Interpretable Phase Detection and Classification with Persistent Homology

* consider also: https://doi.org/10.1103/PhysRevResearch.2.043308 by Bart Olsthoorn, Johan Hellsvik, and Alexander V. Balatsky
Research interest in ultracold atoms:
- Detections (single-shots) are point clouds
- Features may be tough to extract or understand
- Persistent homology works with point clouds → maybe very versatile
Upshot: Persistent homology for feature extraction

- Technique from topological data analysis – *persistent homology*
- Unsupervised feature extraction
  - Number of phases
  - Their properties
- Phase classification: logistic regression with persistence diagrams (results of persistent homology)

### 2D spin models (Drosophilae)

<table>
<thead>
<tr>
<th></th>
<th>Unfrustrated</th>
<th>Frustrated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Discrete</td>
<td>Ising (Section 3.2)</td>
<td>Square-ice (Section 3.3)</td>
</tr>
<tr>
<td></td>
<td>$H_u = - \sum_{i,j} s_i s_j$</td>
<td>$H_{sq} = \sum_{\kappa} (\sum_{\alpha} n_{\kappa})^2$</td>
</tr>
<tr>
<td>Continuous</td>
<td>XY (Section 3.4)</td>
<td>Fully-frustrated XY (Section 3.5)</td>
</tr>
<tr>
<td></td>
<td>$H_{xy} = - \sum_{i,j} \cos \theta_i, \theta_j$</td>
<td>$H_{fxy} = - \sum_{i,j} J_{ij} \cos \theta_i, \theta_j$</td>
</tr>
</tbody>
</table>
How does (persistent) homology work?

A unified description of topological features of all dimensions is given by algebraic topology, and the hierarchical or multiscale version of algebraic topology is persistent homology.\(^1\)

Persistent homology how-to:

- embed data in a discrete complex
- form simplical complexes (0-simplices, 1-simplices, ...)
- simplical complexes are characterized by topological equivalence classes \(H_p\) of \(p\)-cycles (\(p\)-dimensional holes):
  - \(H_0\) are connected components
  - \(H_1\) are non-contractible loops
- That’s homology; add coarse-graining at monotonously increasing scale (“filtration”) \(\rightarrow\) persistent homology

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\(^1\)https://arxiv.org/abs/2009.14231
\(^2\)consider also: https://doi.org/10.1103/PhysRevResearch.2.043308
Filtration (discrete)

A distance function [...] corresponds to a filtration of the simplicial complex, that is a nested sequence of increasing subsets. ³

- points ≡ e.g. all spins of certain orientation
- step-wise coarse graining (α increases)
- features or p-simplexes are created or removed (red lines/areas show most recent ones)

³cf. https://en.wikipedia.org/wiki/Persistent_homology
A persistence diagram characterizes a filtration by points \((X, Y)\); the coordinate \(X\) is the level of the filtration where a feature is “born” and the coordinate \(Y\) is the level at which it “dies”.\(^4\)

\(^4\) cf.: https://en.wikipedia.org/wiki/Persistent_homology
Ising model: persistence diagram and image

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Persistent homology
Phase classification: logistic regression on persistence images

- Generate persistence images from persistent homology
- Label part of the images (extreme temperatures) with phase labels “0” and “1”...
- Use labeled set to obtain regression parameters $\lambda$ (see loss below)
- Optimized regression parameters are useful analogues of order parameters (they tell us which of the persistence images is characteristic for a phase)
- Classify the remainder of the persistence images with learned logistic regression.

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$\sum_k \left( y^{(k)} \log \left[ \sigma(\lambda_0 + \lambda \cdot x^{(k)}) \right] + (1 - y^{(k)}) \log \left[ 1 - \sigma(\lambda_0 + \lambda \cdot x^{(k)}) \right] \right) - C \sum_i \lambda_i^2$$
Ising model: phase classification

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Persistent homology
“Order parameters”

The low-temperature phase has persistent 0-cycles many short-lived 1-cycles (loops around flipped spins).

The high-temperature phase has short-lived 0-cycles and a more uniform distribution of sizes of 1-cycles which are longer-lived.

→ magnetization is an order parameter.

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Persistent homology
Multiscale behavior: 1-cycle feature death probability

- exponential distribution of deaths
- 1-cycle deaths roughly measures the domain sizes and are therefore a measure for correlations
- the exponents in the left panel can be interpreted as correlation lengths
persistent homology is a versatile approach for unsupervised feature extraction

- can be applied to point clouds (discrete or continuous)
- interpretability of extracted order parameters

- but: the classification is supervised; it requires labeling and physical insight into the phase diagram
Filtration (continuous)

- Spin configuration: \( f : \Lambda \rightarrow S^1 \) from the lattice, \( \Lambda \), of \( N \) spin sites to their angles
- Set magnetization to zero: \( f : \Lambda \rightarrow (-\pi, \pi] \)
- Introduce thresholds \( \nu \in S^1 \)
- \( f^{-1}(-\pi, \nu] \) is a filtration of (periodic) cubical complexes
• high-persistence 0-cycles are the stripes
• high-persistence 1-cycles are loops around the stripes
XY model: filtration thresholds and persistence images

\[ \nu = -3.0 \quad \nu = -2.5 \quad \nu = -1.0 \quad \nu = 0.0 \quad \nu = 1.0 \quad \nu = 2.5 \quad \nu = 3.0 \]

\[ H_0 \quad H_1 \]

Death

Birth

Persistence

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Persistent homology
XY model: Classification results

- corners/edges: vortices
as temperature increases, sum of $H_0$ and $H_1$ death probabilities becomes uniform

vortex/antivortex pairs evident from similarity of $H_0$ and $H_1$ (lower panels are averages at low temperature)