TDA for Detecting / Analysing Phase Transitions

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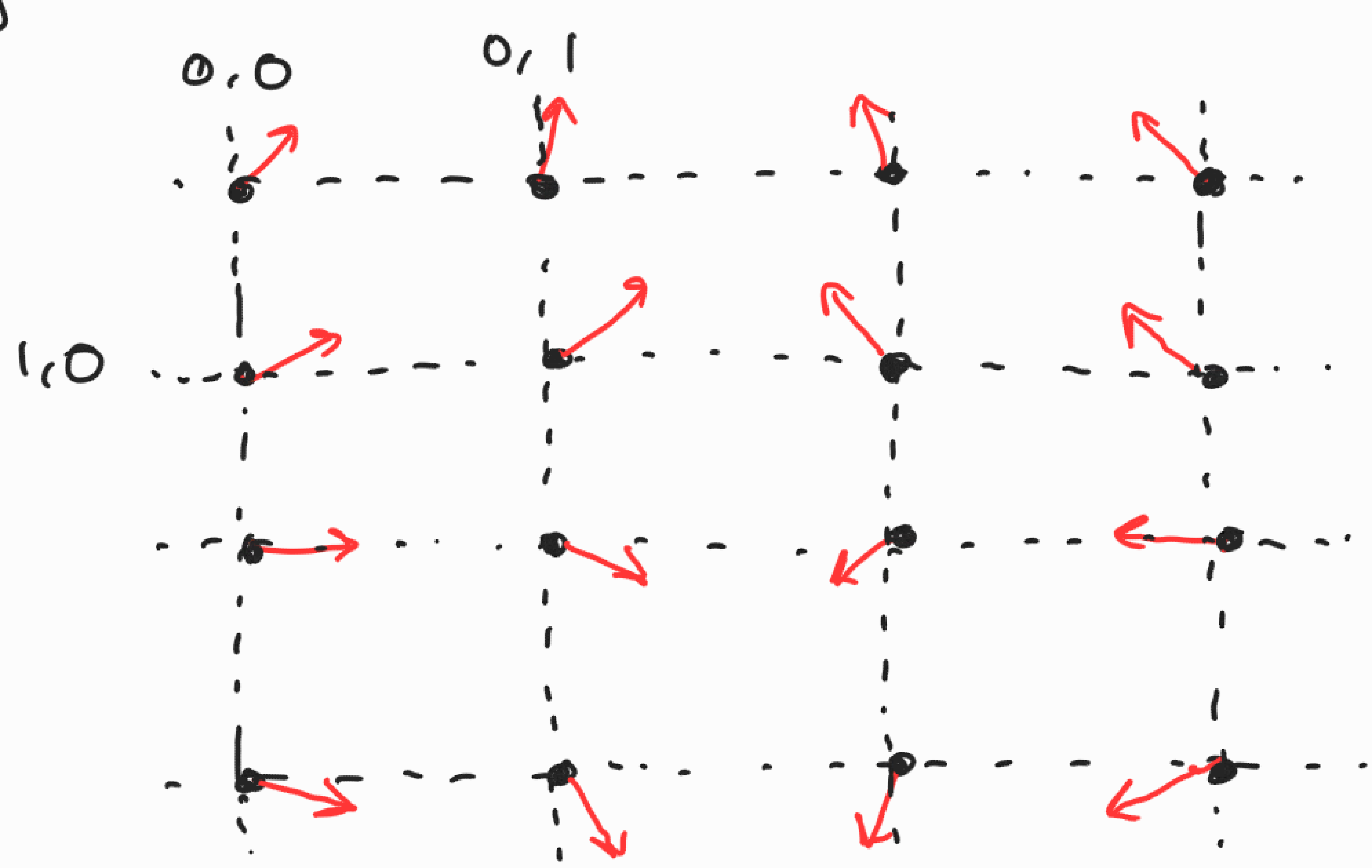
Spin Models

- Lattice Λ with boundary conditions.
- Random 'spin' variable $\theta_i \in \Omega$ at each site $i \in \Lambda$.
- Hamiltonian $H : \Omega^{\Lambda} \longrightarrow \mathbb{R}$.

◦ e.g.: 2D XY Model



$$H(\{\theta_i\}) = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - h \sum_i \cos(\theta_i)$$

- The canonical ensemble:

$$p(\{\theta_i\}) \propto e^{-\beta H(\{\theta_i\})}$$

where $\beta = \frac{1}{kT}$ is essentially inverse temperature.

- The normalising constant

$$Z = \sum_{\{\theta_i\}} e^{-\beta H(\{\theta_i\})}$$

is called the partition function.

- For an observable $A : \Omega^{\Lambda} \longrightarrow X$ the ensemble average is

$$\langle A \rangle = \frac{1}{Z} \sum_{\{\theta_i\}} A(\{\theta_i\}) e^{-\beta H(\{\theta_i\})}$$

- Some important quantities:

  - free energy $F = -\frac{1}{\beta} \ln Z$

  - avg energy $\langle E \rangle = -\frac{\partial F}{\partial \beta}$

  - specific heat $C = -k\beta^2 \frac{\partial \langle E \rangle}{\partial \beta}$

$$= k\beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$$

  - magnetisation $M = \frac{1}{|\Lambda|} \sum_i \theta_i$

$$\langle M \rangle = -\frac{\partial F}{\partial h}$$

  - magnetic susceptibility $\chi = \frac{\partial \langle M \rangle}{\partial h}$

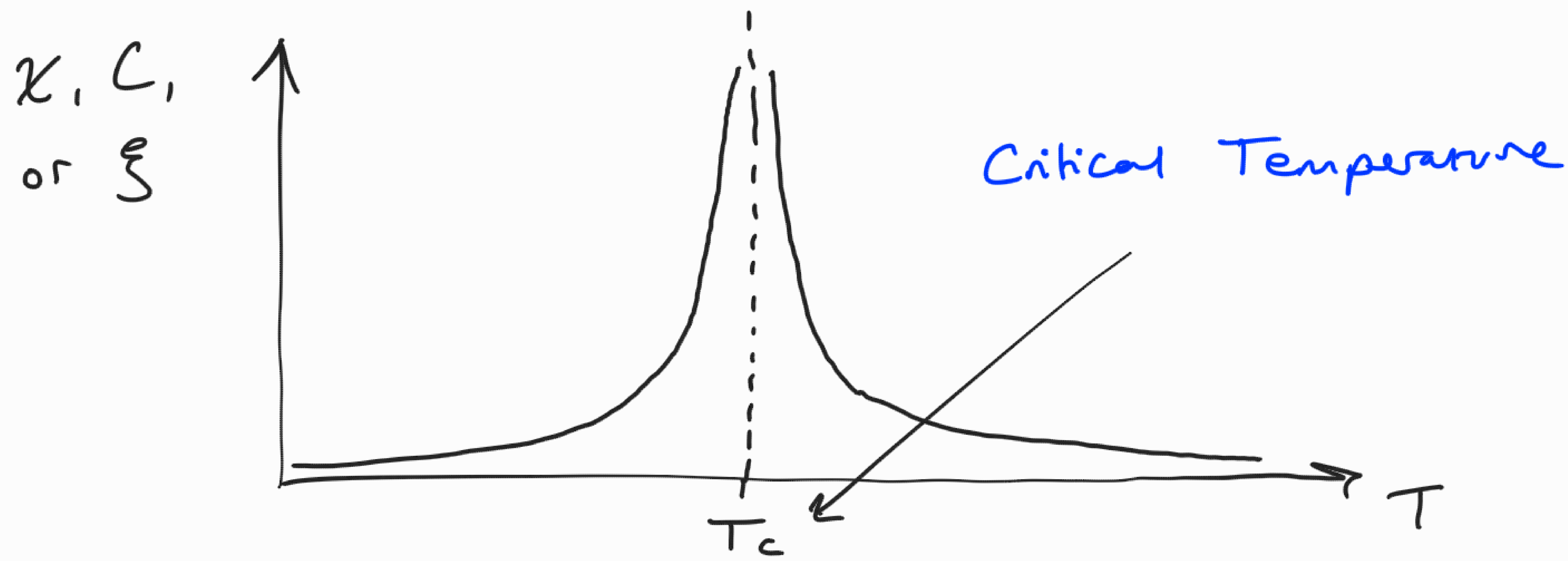
$$= \beta (\langle M^2 \rangle - \langle M \rangle)$$

  - correlation function $C(r) =$

(avg correlation of fluctuations of spins at distance r from each other)

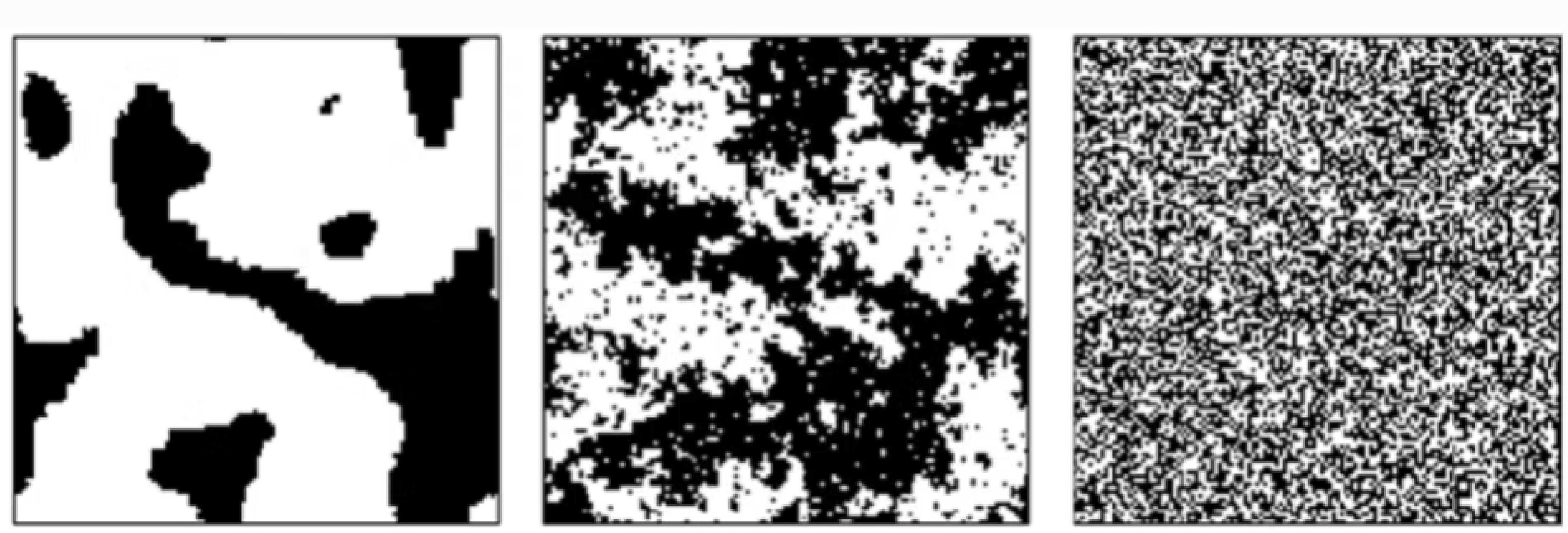
usually $C(r) \approx \frac{1}{r^A} \exp(-r/\xi)$.

- A phase transition is a point where the free energy $F(T, h, \cdots)$ is non-analytic.



- marks the boundary between qualitatively different phases
  - e.g. ordered / disordered phases in the Ising Model:

$$\sigma_i \in \{-1, 1\} \qquad H = -\sum_{\langle ij \rangle} \sigma_i \sigma_j$$



$C(r) \sim e^{-r/\xi}$ $\qquad$ $C(r) \sim \frac{1}{r^{\eta}}$ $\qquad$ $C(r) \sim e^{-r/\xi}$

- Things scale in a nice way near the critical temperature:

$$C(T) \sim |T - T_c|^{-\alpha}$$

$$\chi(T) \sim |T - T_c|^{-\gamma}$$

$$\xi(T) \sim |T - T_c|^{-\nu}$$

- α, γ, ν are critical exponents.

- They depend only on certain large-scale properties of the model like dimension and symmetries.

- This is called universality.

- The critical temperature is not universal.
- Some differences for BKT transitions (as in 2D XY)
- Technically on a finite lattice F is always analytic.

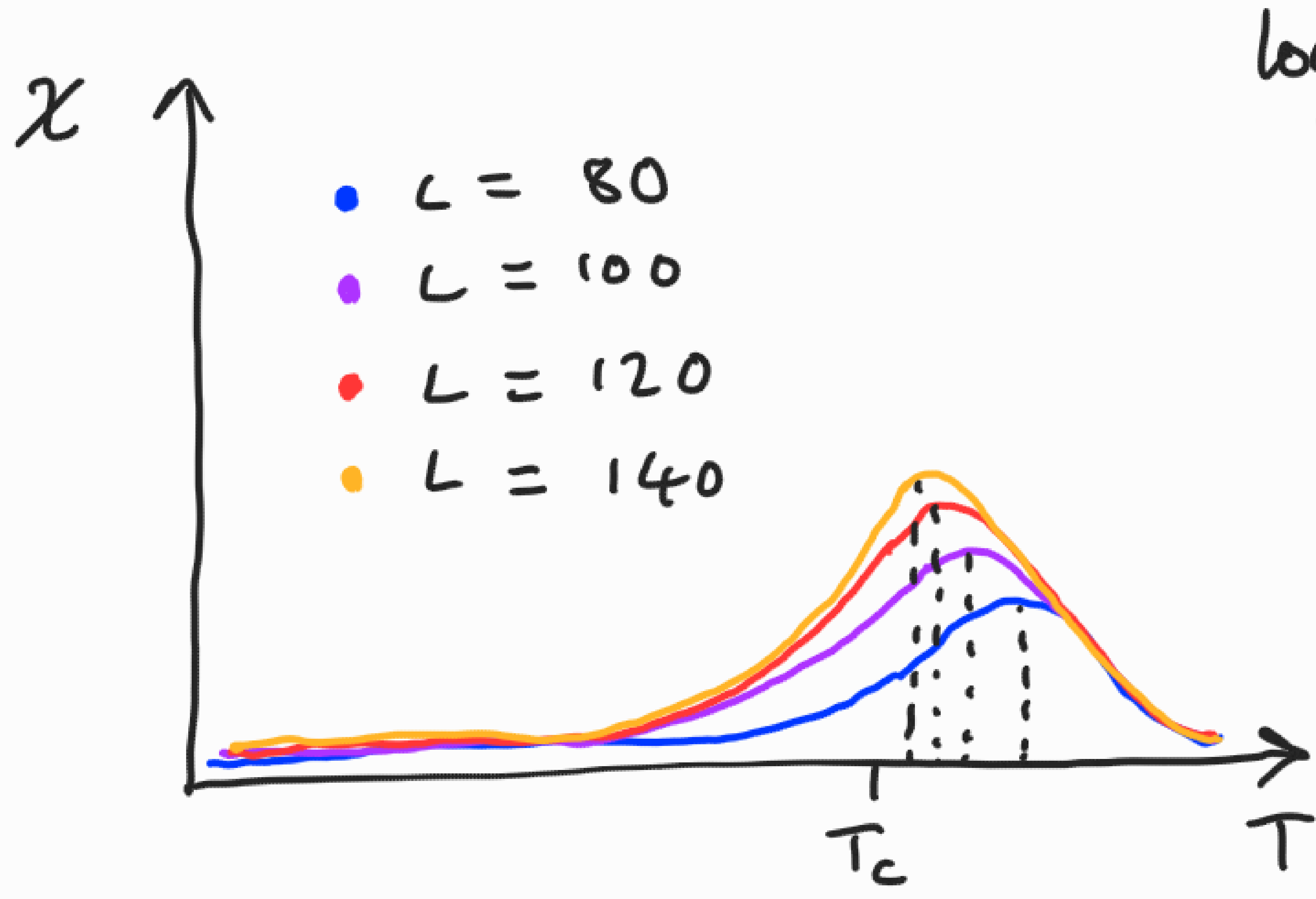
- ξ is bounded above by the length of the lattice L.

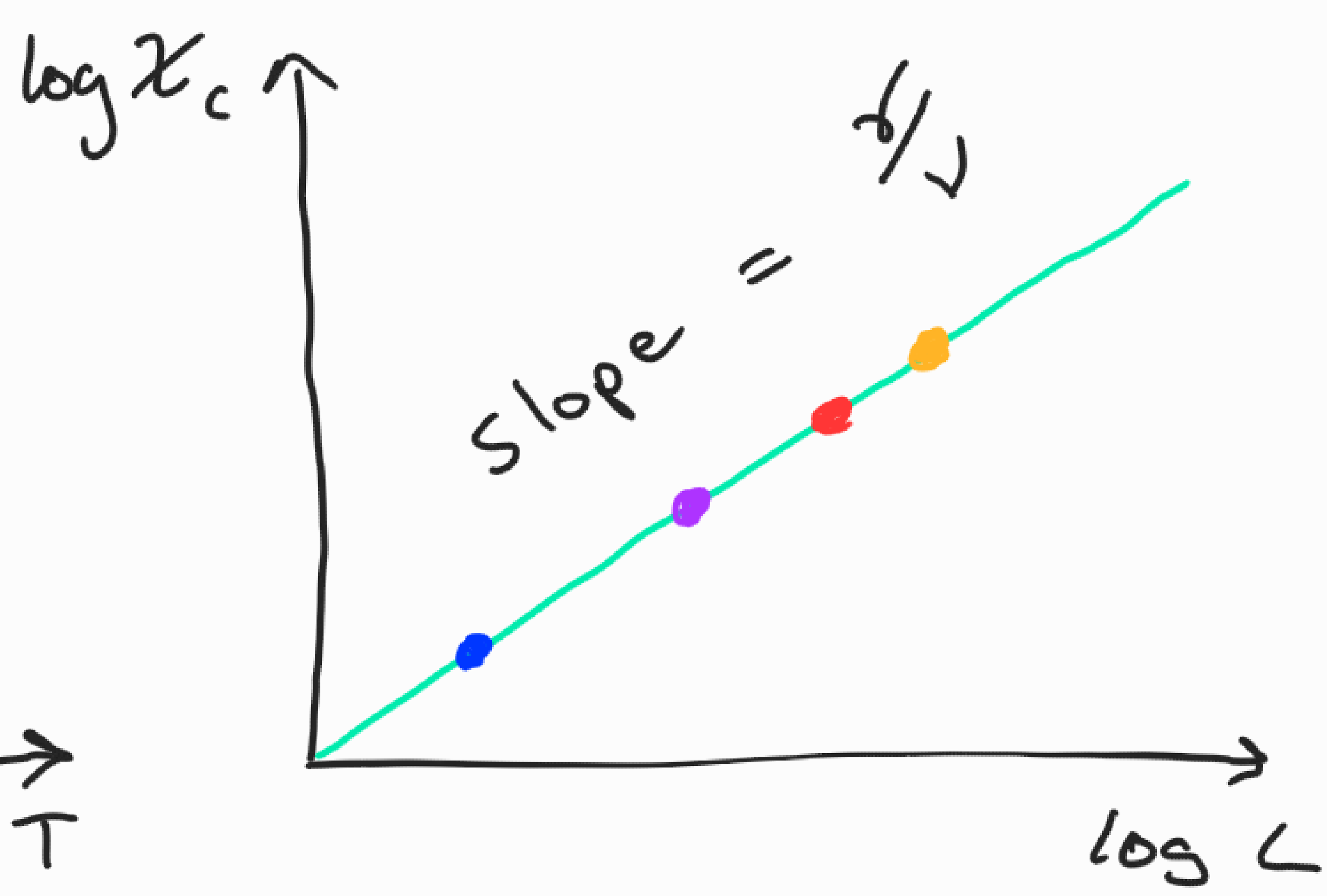
- This is actually useful:

$$|T-T_c|^{-\nu} \sim \xi \sim L$$

so

$$\chi \sim |T-T_c|^{-\gamma} \sim L^{-\gamma/\nu}$$





- We can draw samples from the Boltzmann distribution using Markov Chain Monte Carlo methods — e.g. Metropolis, Wolff.

Persistent homology

- 2 different paradigms:

- Persistent homology in configuration space

Persistent Homology Analysis of Phase Transitions,
Donato et al.

- Topology hypothesis:

phase transitions $\longleftrightarrow$ change in topology of $V^{-1}(-\infty, v]$

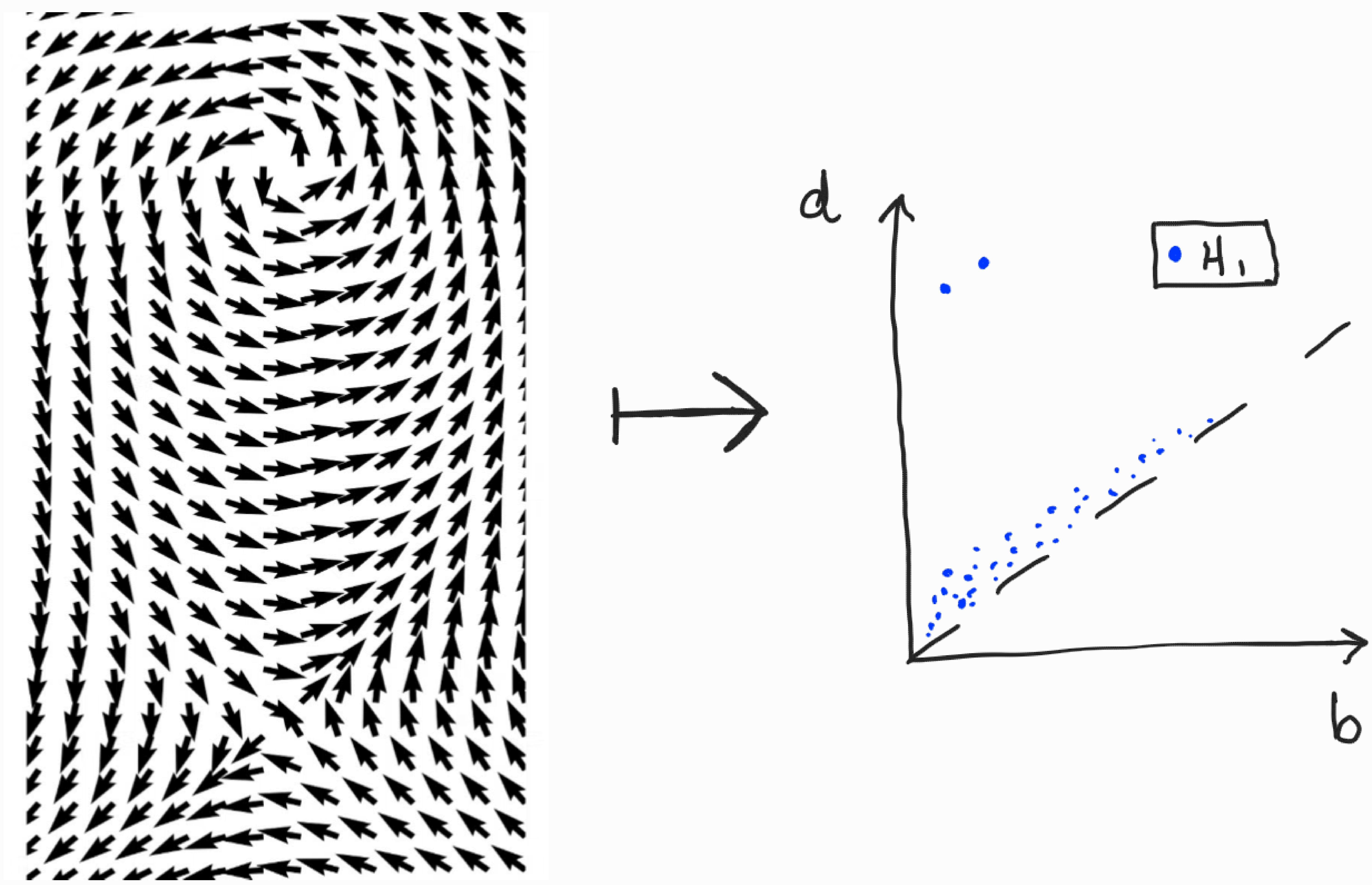
- generate lots of configurations
- define a distance between configurations that may take energy into account

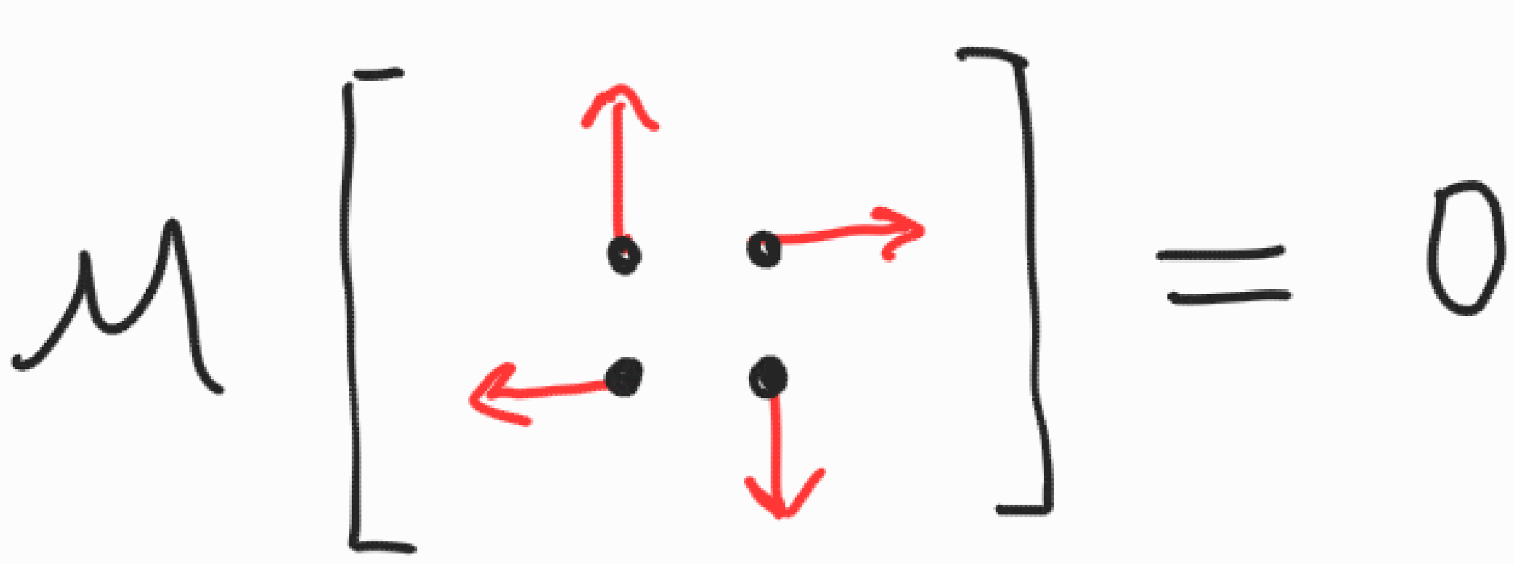
$$d(c_1, c_2) = \int_{c_1}^{c_2} \sqrt{(E - V(q_1, \dots, q_N)) \sum_i^N dq_i^2}$$

- Compute persistence on subsets of configurations within certain energy ranges and compare.

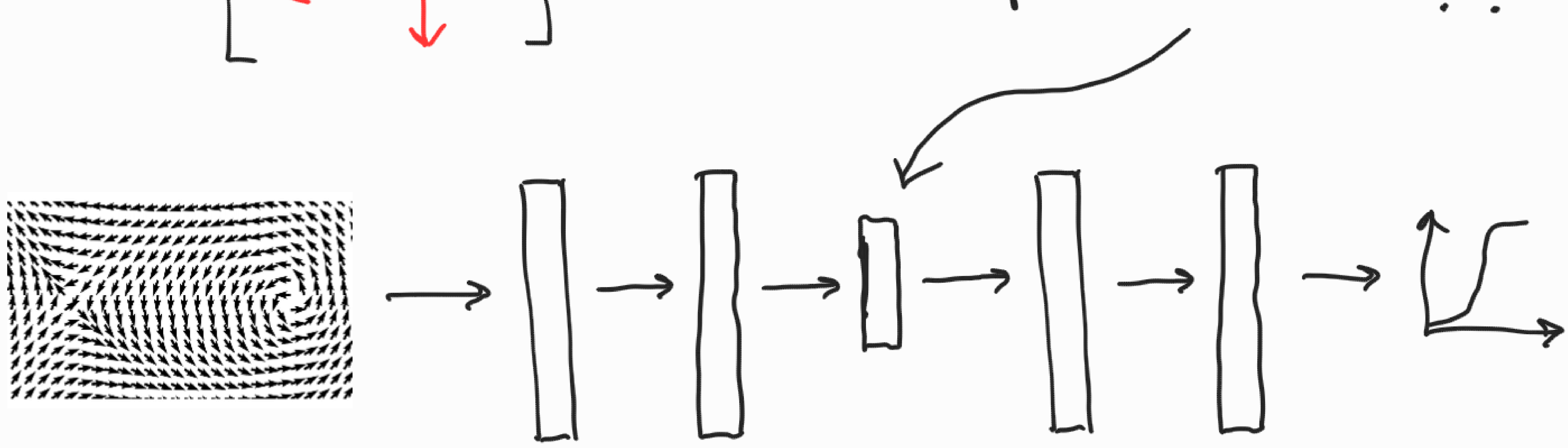
– Persistent Homology as an Observable

- define a filtration on a specific configuration
- can natively capture complex structure in an interpretable way:





Vortices represented here??



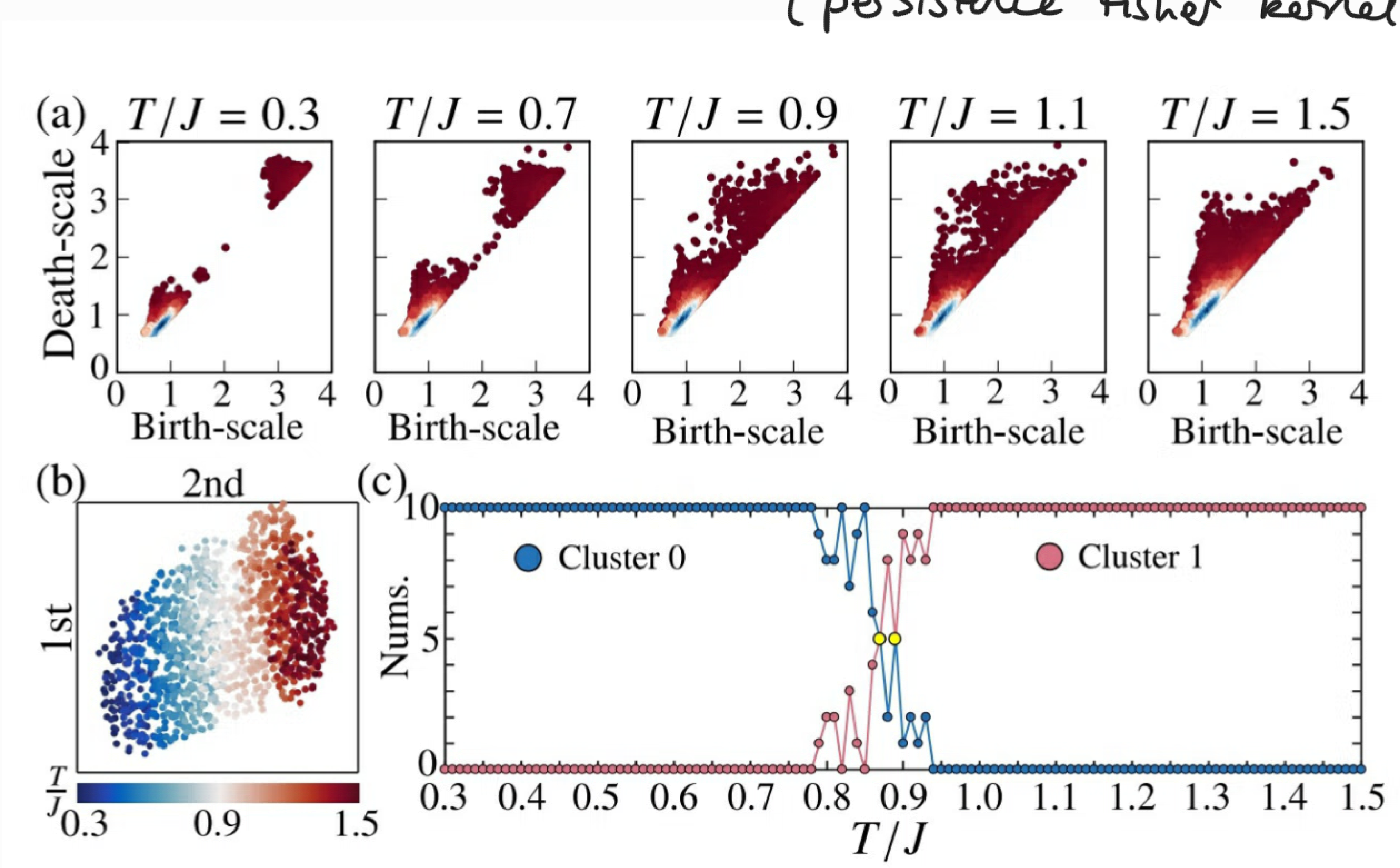
Topological Persistence Machine of Phase Transitions.
Tran, Chen, Hasegawa

- 2D XY Model

$$\{\theta_i\} \longmapsto \{p_i = (x_i, y_i, \theta_i)\}$$

$$d(p_i, p_j) = \xi \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} + (1-\xi)\sqrt{2(1-\cos(\theta_i - \theta_j))}$$

Vietoris-Rips PH $\longmapsto$ Clustering
(persistence Fisher kernel)



Finding hidden order in spin models with persistent homology.
Olsthoorn, Hellsvik, Balatsky

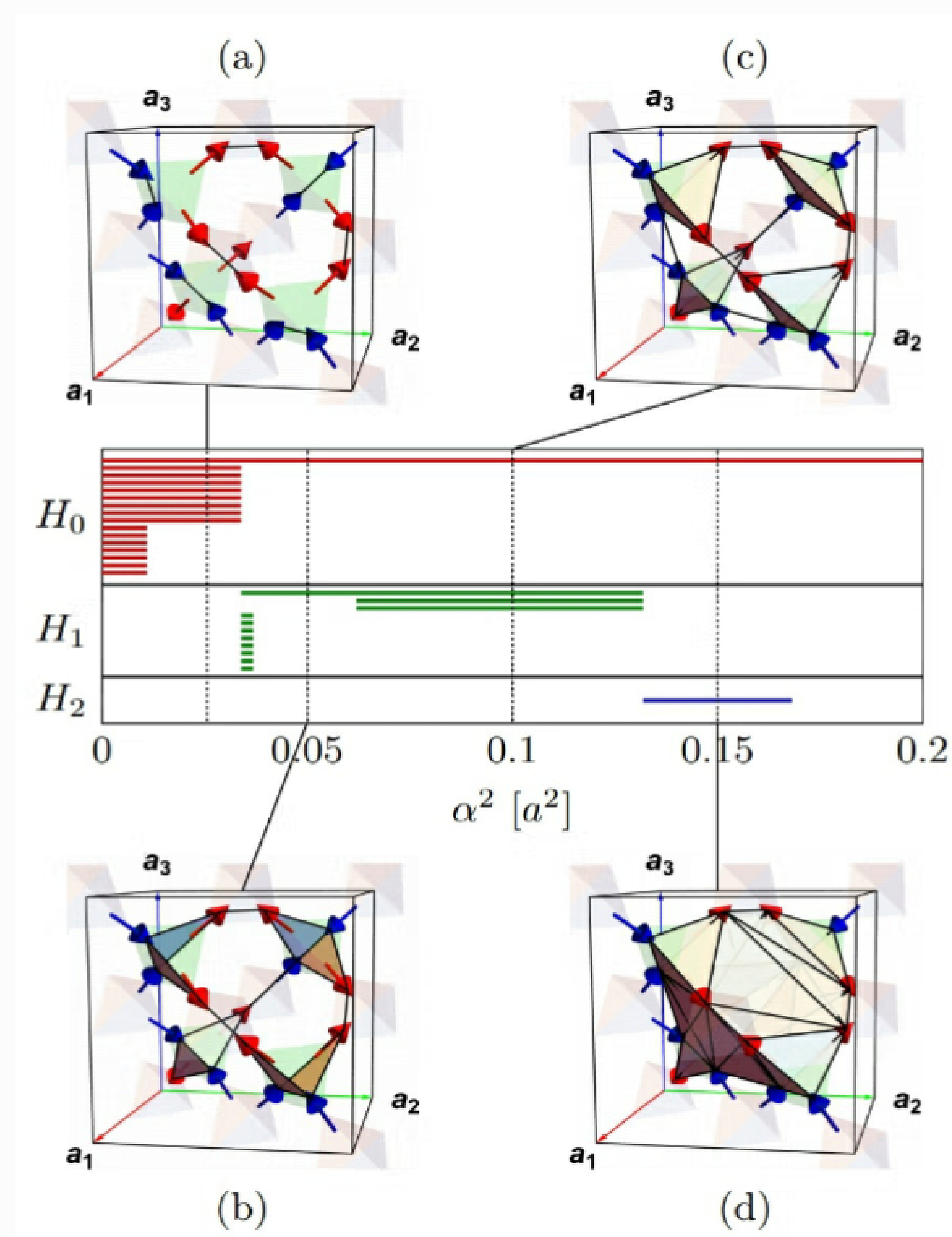
- XXZ model pyrochlore lattice

$$S_i = (S_{i,x}, S_{i,y}, S_{i,z}) \in \mathbb{R}^3 \qquad \|S_i\| = 1$$

$$H = \sum_{\langle ij \rangle} J_{zz} S_{i,z} S_{j,z} - J_{\pm} (S_i^+ S_j^- - S_i^- S_j^+)$$

where $S_i^{\pm} = S_{i,x} \pm S_{i,y}$

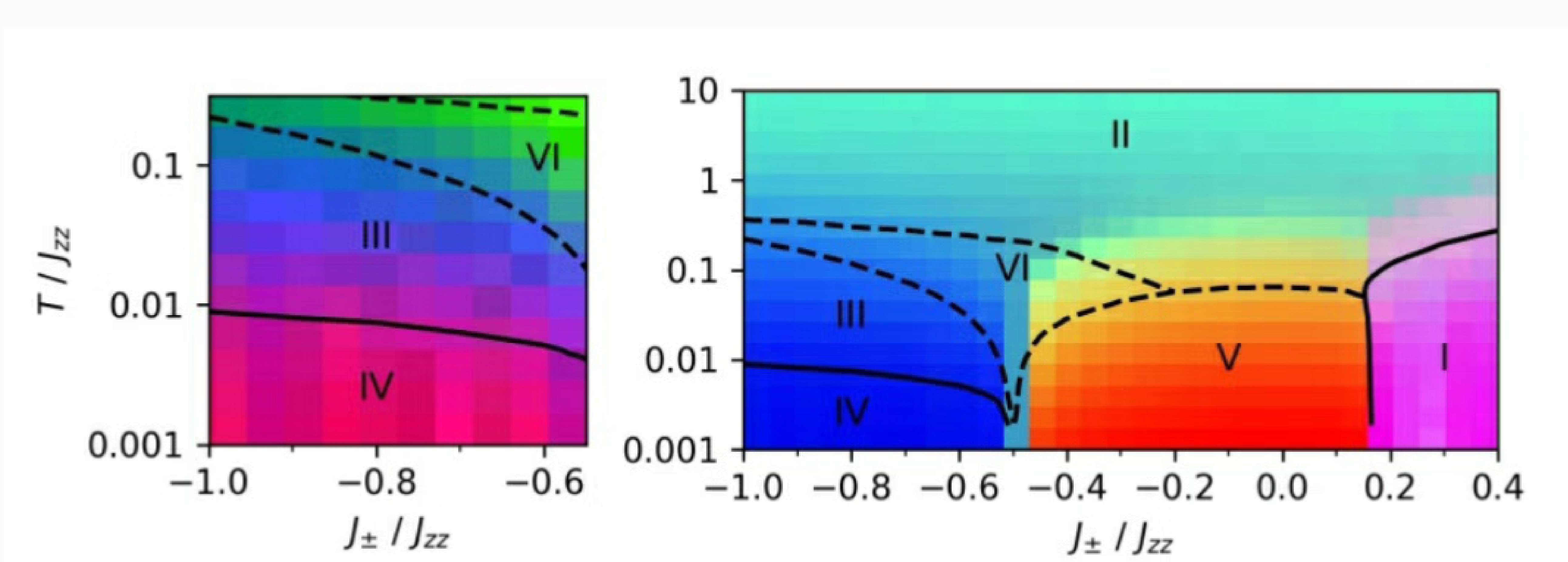
- Has $\underline{6}$ different phases as T and $J_{\pm}$ changed.



- Similar approach to the above:

$$d_{ij} = r(ij) + \frac{1}{2\sqrt{2}} \frac{\|S_i - S_j\|}{4}$$

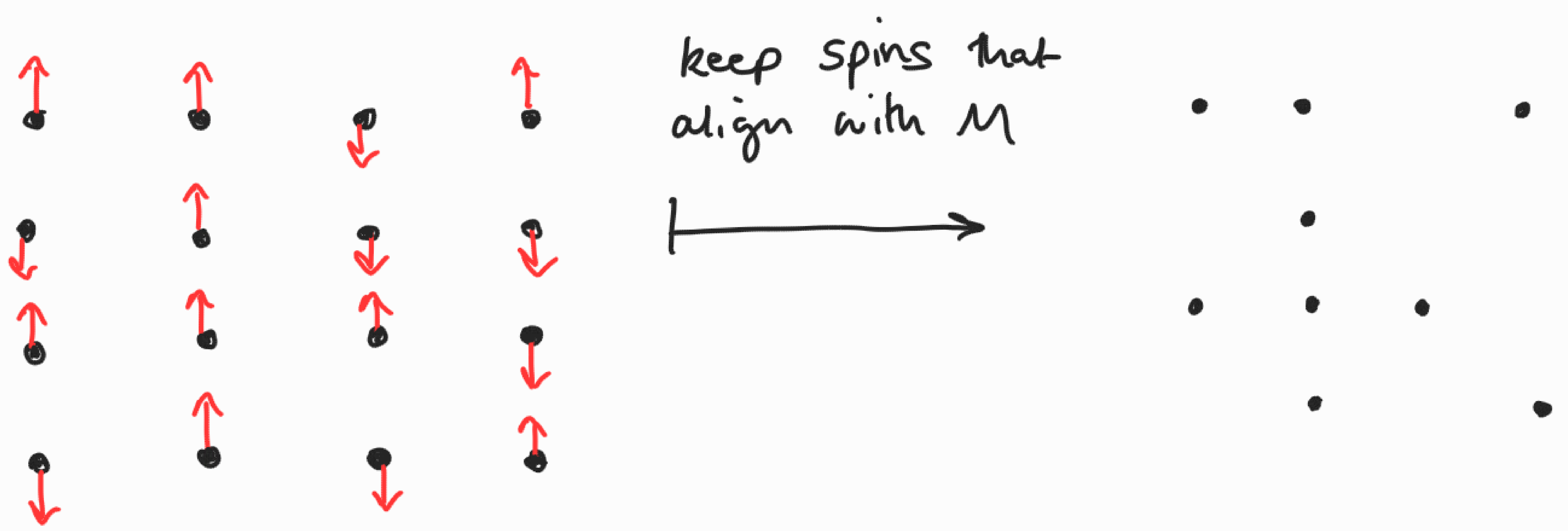
  - α - complexes
  - Sliced Wasserstein distance
  - 'Clustering' by MDS to 3D RGB space



Quantitative and Interpretable Order Parameters for Phase Transitions from Persistent Homology. Cole, Loges, Shiu

- 2D XY, Ising, Square Ice, Fully-frustrated XY
- Filtrations:

Discrete Spins



Then take α-complex filtration.

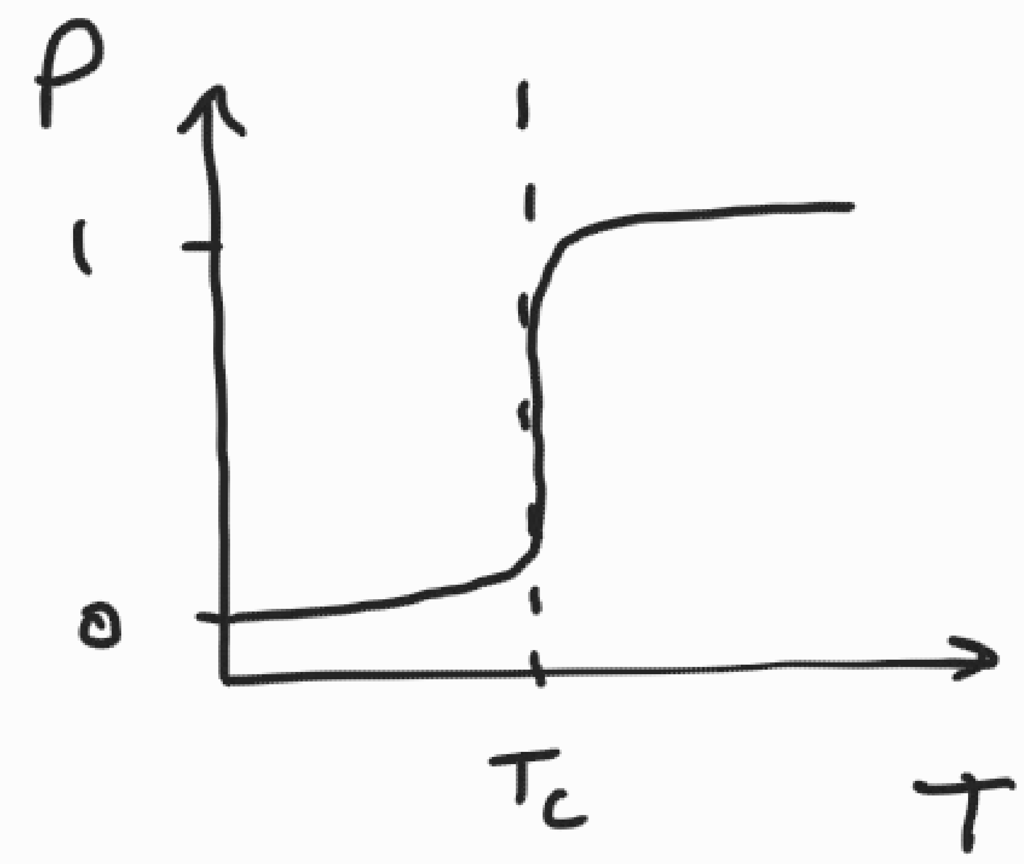
S^1 Spins

Reparameterise all spins so that they lie in $(-\pi, \pi]$ and so the magnetisation points along 0.

Use the sublevel set filtration of $\Lambda \longrightarrow (-\pi, \pi]$ yielding cubical subcomplexes of the lattice.

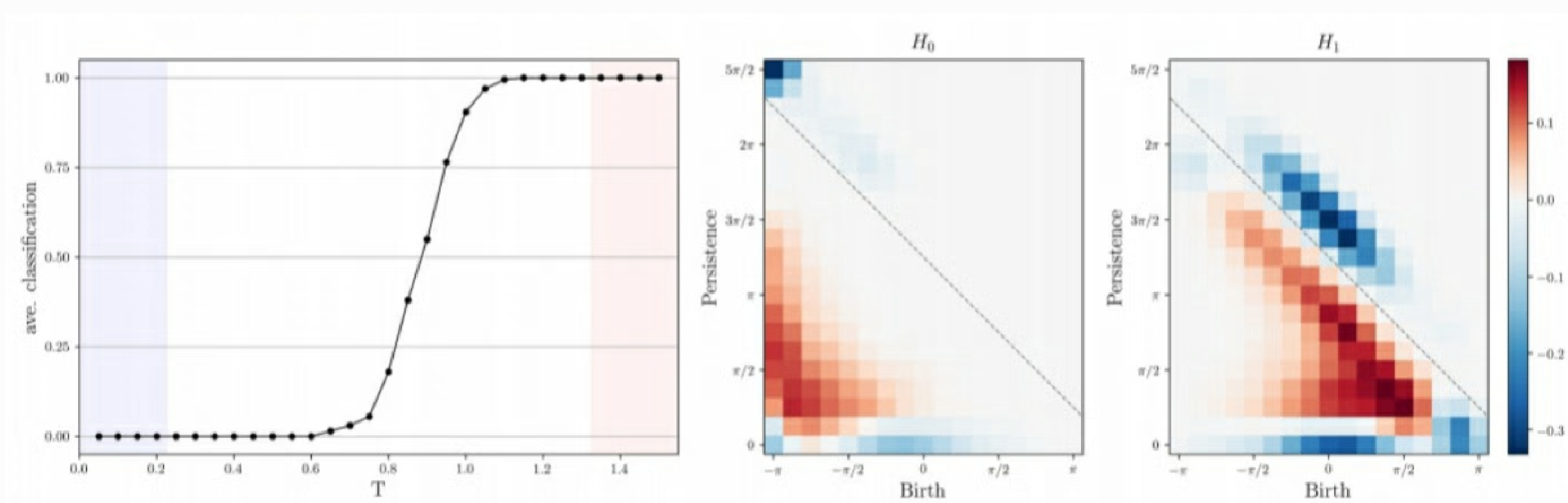
- Configurations $\longrightarrow$ PH $\longrightarrow$ Persistence Images

Logistic Regression (trained on very cold and very hot configs) $\longrightarrow$



'order parameter'

- Similar idea to the ML approaches, but much easier to interpret



Trained in these regions

regression coefficients tell us which parts of the diagrams are used for classification

- For the Ising model they try to fit the distribution of H_1 death times to $D_T(d) = A d^{-\mu} e^{-d/a}$

then argue that $a \sim \xi \sim |T - T_c|^{-\nu}$

My work

- Filtration: Vietoris - Rips

  where $d(i,j) = \begin{cases} |\theta_i - \theta_j| & \text{if } \langle ij \rangle \\ \infty & \text{otherwise} \end{cases}$

- 'Persistence susceptibility'

$$\chi_{PH_n} := \frac{\beta}{L^2} \sum_i \mathrm{Var}_\beta[PI_n^i] = \frac{\beta}{L^2} \mathrm{Tr}\, \mathrm{Cov}_\beta[PI_n]$$

where PI_n^i is the i^{th} component of the H_n persistence image.

- $\chi_{PH_1} \sim |T - T_c|^{-A}$

  and A seems to be constant within universality classes.

- Applying histogram reweighting and bootstrapping to do rigourous quantitative analysis.

- Obtain precise estimates of A and T_c with controlled and quantified error.