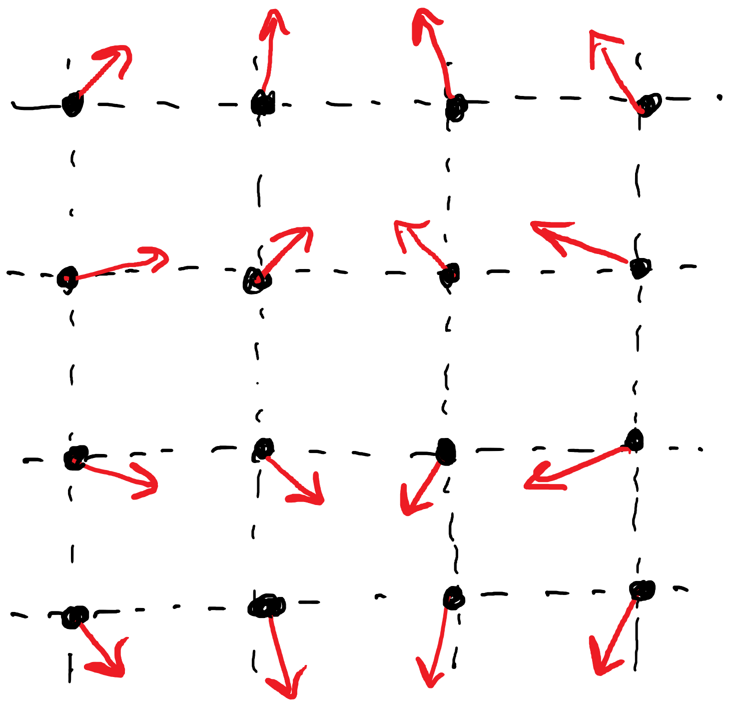
Persistent Homology to Study Phase Transitions

Nick Sale – Centre for TDA Meeting – 27 Nov 2020

Spin Models

- Lattice Λ with boundary conditions
- Spin variables $\theta_i \in \Omega$ at each $i \in \Lambda$
- Hamiltonian $H : \Omega^{\Lambda} \to \mathbb{R}$



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

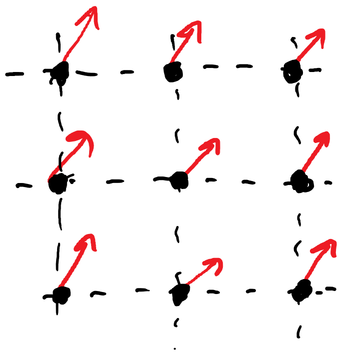
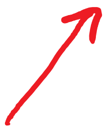
- The Canonical ensemble

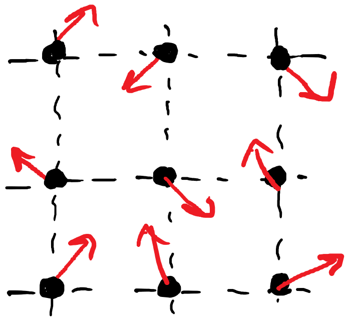
$$p(\{\theta_i\}) \propto e^{-\beta H(\{\theta_i\})}$$

- Ensemble average $\langle A \rangle_\beta = \mathbb{E}_{p(\beta)}[A]$

• e.g: magnetisation

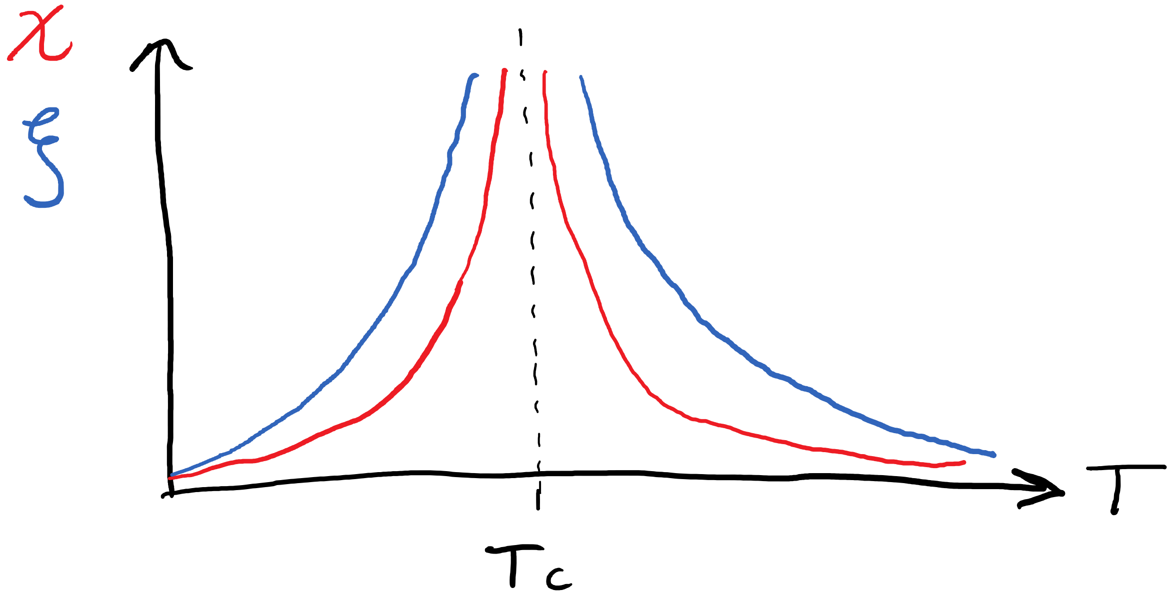
$$M := \frac{1}{|\Lambda|} \sum_{i \in \Lambda} \begin{bmatrix} \cos\theta_i \\ \sin\theta_i \end{bmatrix}$$

$M\Big($  $\Big) =$ 

$M\Big($  $\Big) \approx 0$

- A phase transition occurs when things get non-analytic

$$\chi = \frac{\partial \langle |M| \rangle_\beta}{\partial h} = \frac{1}{\beta}\left(\langle |M|^2 \rangle_\beta - \langle |M| \rangle_\beta^2\right)$$



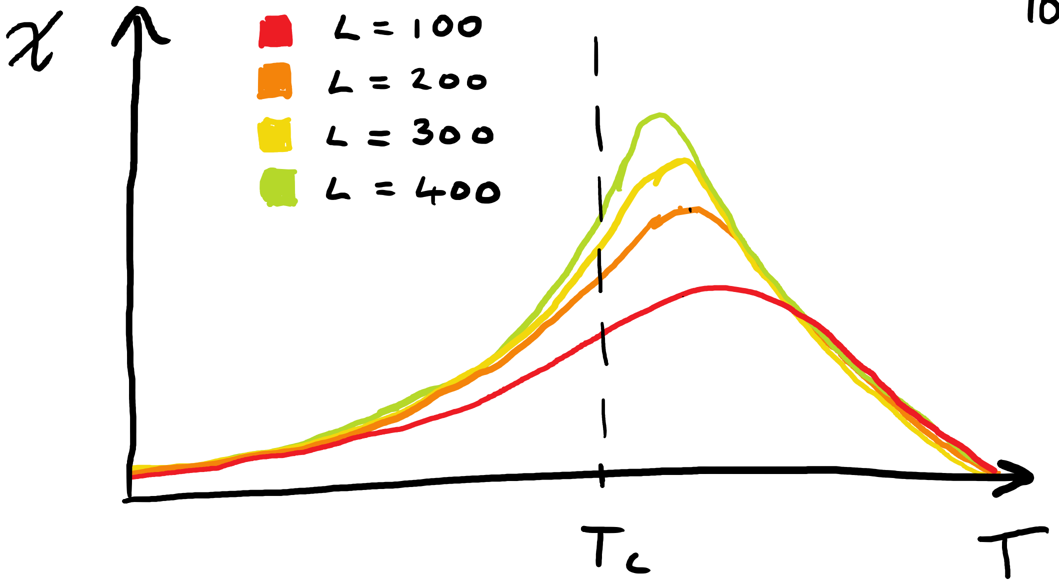
ξ = Correlation length

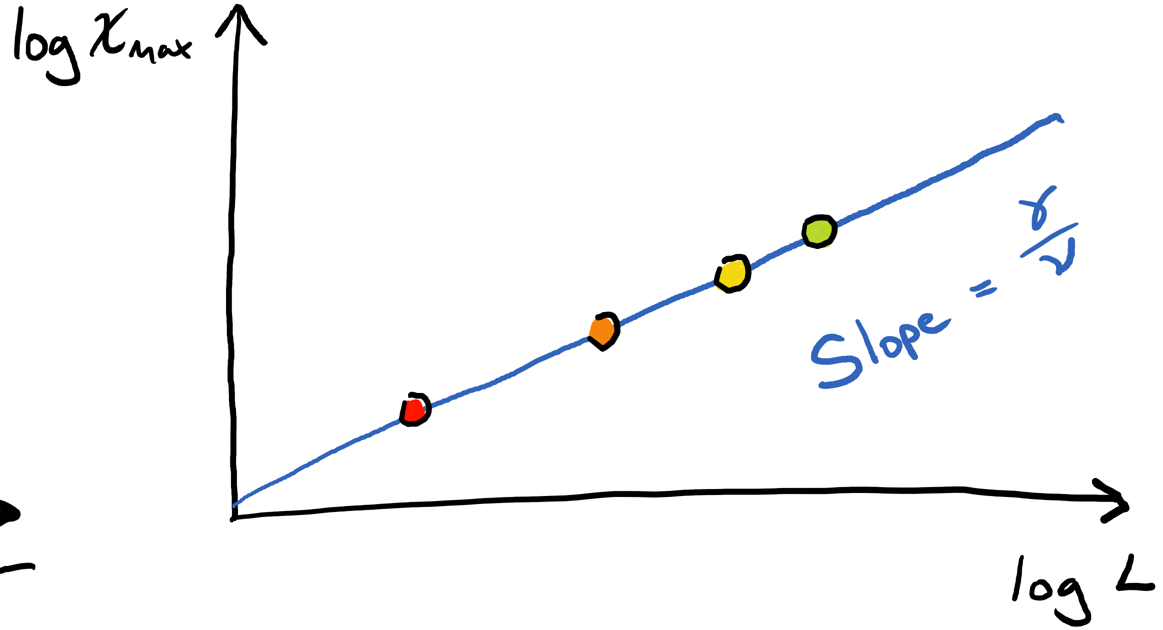
$$\chi(T) \sim |T - T_c|^{-\gamma} \qquad \xi(T) \sim |T - T_c|^{-\nu}$$

- "but models on finite lattices are always analytic..."

e.g. $\xi \leq L$ We can use this!

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





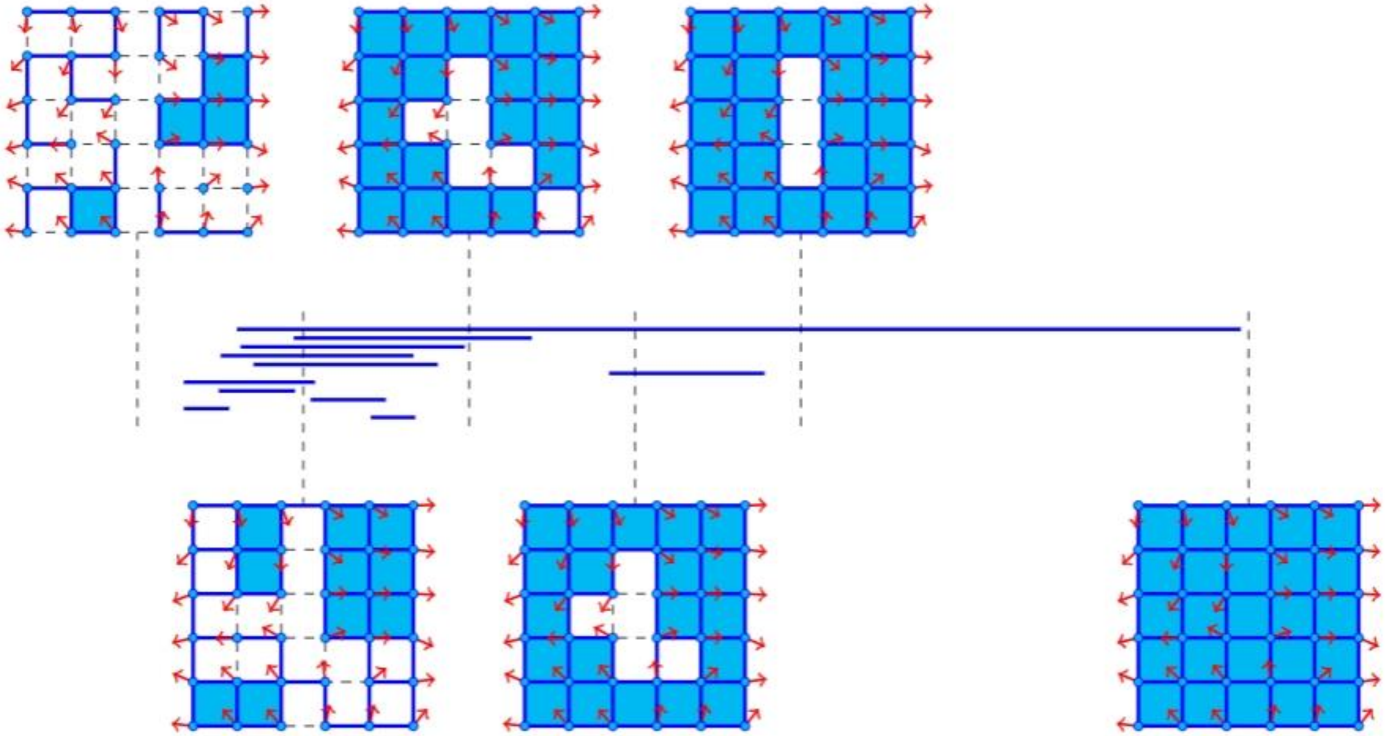
- Why do we need new observables?

- Existing theory relies on the existence of order parameters

- e.g. Magnetisation in the Ising or XY models

- But these don't exist / haven't been found for some models – eg. lattice QCD

PH as an Observable

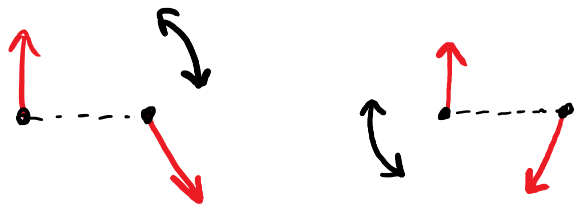


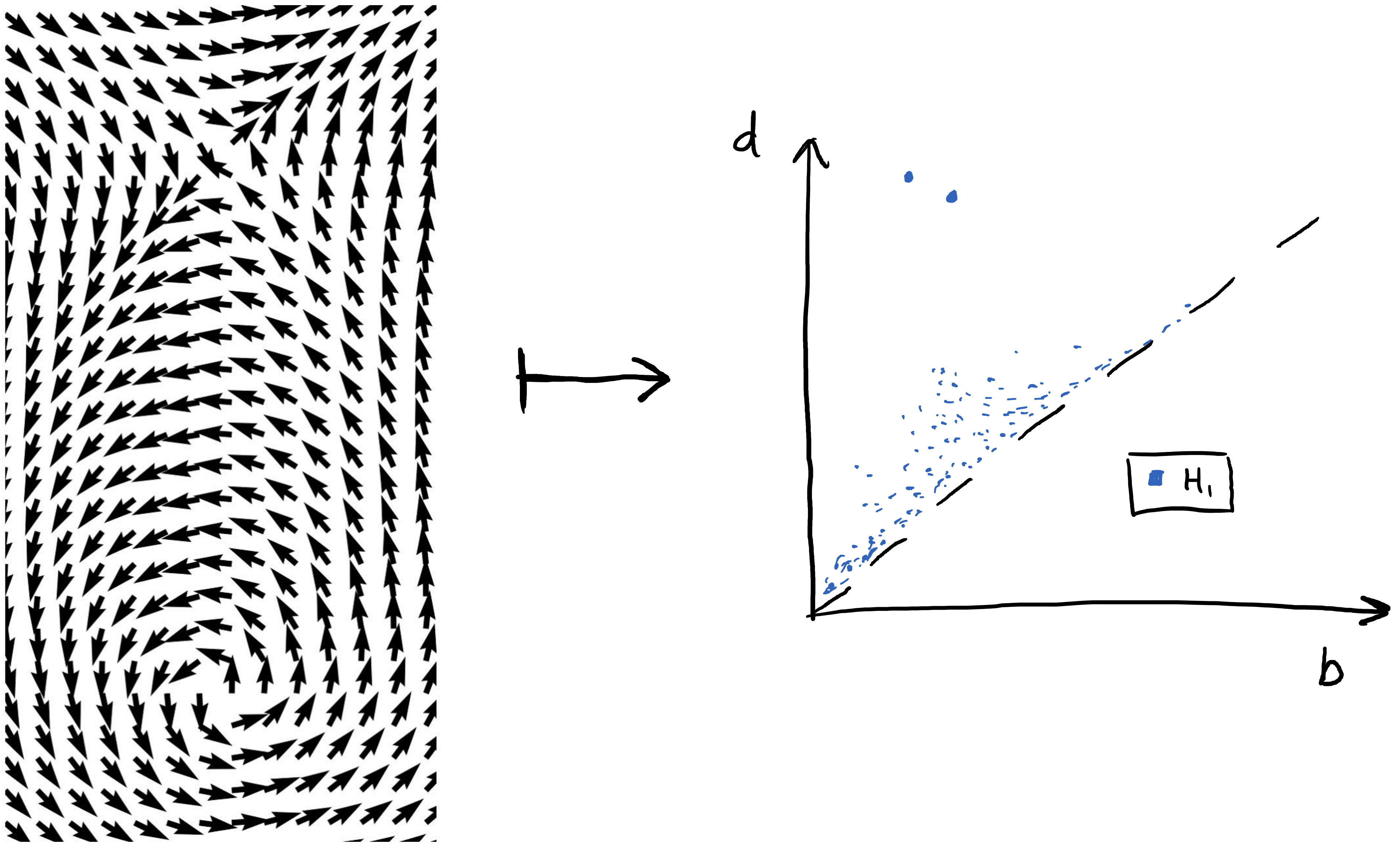
- Filter lattice by energy contribution

e.g. XY model

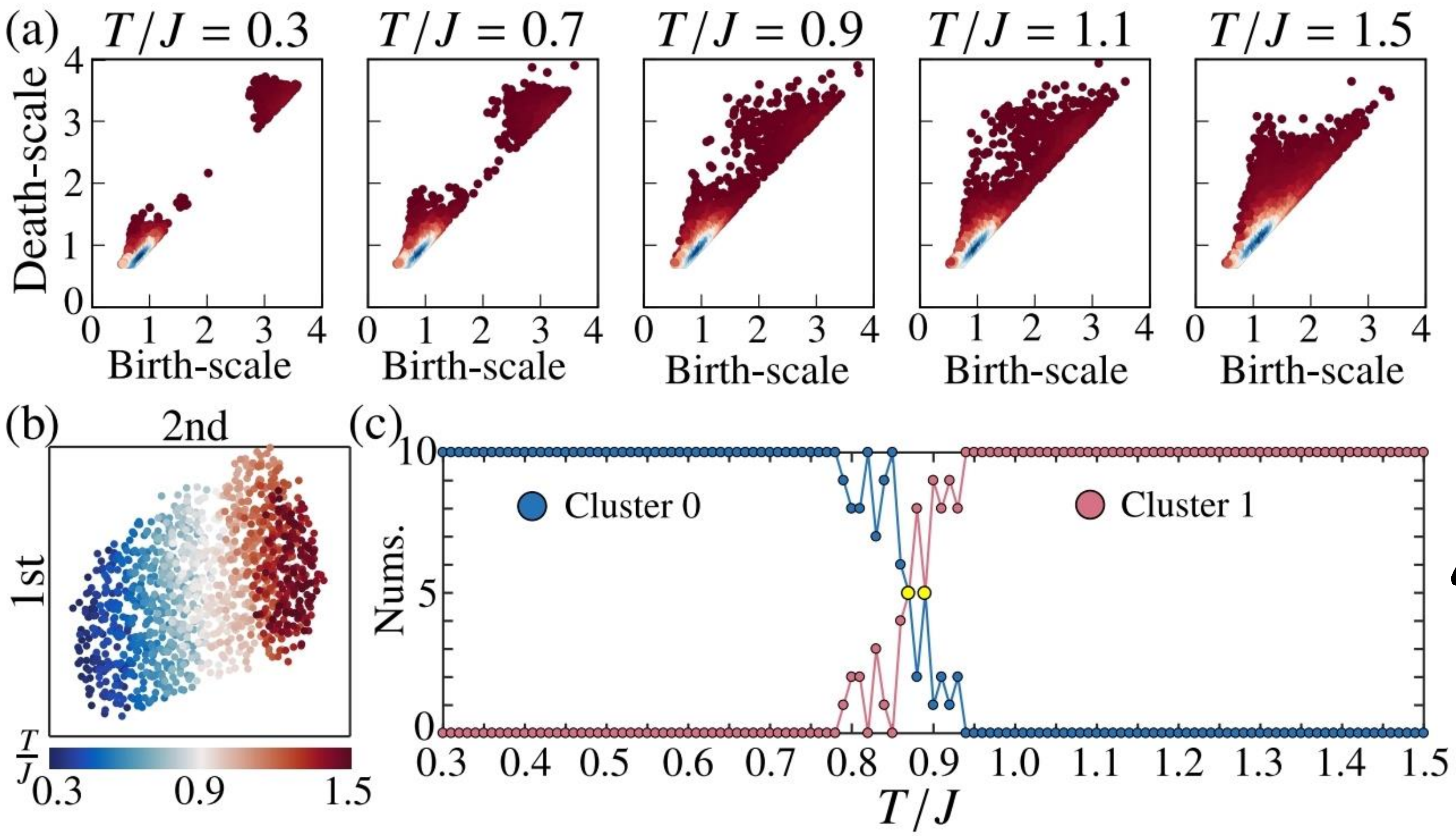
- vertices at $t = 0$
- edges $\langle ij \rangle$ at $t = |\theta_i - \theta_j|$
- plaquettes $\square$ at $t = \max_{ij \in \square} |\theta_i - \theta_j|$

$|\theta_i - \theta_j|$:





d
b
H1



Spectral clustering of Persistence Fisher Kernel

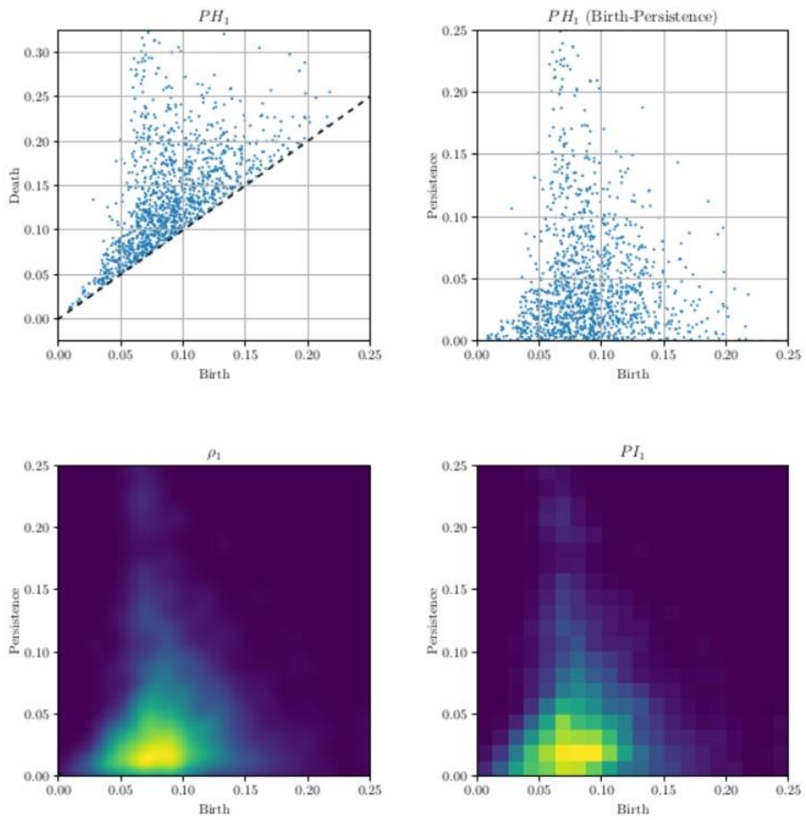
Topological persistence machine of phase transitions – Tran, Chen, Hasegawa

- Fluctuation in Persistence

$$\chi_M = \frac{\beta}{L^2}\left(\langle M^2\rangle_\beta - \langle M\rangle_\beta^2\right) = \frac{\beta}{L^2}\,\mathrm{Var}_\beta M$$

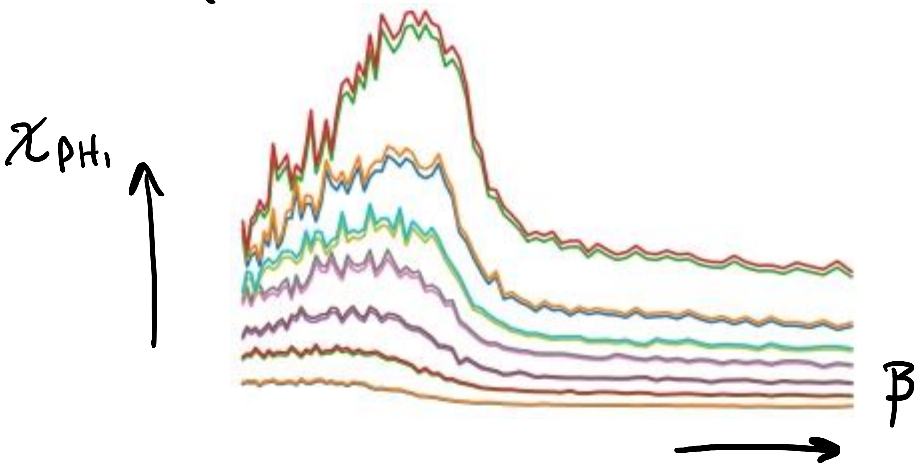
$$\chi_{PH_1} := \frac{\beta}{L^2}\,\mathrm{Tr}\left[\mathrm{Cov}_\beta\, PI_1\right]$$

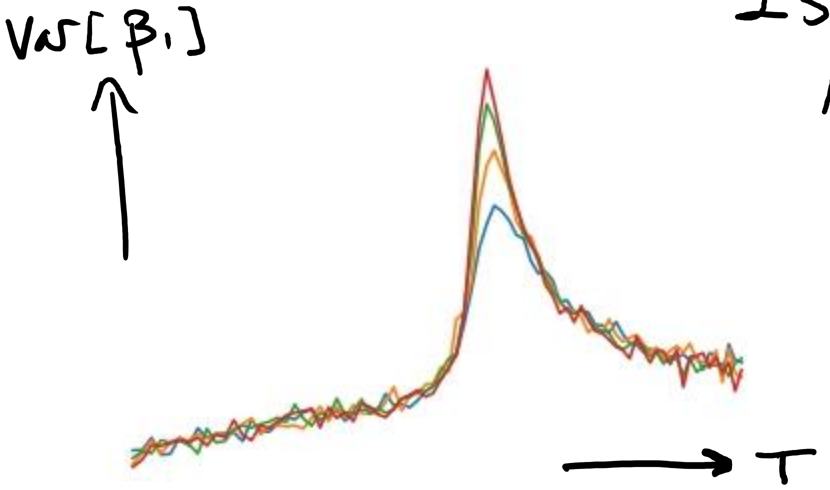
$$= \frac{\beta}{L^2}\sum_i \mathrm{Var}_\beta\left[PI_1^i\right]$$

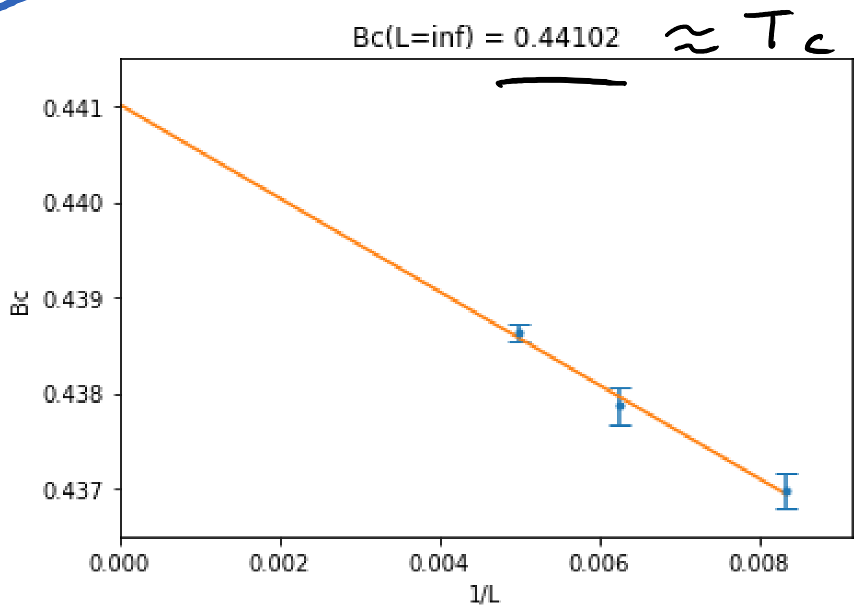


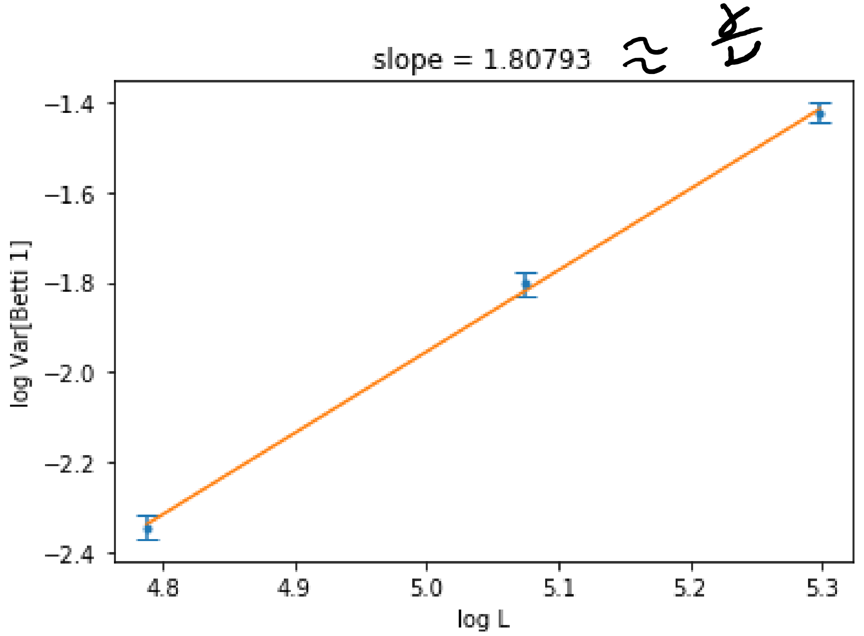
XY Model

Ising Model



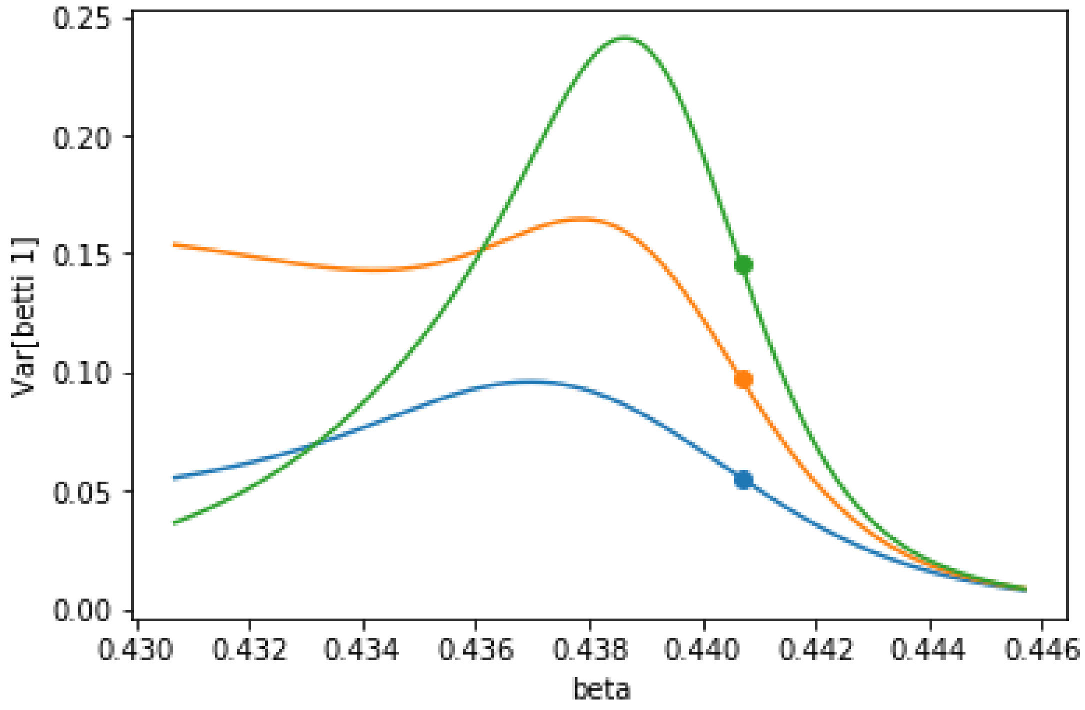






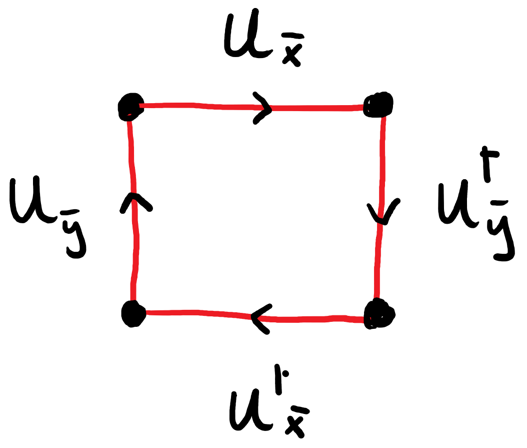
- Histogram Reweighting

$$\langle A \rangle_{\beta'} = \frac{\langle A e^{-(\beta'-\beta)H} \rangle_\beta}{\langle e^{-(\beta'-\beta)H} \rangle_\beta}$$



- Next steps:

  - Lattice Gauge models



$$H = \sum_{\square} \mathrm{Tr}\left[\prod_{i \in \square} U_i\right]$$

  - 'Phase transitions' in other contexts?