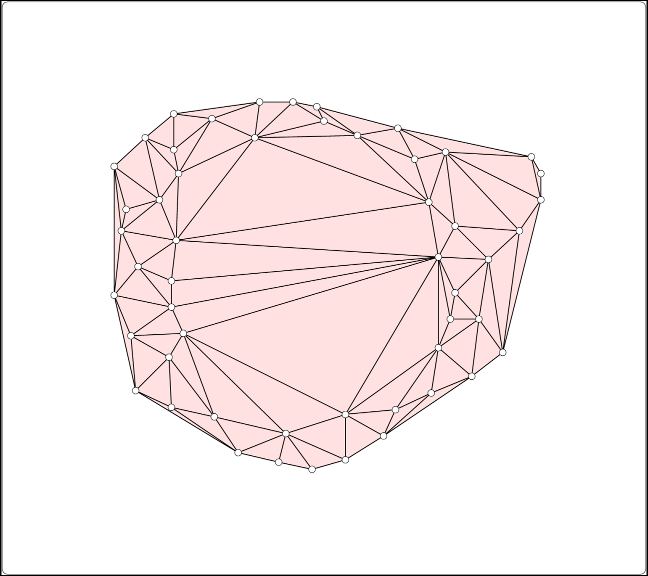


From a talk by H. Edelsbrunner

(Asymptotic) persistence pair distribution

$(D_i)_{i\in\mathbb{N}} \subset \mathscr{D}$ be ensemble of persistence diagrams. *Persistence pair distribution* of D_i:

$$\mathfrak{P}_i(r'_b, r'_d) := \sum_{(r_b,r_d)\in D_i} \delta(r'_b - r_b)\,\delta(r'_d - r_d).$$

Define the **asymptotic persistence pair distribution**, $\langle\mathfrak{P}\rangle$, implicitly, requiring that for a functional summary F,

$$\int_0^\infty dr'_b \int_0^\infty dr'_d\, F(\{(r'_b, r'_d)\})(s)\,\langle\mathfrak{P}\rangle(r'_b, r'_d)$$
$$:= \lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} \int_0^\infty dr'_b \int_0^\infty dr'_d\, F(\{(r'_b, r'_d)\})(s)\,\mathfrak{P}_i(r'_b, r'_d).$$

Rigorous construction see DS, Wienhard, arXiv:2012.05751.

Functional summaries of interest

Distributions of birth and death radii,

$$\langle \mathcal{B} \rangle(r_b) := \int_0^\infty dr_d \, \langle \mathfrak{P} \rangle(r_b, r_d), \qquad \langle \mathcal{D} \rangle(r_d) := \int_0^\infty dr_b \, \langle \mathfrak{P} \rangle(r_b, r_d).$$

Persistence distribution (distribution of $r_d - r_b$),

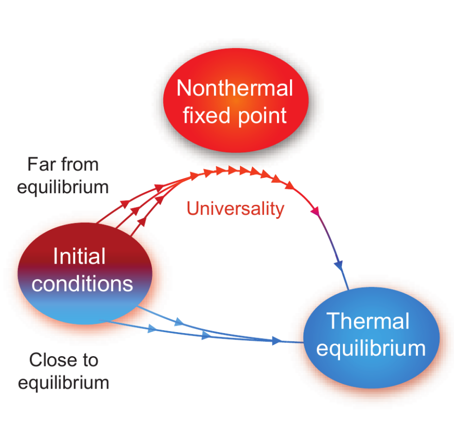
$$\langle \mathcal{P} \rangle(r) := \int_0^\infty dr_d \, \langle \mathfrak{P} \rangle(r_d - r, r_d).$$

Distribution of Betti numbers,

$$\langle \beta \rangle(r) := \int_0^r dr_b \int_r^\infty dr_d \, \langle \mathfrak{P} \rangle(r_b, r_d).$$

Contents

Generic evolution towards thermal equilibrium

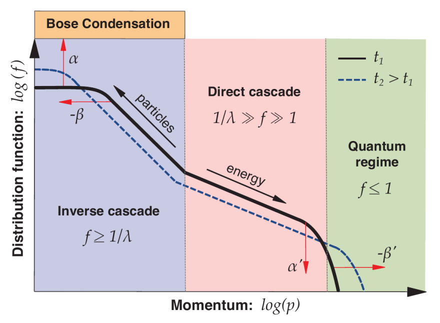


Picture reprinted from Berges 2015.

Universality far from equilibrium: Nonthermal fixed points

Rescaling approach to occupation number distribution:

$$f(t, \boldsymbol{p}) = t^{\alpha} f_S(t^{\beta}|\boldsymbol{p}|).$$



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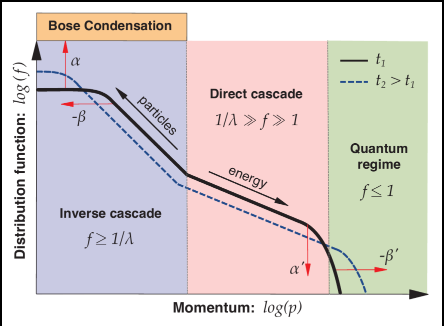


Picture reprinted from Berges 2015.

Goal: Reveal universal dynamics beyond *n*-point correlation functions via persistent homology observables.

Self-similar scaling ansatz

Let $\langle\mathfrak{P}\rangle(t, r_b, r_d)$ be a time-dependent asymptotic persistence pair distribution. Say $\langle\mathfrak{P}\rangle(t, r_b, r_d)$ **scales self-similarly**, if exponents η_1, η_1' and η_2 exist, s.t. for all times t, t',

$$\langle\mathfrak{P}\rangle\big(t, r_b, r_d\big) = (t/t')^{-\eta_2}\,\langle\mathfrak{P}\rangle\big(t', (t/t')^{-\eta_1} r_b, (t/t')^{-\eta_1'} r_d\big).$$

$\Longrightarrow$ Rigorously defined in DS, Wienhard, arXiv:2012.05751.

Geometric intuition: Persistence length scales computed from $\langle\mathfrak{P}\rangle(t)$ blow up in time as a power-law $\sim t^{\eta_1}$ (assuming $\eta_1 = \eta_1'$).

Packing relation: heuristics

Set $\eta_1 = \eta_1'$. Assume point clouds are dominated by a length scale $L(t)$, but restricted to lattice volume V. In d spatial dimensions, find that a number $n(t)$ of top-dimensional homology classes fits into V:

$$\langle n \rangle(t) \simeq \frac{V}{L(t)^d} \propto \left(\frac{t}{t'}\right)^{-d\eta_1}.$$

Now,

$$\langle n \rangle(t) = \int r_b \int r_d \, \langle \mathfrak{P}_{d-1} \rangle(t, r_b, r_d) = \left(\frac{t}{t'}\right)^{-\eta_2 + 2\eta_1} \langle n \rangle(t').$$

Thus,

$$\eta_2 = (2 + d)\eta_1.$$

Can be derived mathematically rigorous in a very broad setting exploiting ergodicity and persistence inequalities (DS, Wienhard, arXiv:2012.05751).

Contents

The classical-statistical approximation

Can to a controlled accuracy map quantum dynamics onto a classical-statistical ensemble. Classical-statistical simulations proceed as follows:

1. Monte Carlo **sampling of quantum initial conditions**,
2. evolution in time of such a configuration via **classical equation of motion**,
3. expectation value of a physical observable computed by **averaging** over classical field trajectories' outcomes.

Regime of validity: large occupation numbers and weak couplings.

Simulating the $d = 2$ Bose gas

Bose gas governed by Gross-Pitaevskii equation,

$$\left(-\frac{\nabla^2}{2m} + g\,|\psi(t,\mathrm{x})|^2\right)\psi(t,\mathrm{x}) = i\partial_t\psi(t,\mathrm{x}).$$

Equation numerically solved on a spatial lattice, describes Bose-Einstein condensate dynamics.

Non-linearities arise via the **interaction** term, rendering GPE quantum dynamics highly non-trivial.

$d = 2$ results: analytics

Different analytic predictions exist for IR universal scaling exponents:

- 2PI $1/N$ expansion result: $\beta = 0.5$. Surprisingly, works also for $N = 1$. (Orioli, Boguslavski, Berges, PRD 92, 2015)
- Vortices yield anomalous $\beta = 0.2$ (Karl & Gasenzer, New J Phys 19, 2017).

$\Longrightarrow$ Confirmed depending on initial conditions (Deng *et al.*, PRA 97, 2018; Karl & Gasenzer, New J Phys 19, 2017)

Point clouds from simulations

Restrict construction of persistent homology observables to classical-statistical approximation in this work.

Work on lattice,

$$\Lambda = \{(an_1, \ldots, an_d) \,|\, n_i \in \{1, \ldots, N\}\}, \qquad a = L/N.$$

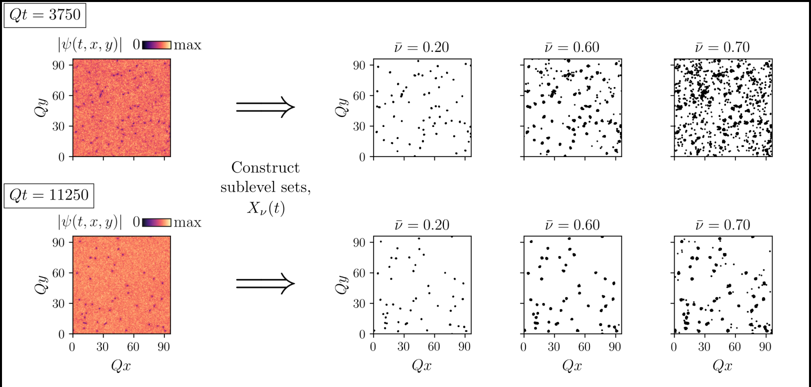
Immense freedom of choice exists in constructing point clouds from individual field configurations, e.g., by means of sublevel sets of a filtration function (a map from a field configuration to $\mathbb{R}$).

Here, for all $\nu \in [0, \infty)$ point clouds generated as

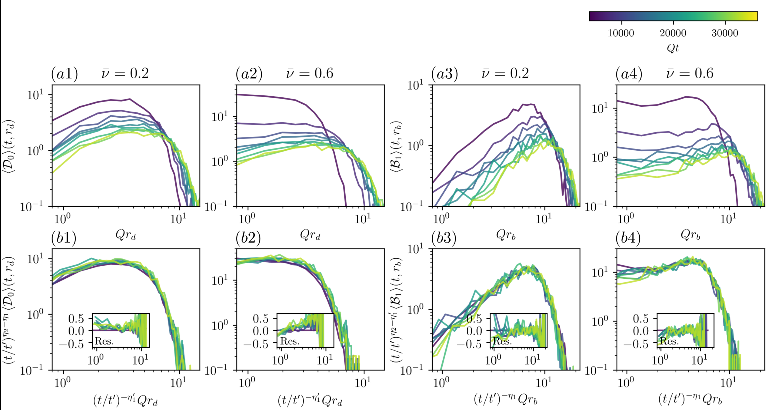
$$X_\nu(t) := |\psi(t, \cdot)|^{-1}[0, \nu] = \{\mathrm{x} \in \Lambda \,|\, |\psi(t, \mathrm{x})| \leq \nu\}.$$

Interested in sequence of alpha complexes of $X_\nu(t)$ for fixed ν.

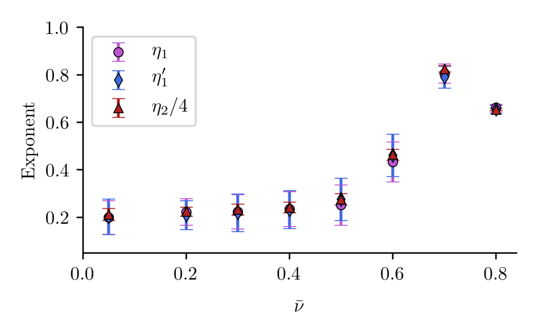
Point clouds



Birth and death radii distributions in IR NTFP vicinity



Persistent homology scaling exponents



Contents

Conclusions

- Introduced persistent homology observables to the analysis of dynamical quantum phenomena.
- Discussed corresponding manifestations of universal behavior, including a packing relation between occurring scaling exponents.
- In the $d = 2$ nonrelativistic Bose gas found scaling behavior in the IR and accurately confirmed the deduced packing relation.

Outlook

- What effect does the employed filtration function have in general?
- How about scaling of persistent homology observables in other theories?
- What further constructions related to persistent homology turn out useful to understand quantum dynamics?