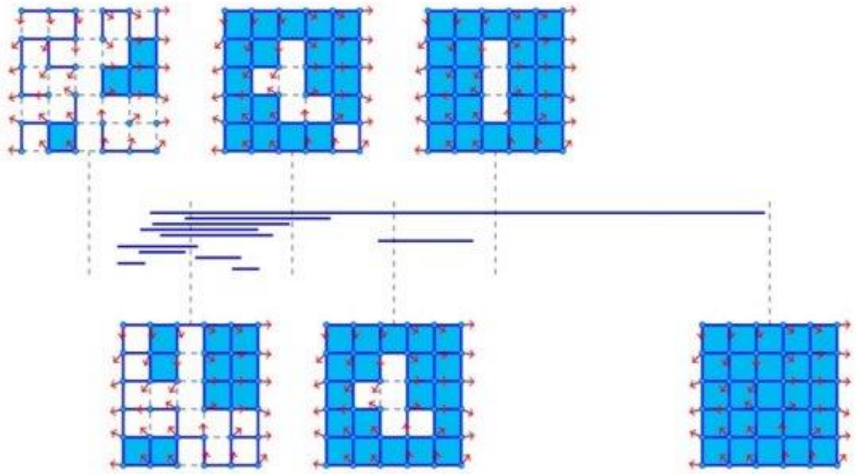
Quantitative Analysis of Phase Transitions Using Persistent Homology



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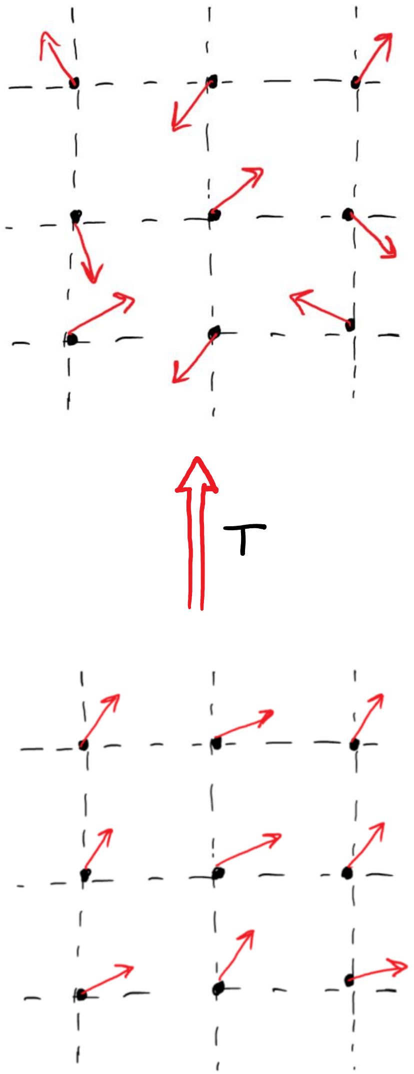
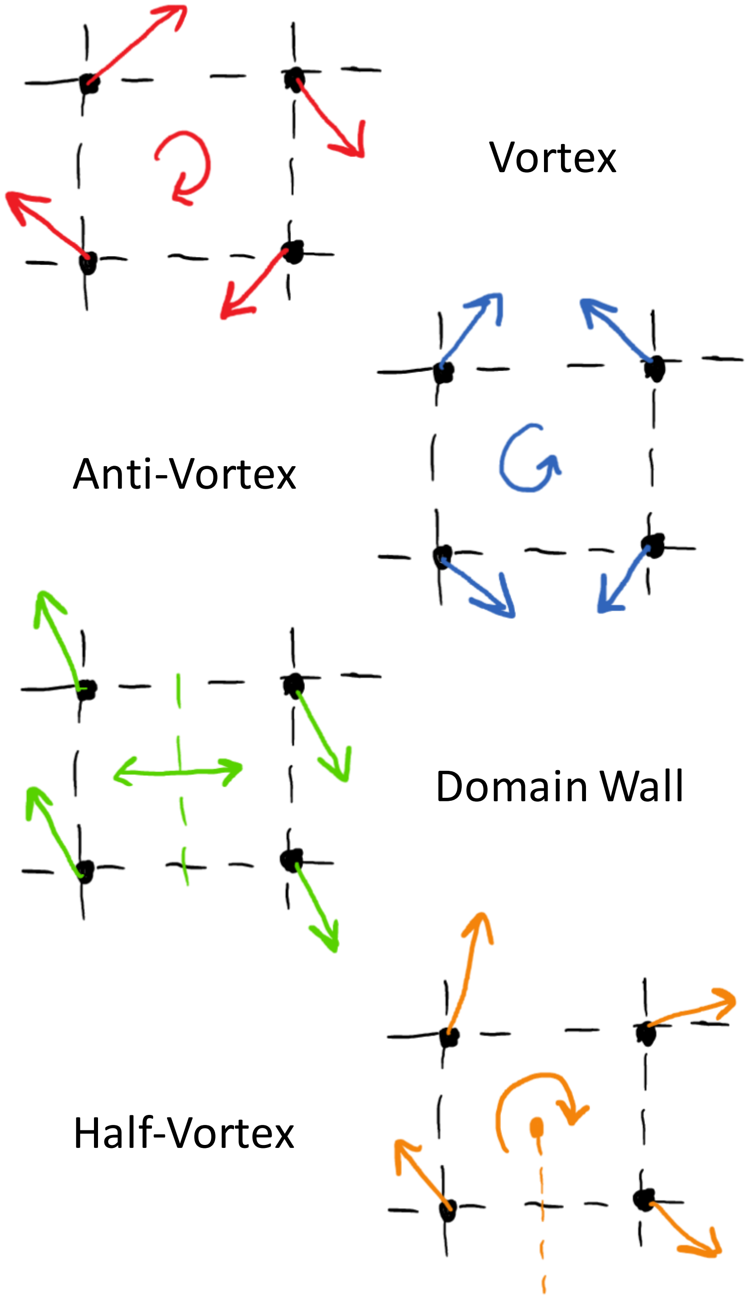
XY Models

- Finite 2-dimensional square lattice Λ
- Spin variable $\theta_i \in S^1$ at each site $i \in \Lambda$
- Hamiltonian $\mathcal{H} : (S^1)^\Lambda \longrightarrow \mathbb{R}$
  - e.g. $\mathcal{H} = -\sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$
- Canonical ensemble $\Pr(\underline{\theta}) \propto e^{-\frac{1}{T}\mathcal{H}(\underline{\theta})}$
- Phase transition(s) as T increases
- Typically analysed by measuring various correlations from Monte Carlo simulations



Why Persistent Homology?

- Transitions driven by / introduce topological defects
- Arise from non-triviality of $\pi_1(S^1)$
- Different models have different defects
  - More in higher dimensions
- Want to detect these in a robust way
  - Stability is desirable

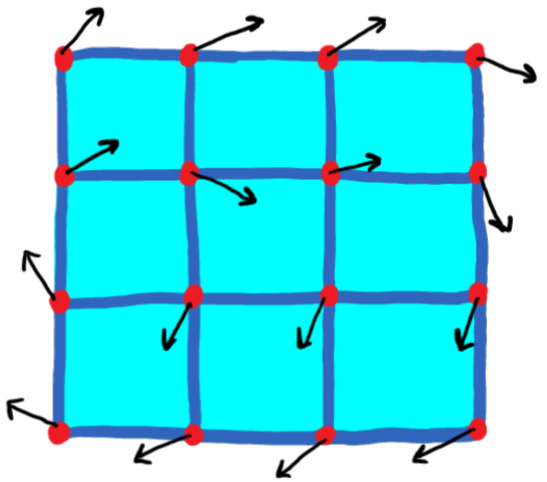


Filtration

- Sequence of cubical complexes
- We construct our filtration as increasing subcomplexes of "filled in" lattice
- Encode defects as 1-dimensional holes
  - Only need to look at H_1
  - Higher dimensional defects may require higher homology groups
- Straightforward to show stability via interleaving

$$\mathcal{F} : \mathbb{R} \longrightarrow \text{Cubical Complex}$$

$$\mathcal{F}(r) = f^{-1}((-\infty, r])$$



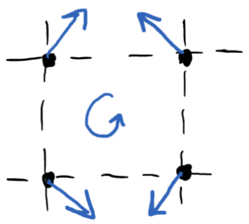
$$f(\bullet) = 0$$

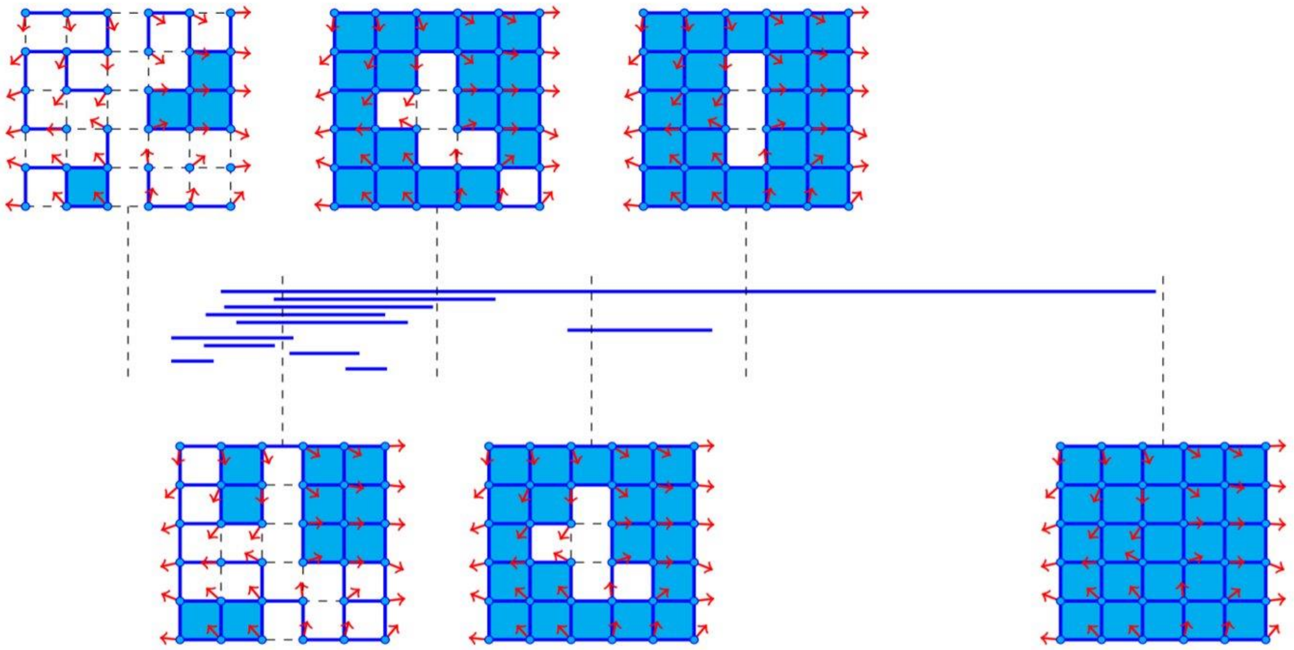
$$f(—) = |\theta_i - \theta_j|$$

$$f(\blacksquare) = \max_{ij \in \square} \{ |\theta_i - \theta_j| \}$$

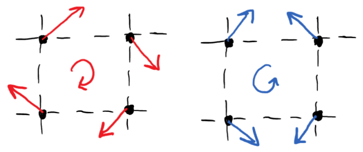
Example

- Configuration with anti-vortex
- H_1 barcode shows one long bar and many short bars all born early on





Resulting Persistence Images



- Classical XY Model

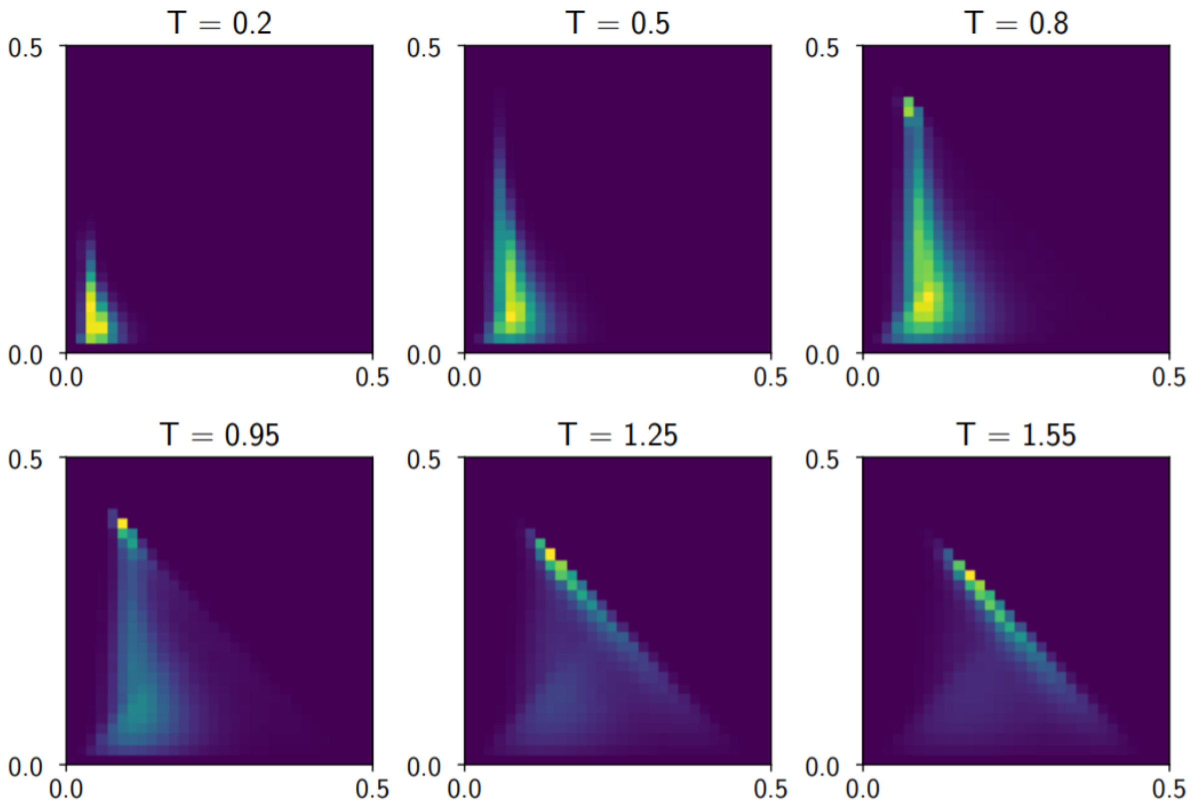
  - Hamiltonian

$$\mathcal{H}(\underline{\theta}) = \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$

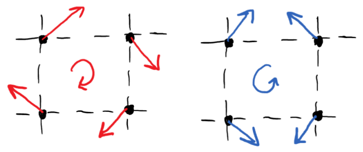
  - BKT transition at

$$T \approx 0.893$$

[Hasenbusch 2005]



Resulting Persistence Images



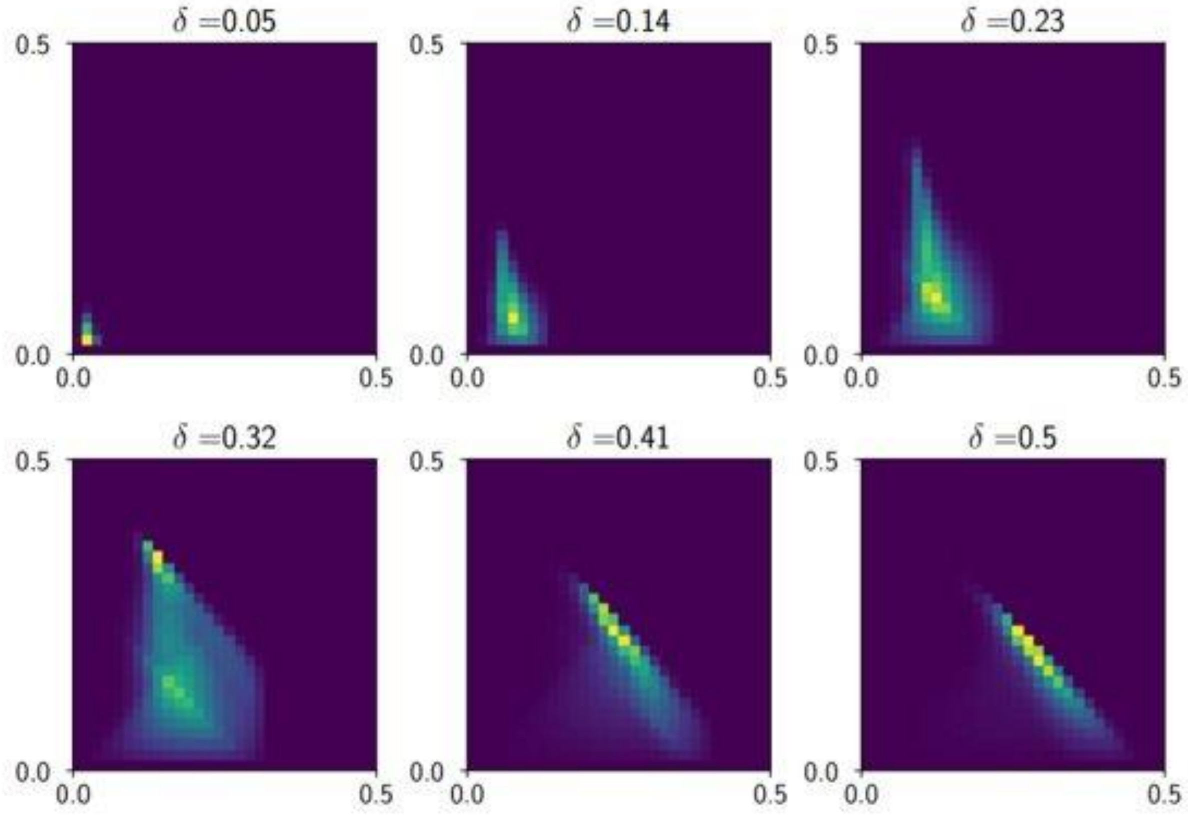
- Constrained XY Model

  - Hamiltonian

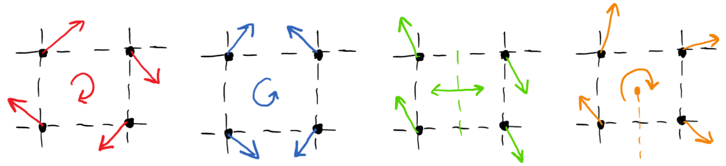
$$\mathcal{H}_\delta(\underline{\theta}) = \begin{cases} \infty & \text{if } \exists \langle ij \rangle .\ |\theta_i - \theta_j| > \delta \cdot 2\pi \\ 0 & \text{otherwise} \end{cases}$$

  - BKT transition at
    $\delta \approx 0.2825$

    [Bietenholz et al. 2005]



Resulting Persistence Images

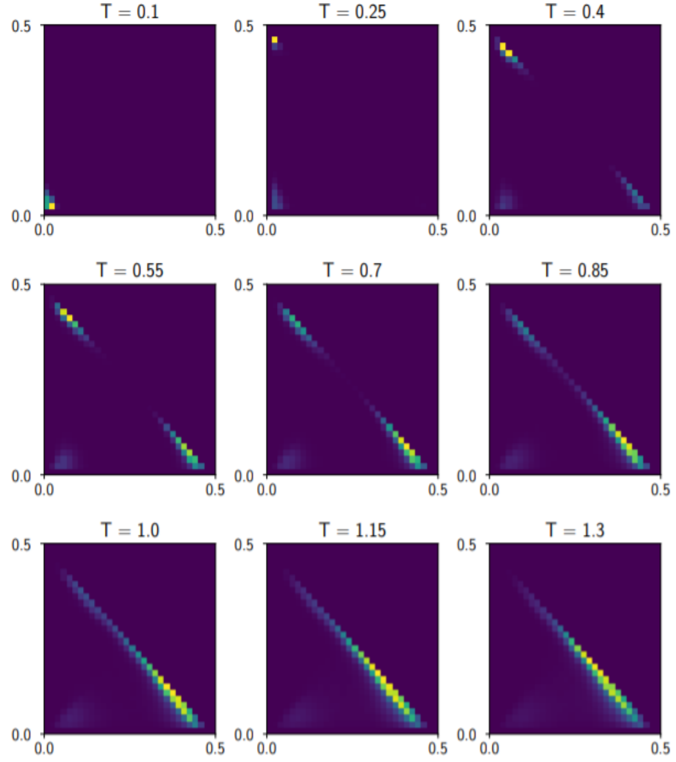


- Nematic XY Model
  - Hamiltonian $\Delta = 0.15$

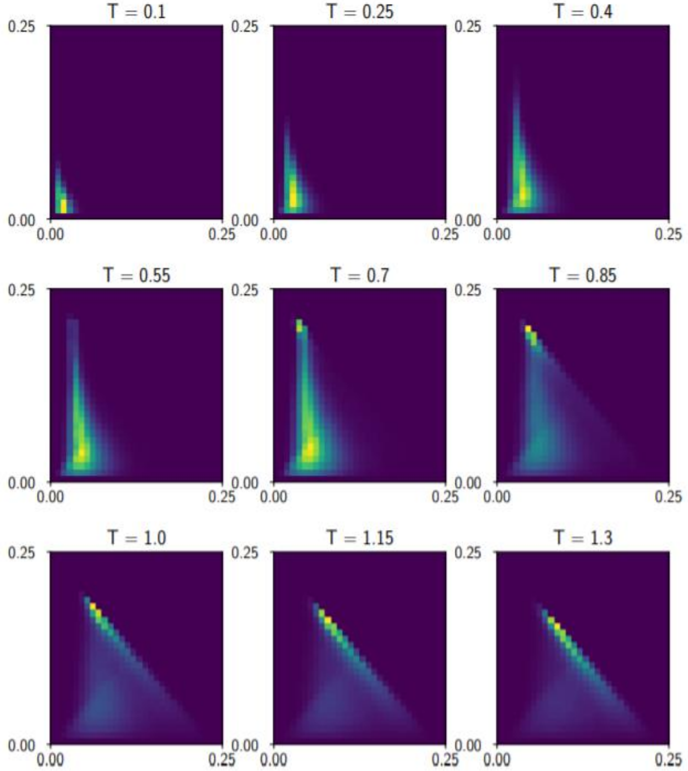
$$\mathcal{H}_{\Delta}(\underline{\theta}) = -\sum_{\langle ij \rangle}\left[\Delta \cos(\theta_i - \theta_j) + (1-\Delta)\cos(2\theta_i - 2\theta_j)\right]$$

  - 2nd order transition at $T \approx 0.331$
  - BKT transition at $T \approx 0.795$

[Nui et al. 2018]
and analysis of magnetic susceptibility



Normal Filtration



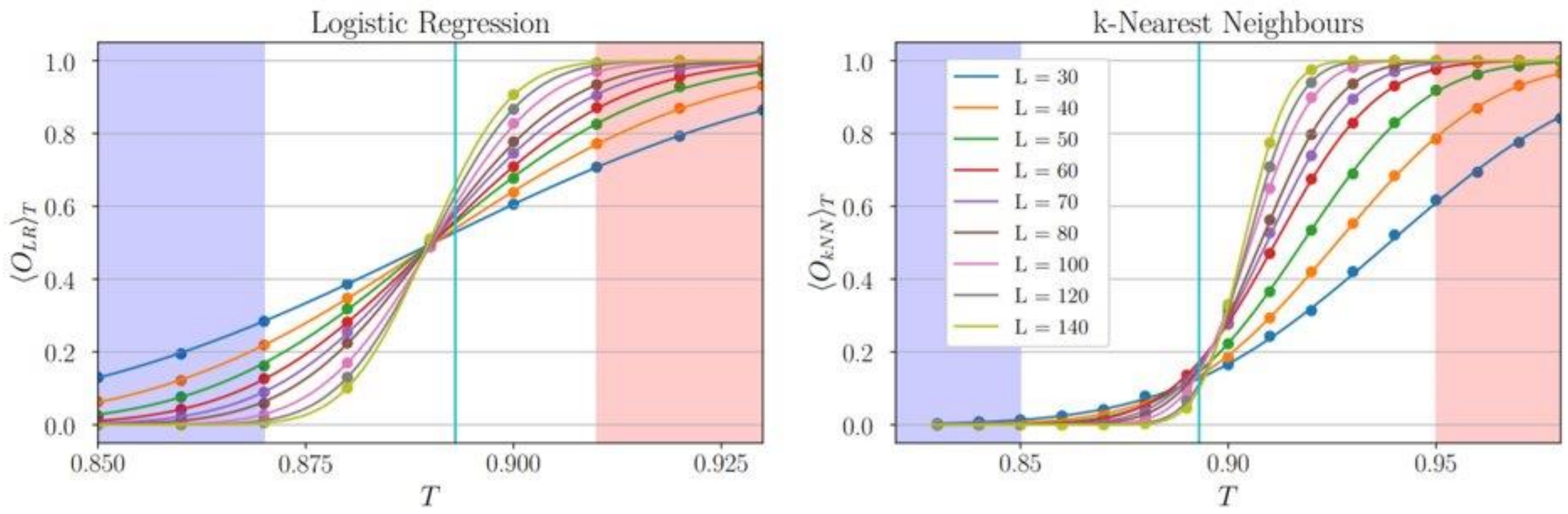
Nematic Filtration

Analysis Outline

- Like Cole, Loges and Shiu, we will use persistence images and binary classification models to learn the transition point
- Logistic regression and k-nearest neighbours
- Train and analyse much closer to the transition point
  - Making use of histogram reweighting for precise estimates
- Look for finite-size scaling behaviour to extrapolate critical temperatures and determine critical exponent of correlation length via curve collapse approach
- Bootstrap for error estimates

Observables

- Sample model over a range of temperatures
- Train classifier on persistence images away from T_c
- Look at the mean $\langle o \rangle$ and variance $\langle o^2 \rangle - \langle o \rangle^2$ of classifier output close to T_c
- Use histogram reweighting to interpolate



Finite-Size Scaling

- True phase transitions only occur in the continuum limit $L \to \infty$
  - Divergence of correlation length ξ, etc...
- On finite lattices we see a squashed version $\xi \sim L$
- Quantities of interest "squash" in a predictable way governed by the critical exponents and temperature of the transition

$$Q(L,t) = \begin{cases} L^{q/\nu}\, \hat{Q}\left(L \exp(-bt^{-\nu})\right) & \text{if BKT} \\ L^{q/\nu}\, \hat{Q}\left(L^{1/\nu} t\right) & \text{if 2}^{\text{nd}}\text{ order} \end{cases}$$

$$t = \frac{T - T_c}{T_c}$$

Finite-Size Scaling

- As we change lattice size, the peak temperature of the classification variance should fit

$$(T_c(L) - T_c) \propto \begin{cases} \log(L)^{-\frac{1}{\nu}} & \text{if BKT} \\ L^{-\frac{1}{\nu}} & \text{if 2}^{\text{nd}}\text{ order} \end{cases}$$

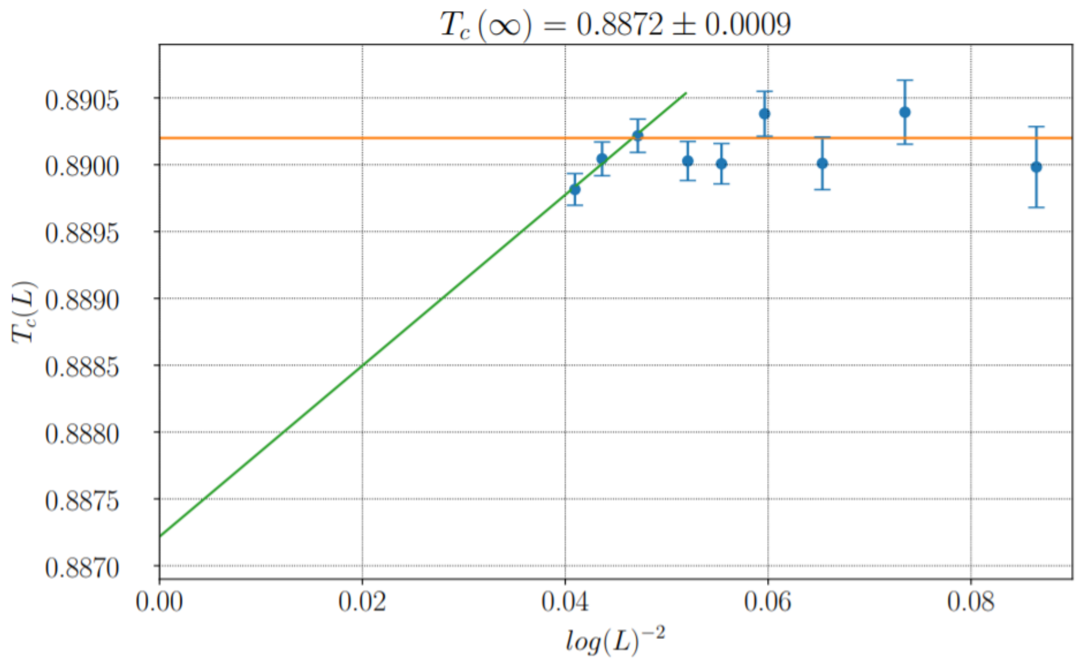
- We can also plot the variance curves for different lattice sizes against

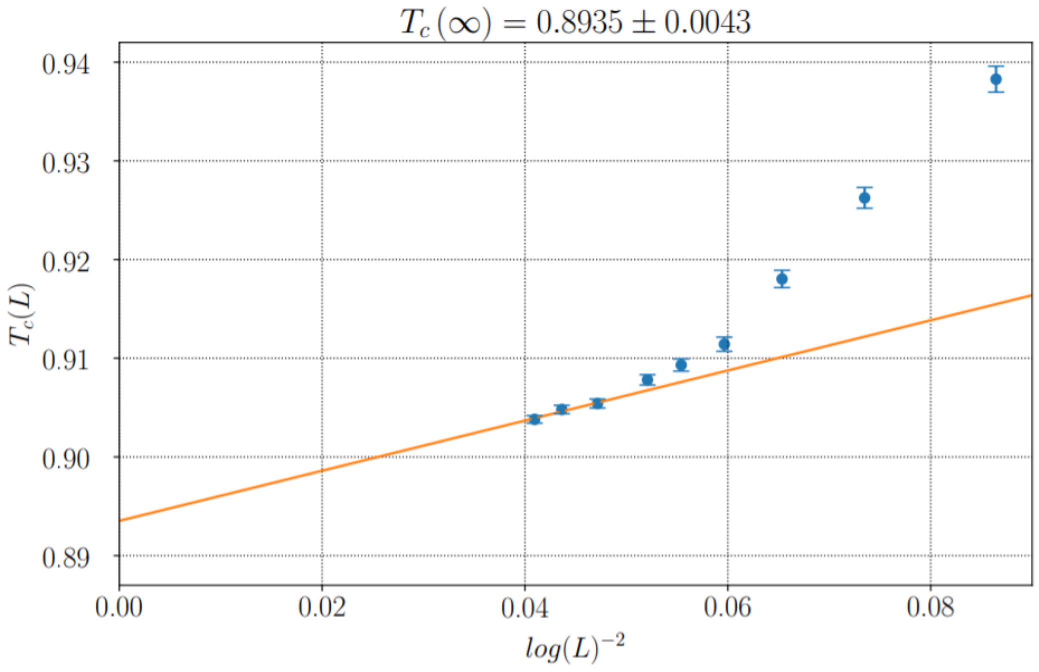
$$x = L\exp(-bt^{-\nu}) \quad \text{or} \quad L^{\frac{1}{\nu}}t$$

and optimise the unknown critical temperature / exponents to obtain the best fit (curve collapse)

Classical XY Model

$T_c = 0.8929$, $\nu = 0.5$





Logistic Regression

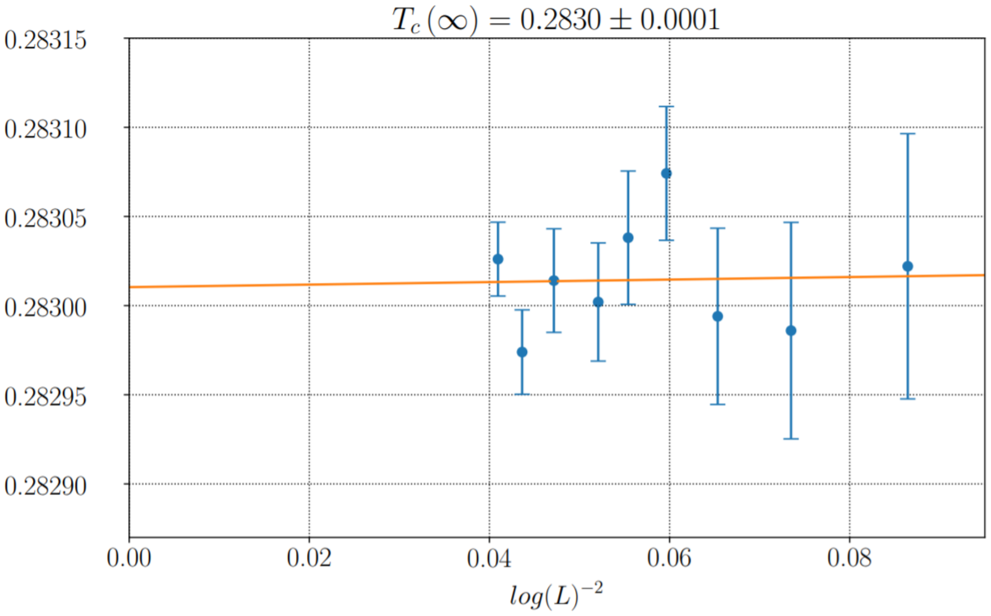
K-NN

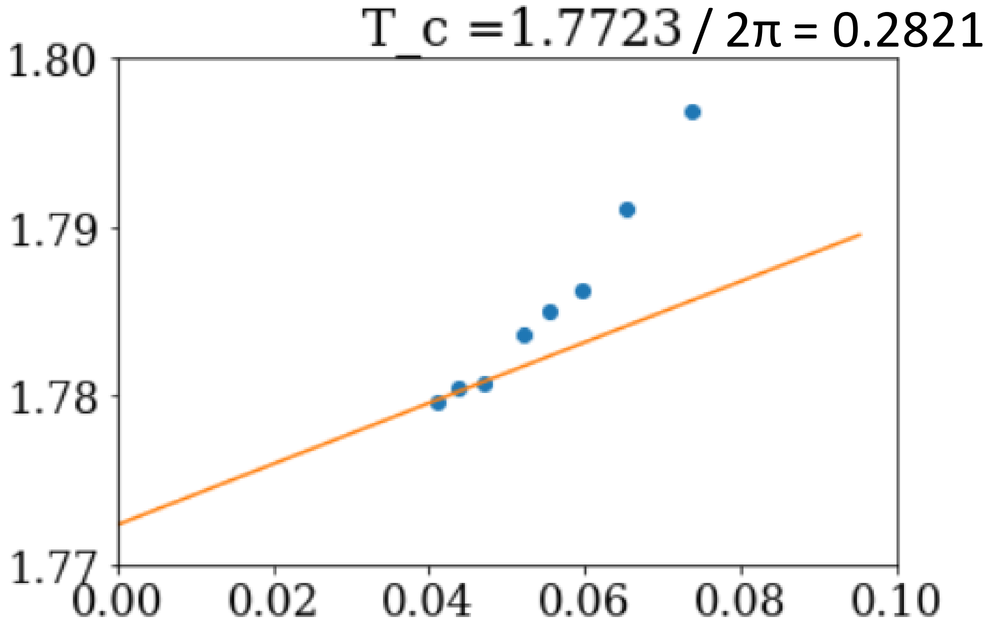
Curve collapse: $T_c = 0.8964 \pm 0.0064$, $\nu = 0.5266 \pm 0.0250$

Curve collapse: $T_c = 0.8918 \pm 0.0033$, $\nu = 0.4972 \pm 0.0264$

Constrained XY Model

$\delta_c = 0.2825$, $\nu = 0.5$



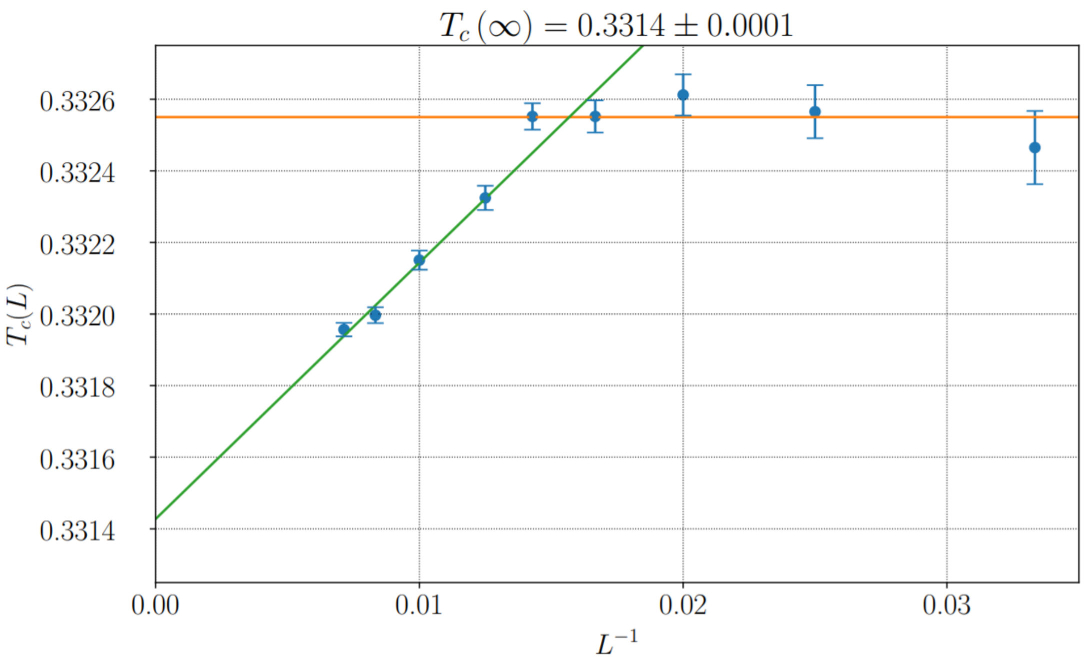


Logistic Regression

Curve collapse: $T_c = 0.2857 \pm 0.0014$
$\nu = 0.5186 \pm 0.0251$

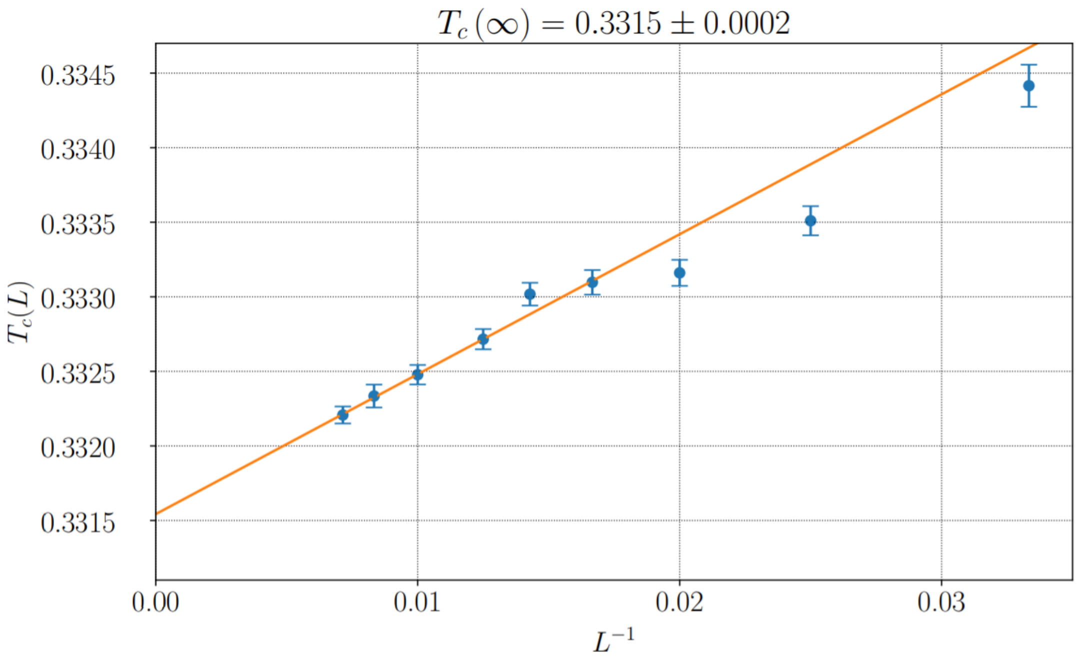
Nematic XY Model – 2nd Order Transition

T_c = 0.3314, v = 1



Logistic Regression

Curve collapse: $$T_c = 0.3315 \pm 0.0001$$ $$\nu = 1.168 \pm 0.014.$$

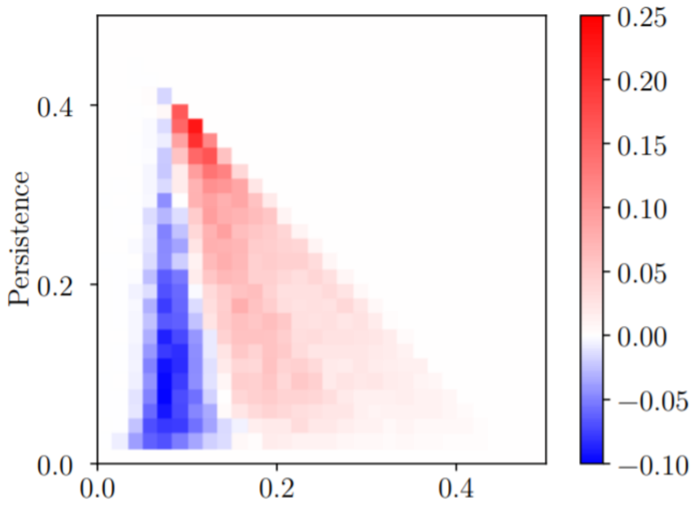


K-NN

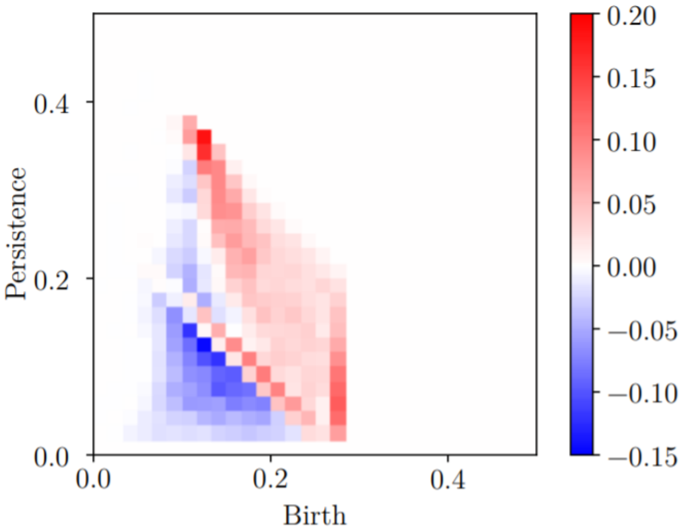
Curve collapse: $$T_c = 0.3316 \pm 0.0002$$ $$\nu = 1.047 \pm 0.0240,$$

Logistic Regression Coefficients

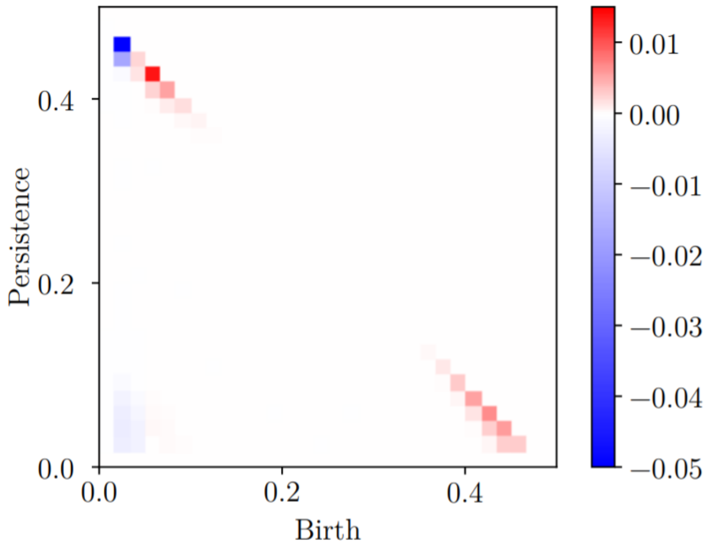
Classical



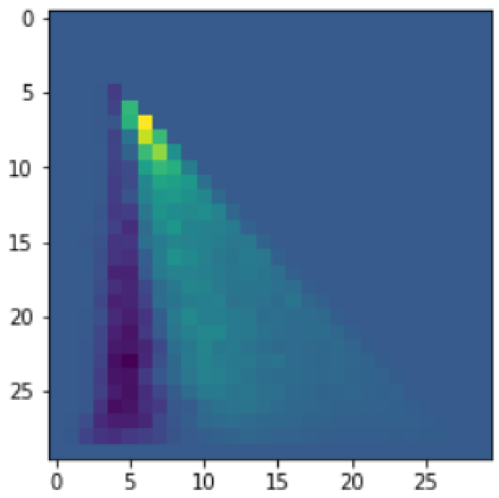
Constrained



Nematic
2nd order



Nematic
BKT



Summary

- Introduced a new class of filtrations for looking at lattice spin models which yield stable persistence
- Able to successfully identify critical temperature and exponent of correlation length to reasonable accuracy using k-NN and finite-size scaling analysis for both BKT transitions and a 2nd order transition in the Ising universality class
- Found that different filtrations identify different phase transitions even within the same model

Future Work

- A lot!
- Extension to more complex models e.g. lattice gauge theories
- Universality of persistence?
- What do the different filtrations that have been introduced tell us? Compared to classical observables?
- Can we do without the classification step? Fréchet means/variances?