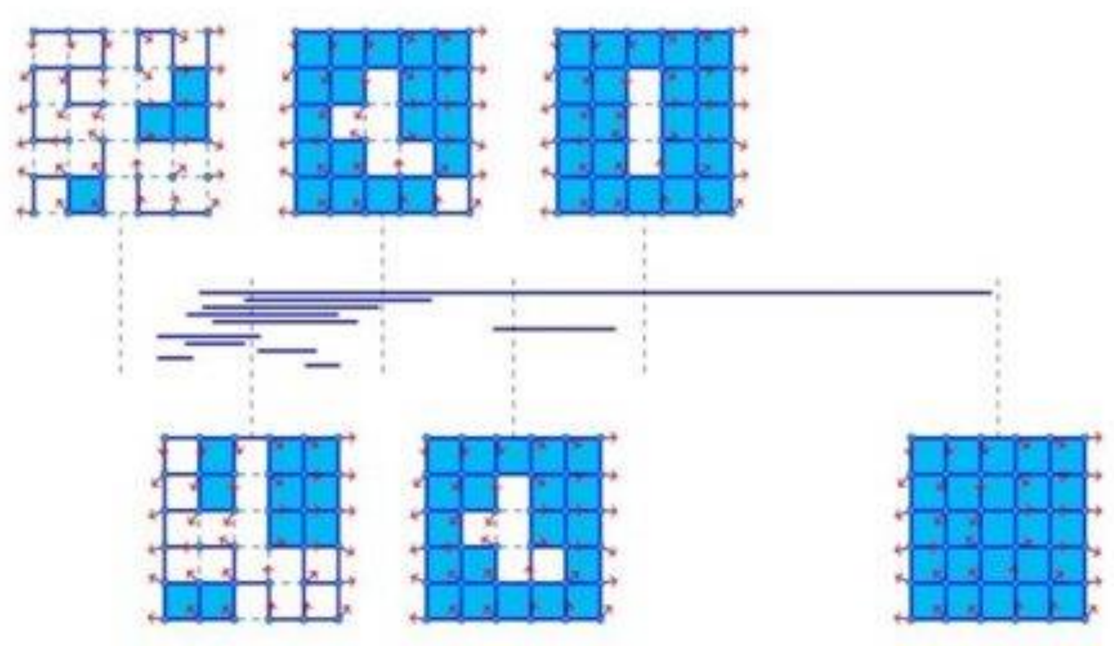
Quantitative analysis of phase transitions in two-dimensional XY models using persistent homology

Nicholas Sale – 29th September 2021 –
ECT* Workshop on Machine Learning for High Energy Physics

Joint work with Jeff Giansiracusa and Biagio Lucini



What is Persistent Homology?

- A tool from the emerging field of Topological Data Analysis (TDA)
- A way to quantitatively summarise the topological / structural features of data
- Essentially just counting and tracking connected components and holes (of various dimension) via linear algebra

Data →

"Filtration" (sequence of geometric complexes) →

Persistence "barcode"

What is Persistent Homology?

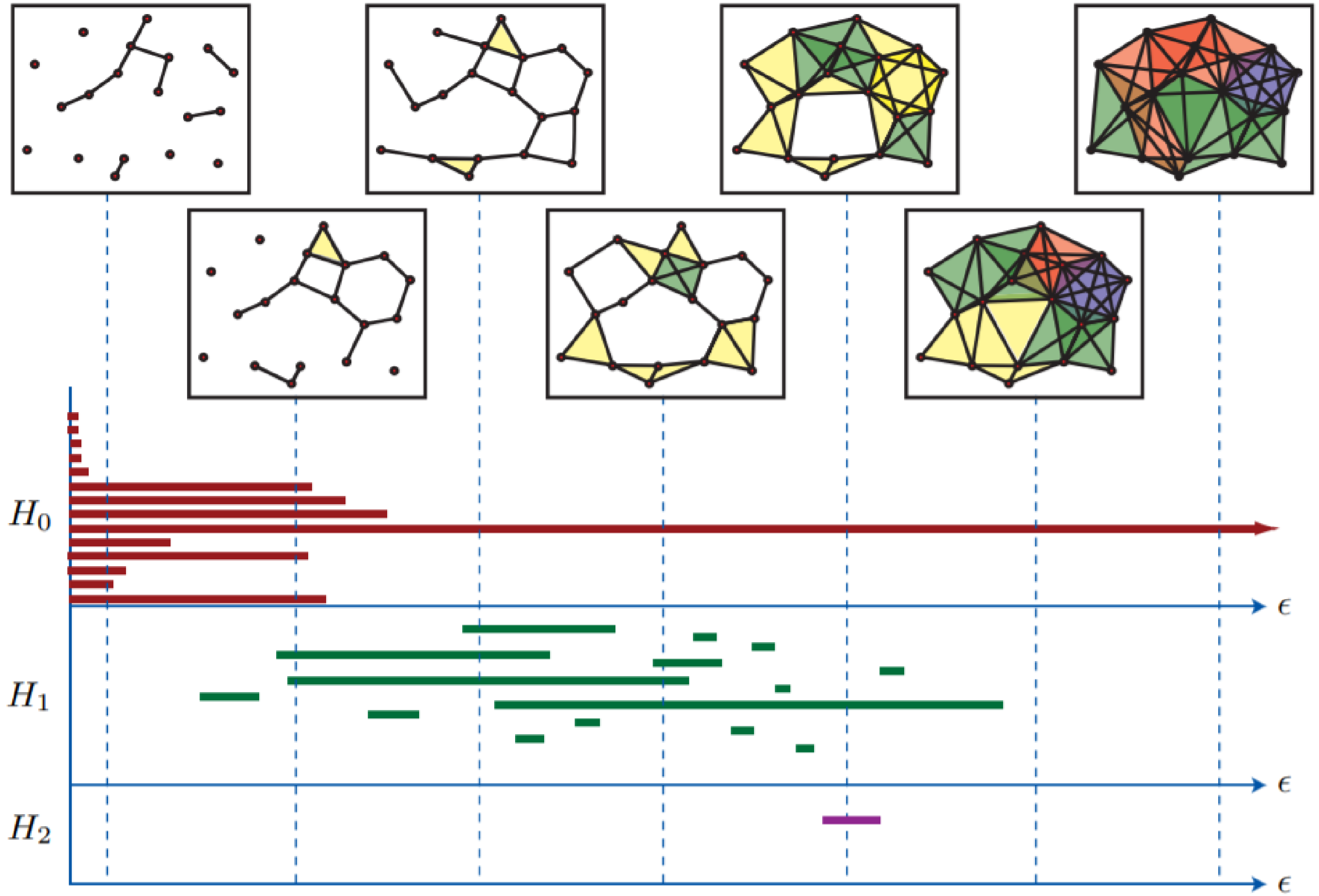
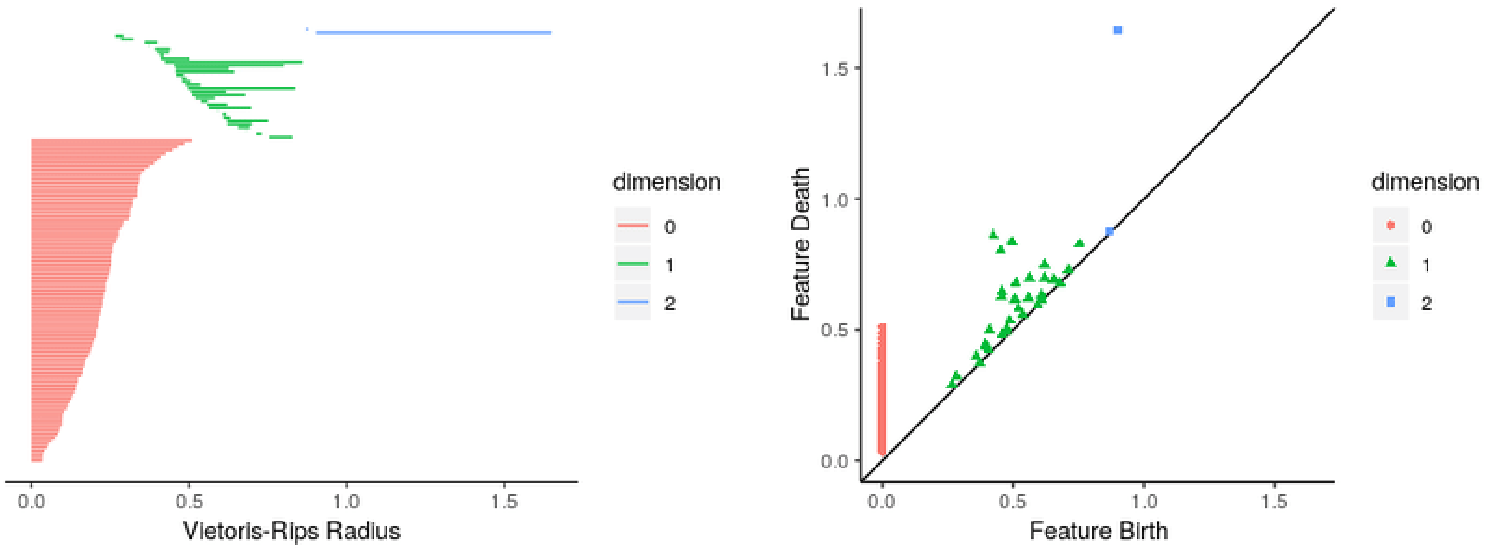


Figure reproduced from: Ghrist, R.. "Barcodes: The persistent topology of data." *Bulletin of the American Mathematical Society* 45 (2007): 61-75.

What is Persistent Homology?

- We will often represent the barcode as a persistence diagram



- For many choices of filtration, the barcode/diagram is *stable* with respect to small changes in the input data

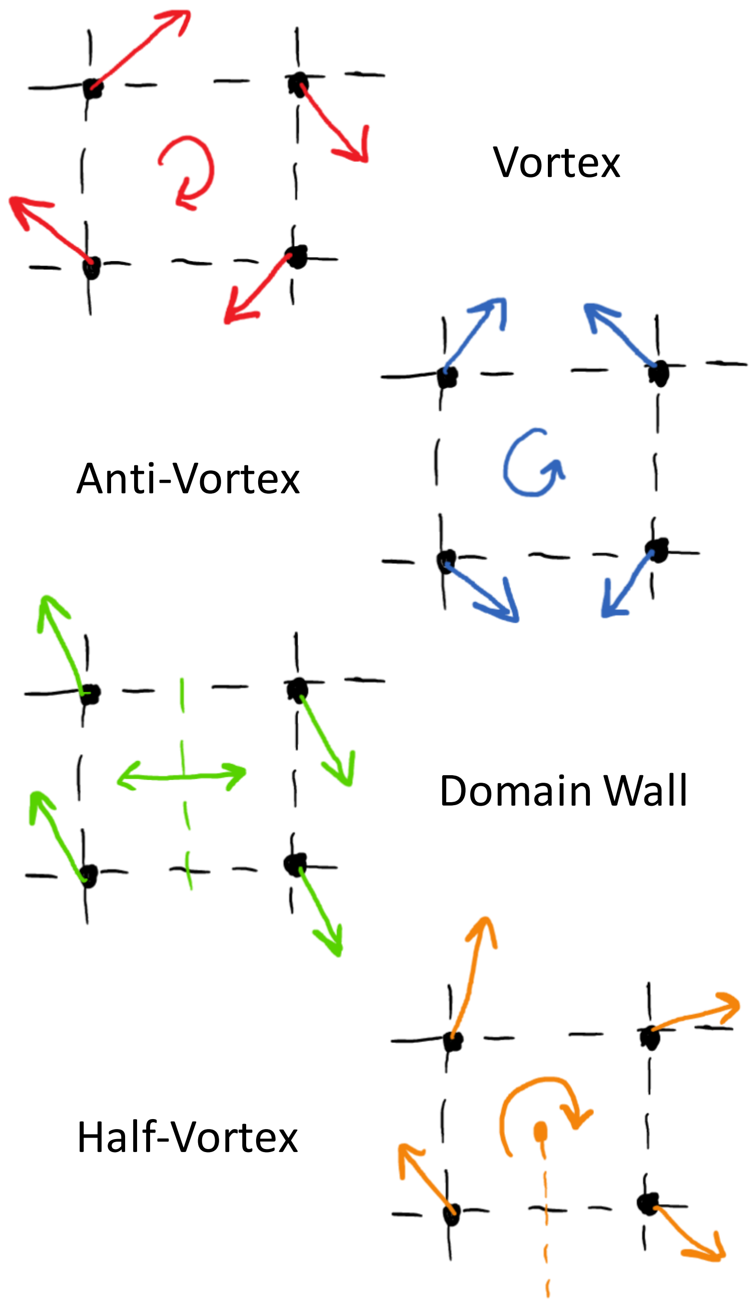
Figure reproduced from: Wadhwa, Raoul & Williamson, Drew & Dhawan, Andrew & Scott, Jacob. (2018). TDAstats: R pipeline for computing persistent homology in topological data analysis. Journal of Open Source Software. 3. 860. 10.21105/joss.00860.

Persistent Homology and Statistical Physics

- Two paradigms:
- *Persistent homology of configuration space*:
  - Look for a topological change in energy sublevel sets of the (very large) space of configurations
  - Donato, I. et al. “Persistent homology analysis of phase transitions.” Physical review. E 93 5 (2016): 052138
- *Persistent homology as an observable*:
  - Given a single configuration, compute persistence to reduce the degrees of freedom and capture the important features
  - T. Hirakida, K. Kashiwa, J. Sugano, J. Takahashi, H. Kouno, and M. Yahiro, Persistent homology analysis of deconfinement transition in effective polyakov-line model (2018)
  - Q. H. Tran, M. Chen, and Y. Hasegawa, Topological persistence machine of phase transitions, Phys. Rev. E 103,052127 (2021)
  - B. Olsthoorn, J. Hellsvik, and A. V. Balatsky, Finding hidden order in spin models with persistent homology, Phys. Rev. Research 2, 043308 (2020)
  - A. Cole, G. J. Loges, and G. Shiu, Quantitative and interpretable order parameters for phase transitions from persistent homology (2020)

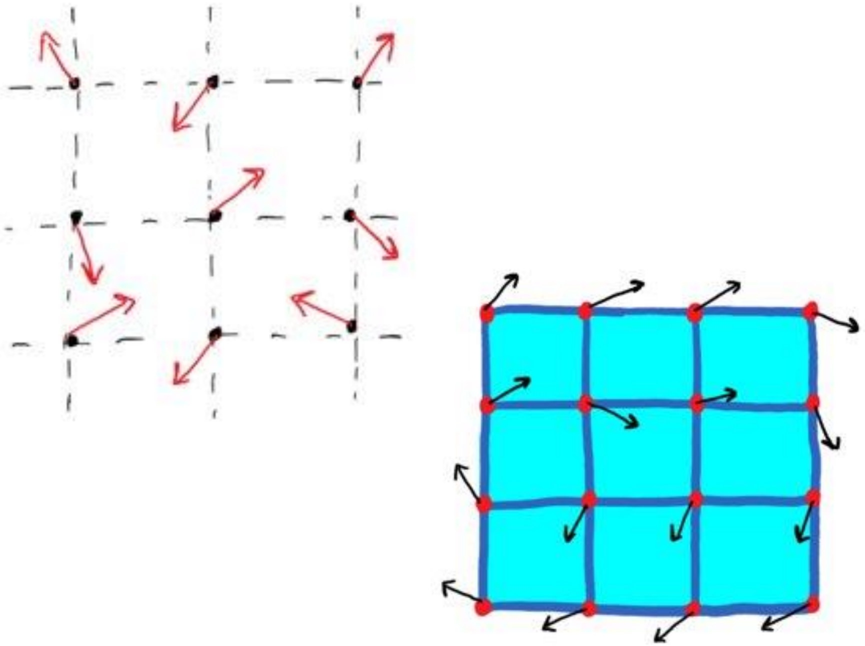
Why Persistent Homology as an Observable?

- Many phase transitions driven by / involve topological defects
- Many types of defects in different dimensions
- Want to detect these in a robust way



Our Filtration

- Given a configuration of a two-dimensional XY model we want to obtain a 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 1-dimensional persistence
  - Higher dimensional defects may require higher homology groups
- Easy to show stability



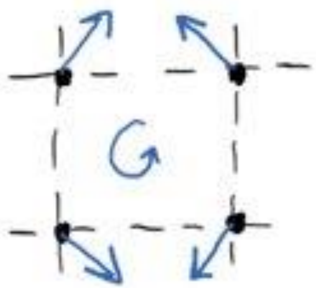
$$F(r) = f^{-1}((-\infty, r])$$

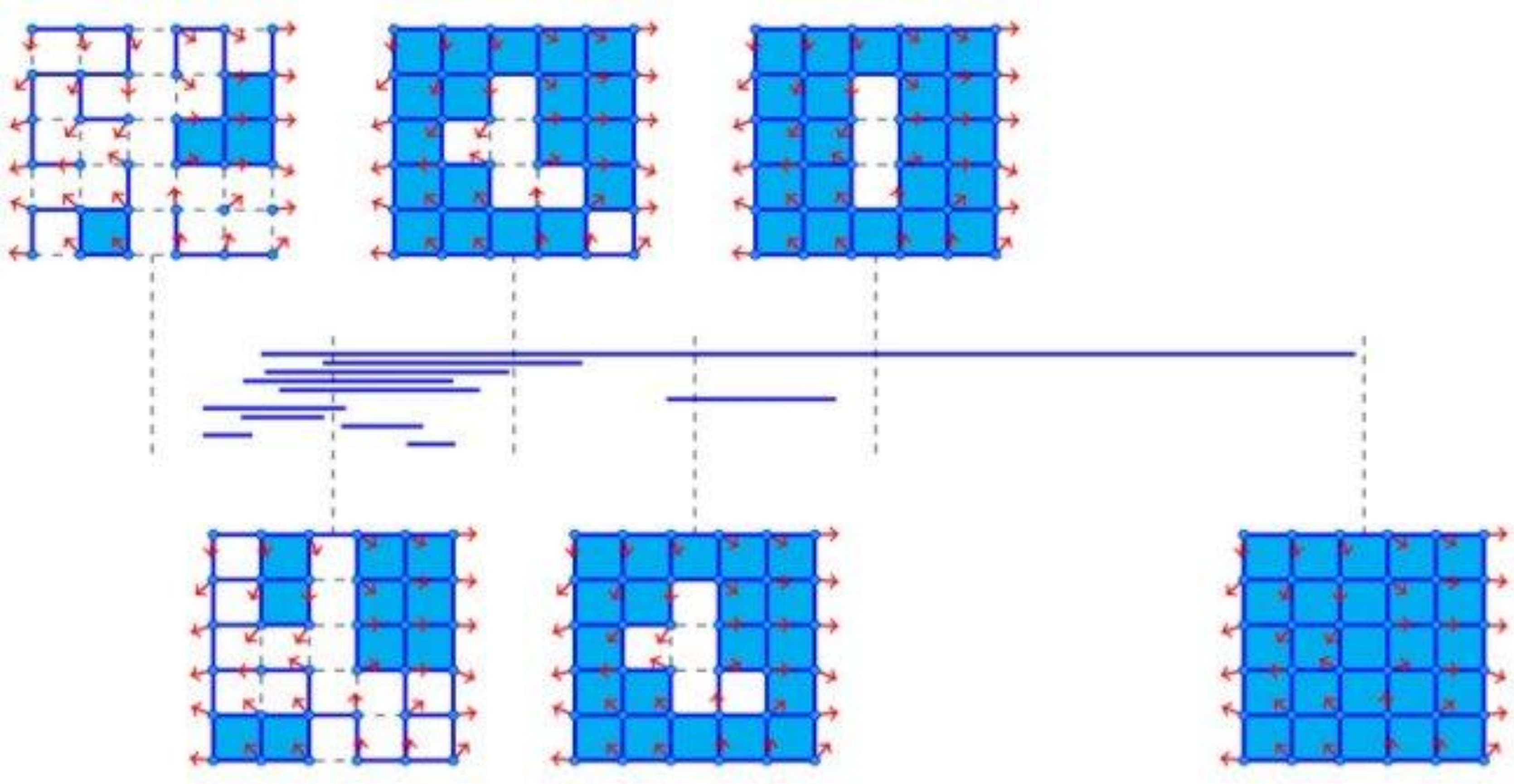
$$f(\bullet) = 0$$

$$f(\text{—}) = |\theta_i - \theta_j|$$

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

Example



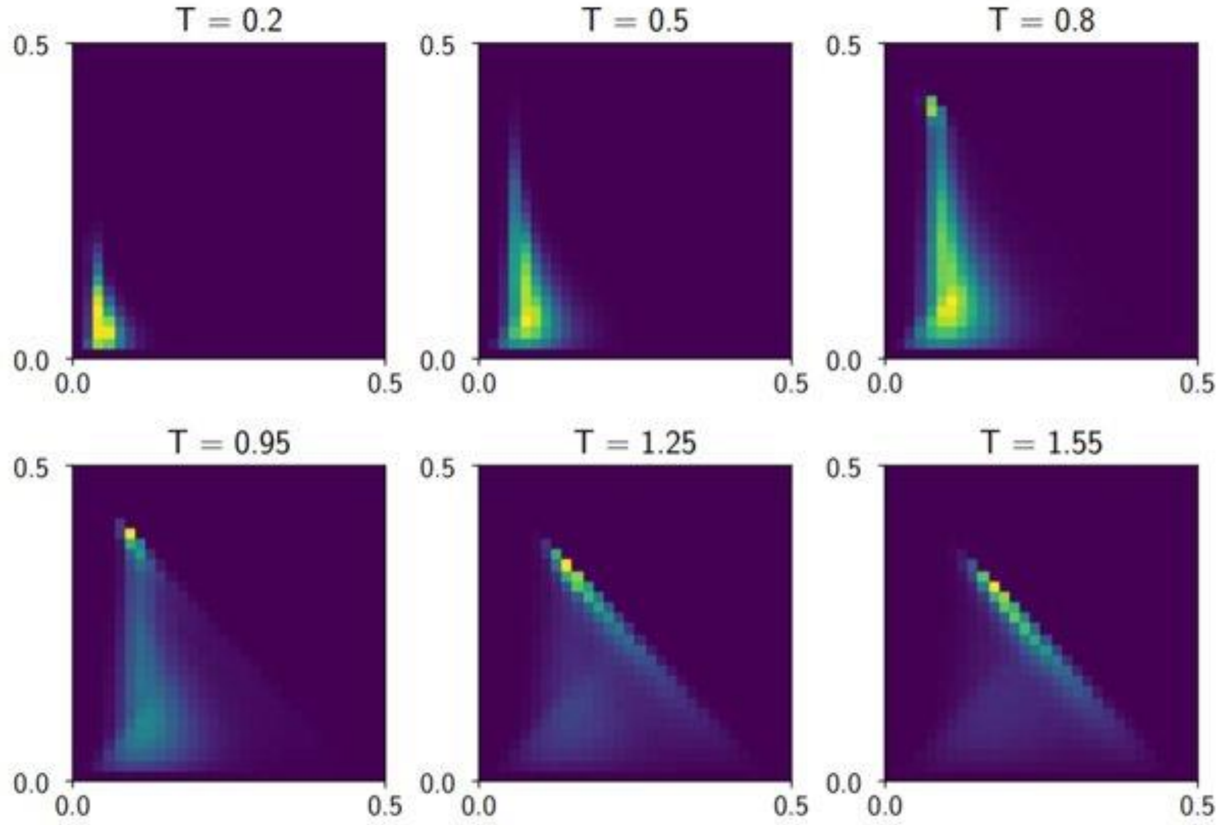


Models

- Classical XY

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

- Vortex-antivortex pairs

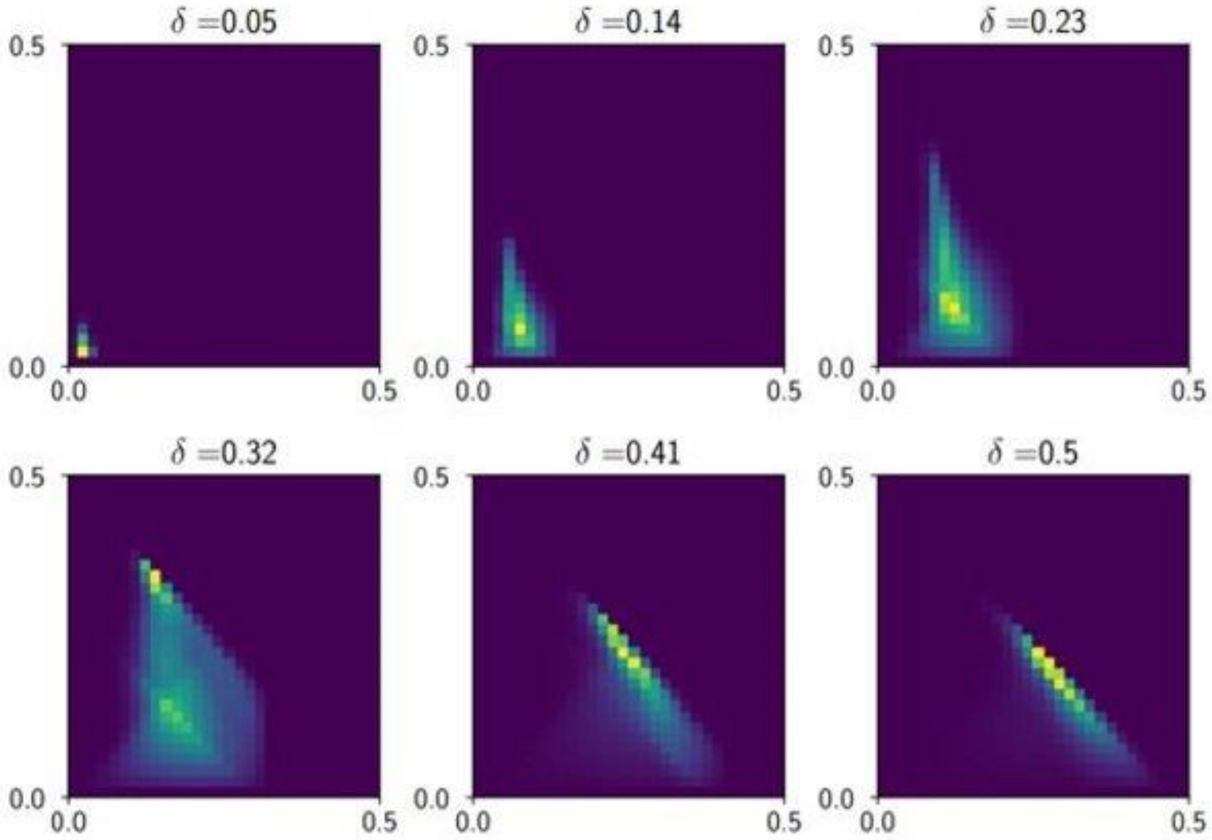


Models

- Constrained XY

$$H(\boldsymbol{\theta}) = \begin{cases} 0 & \text{if } \frac{1}{2\pi}|\theta_i - \theta_j| \leq \delta \text{ for all } \langle i, j \rangle \\ \infty & \text{otherwise.} \end{cases}$$

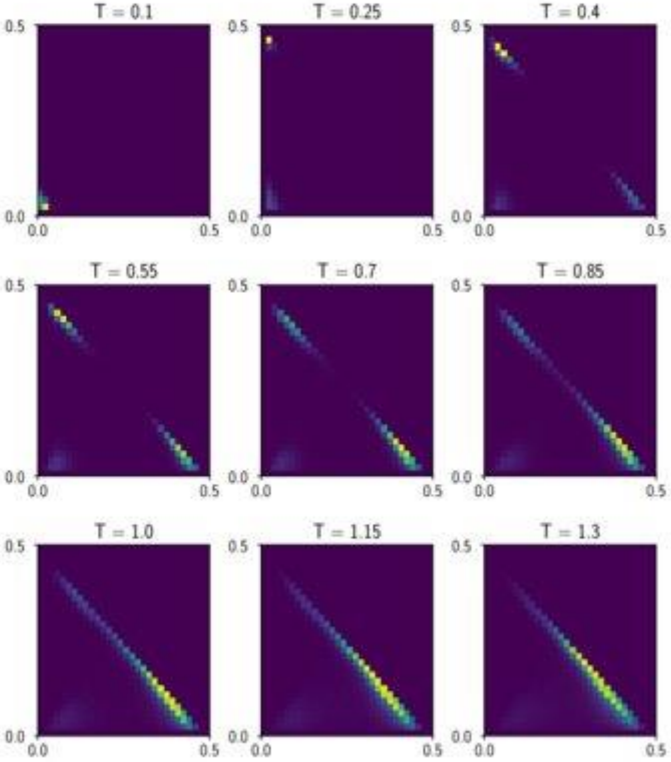
- Vortices suppressed for low delta

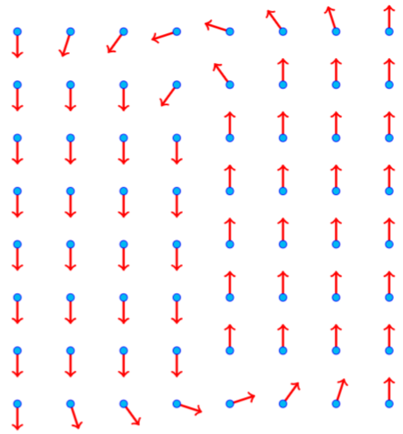


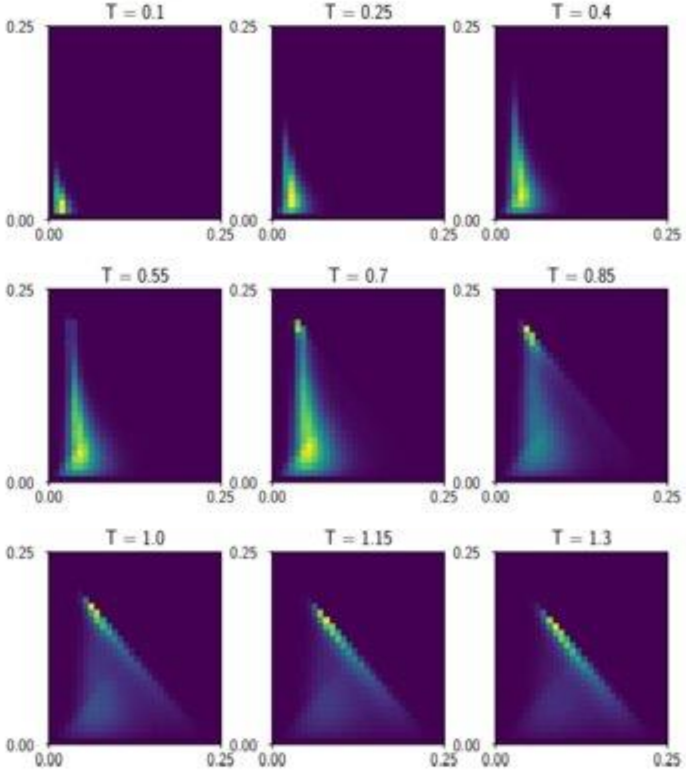
Models

- Nematic XY

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





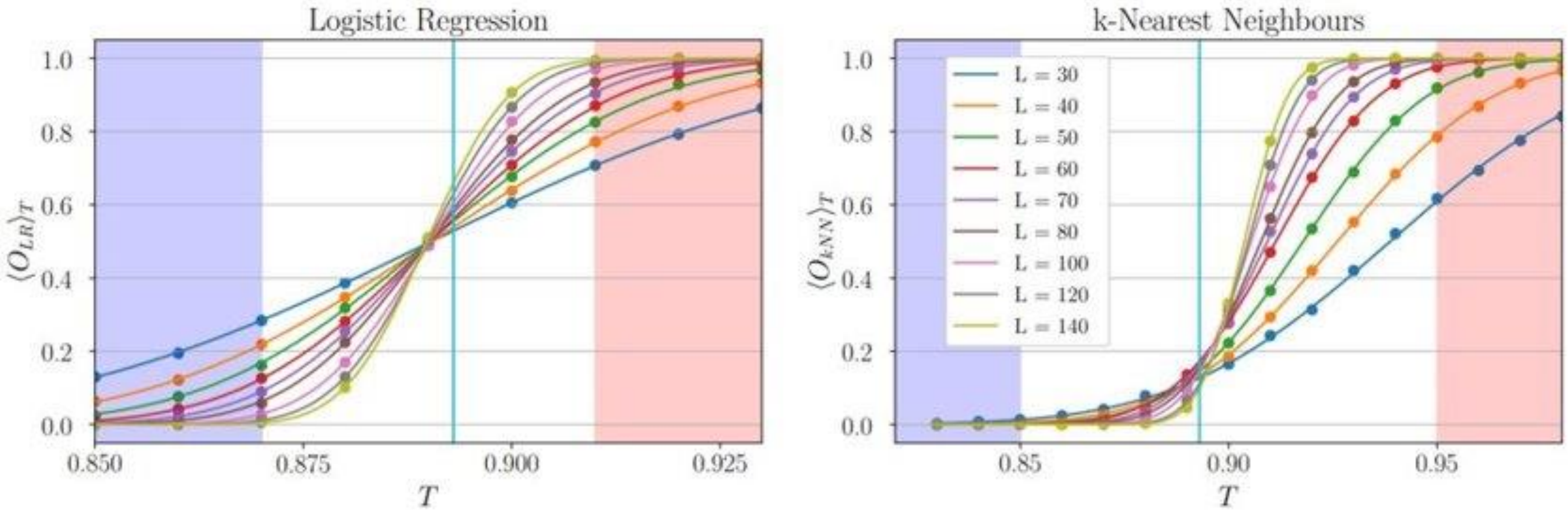


- Two phase transitions:
  - Magnetic-Nematic transition in Ising class
  - Nematic-Paramagnetic BKT transition

- Vortices stretch out into pairs of half-vortices connected by domain walls

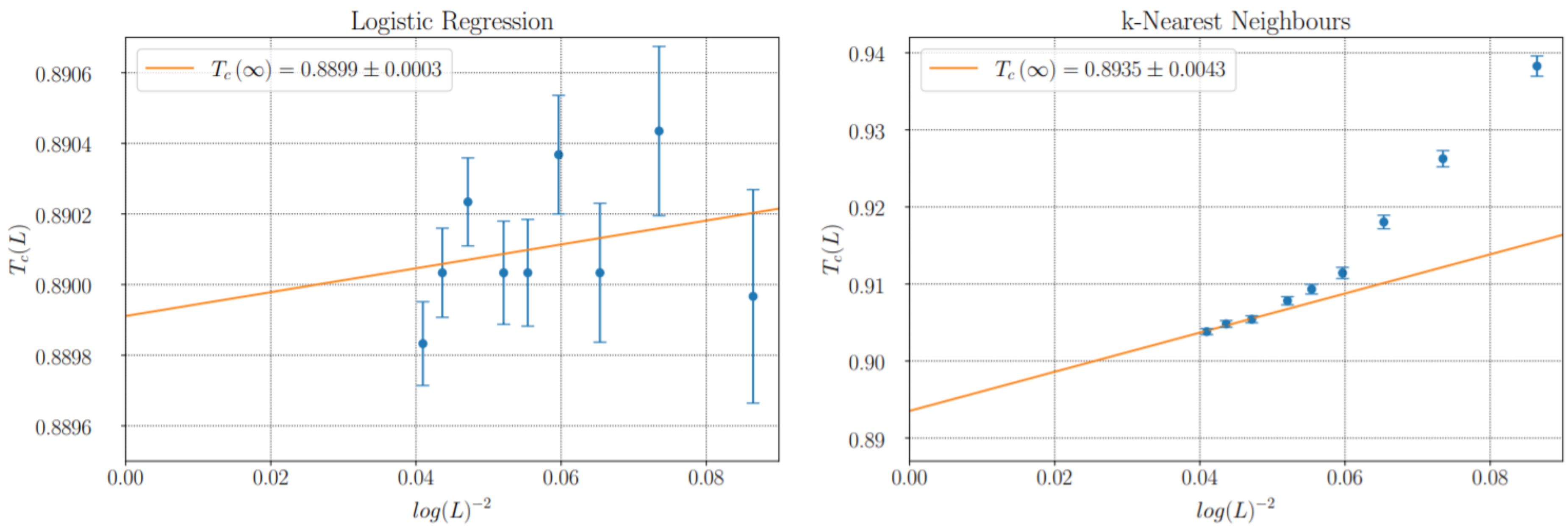
Analysis

- Classify phases with logistic regression and k-nearest neighbours
- Train on either side of the transition
- Histogram reweight to obtain point of most uncertainty



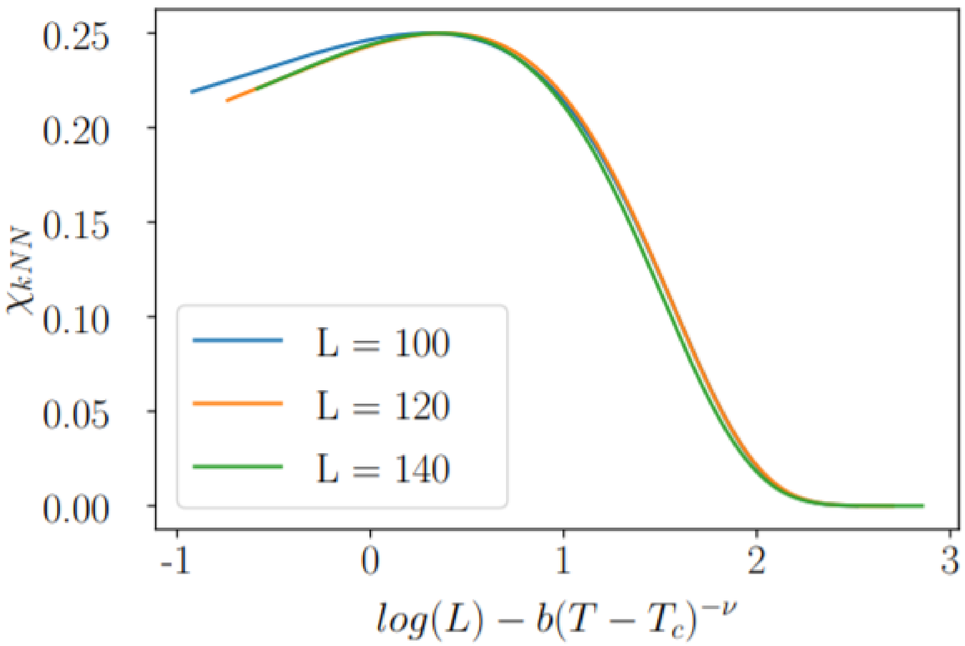
Analysis

- Look for finite-size scaling behaviour to extrapolate critical temperatures
- Bootstrap for error estimates



Analysis

- Determine critical exponent of correlation length via curve collapse approach



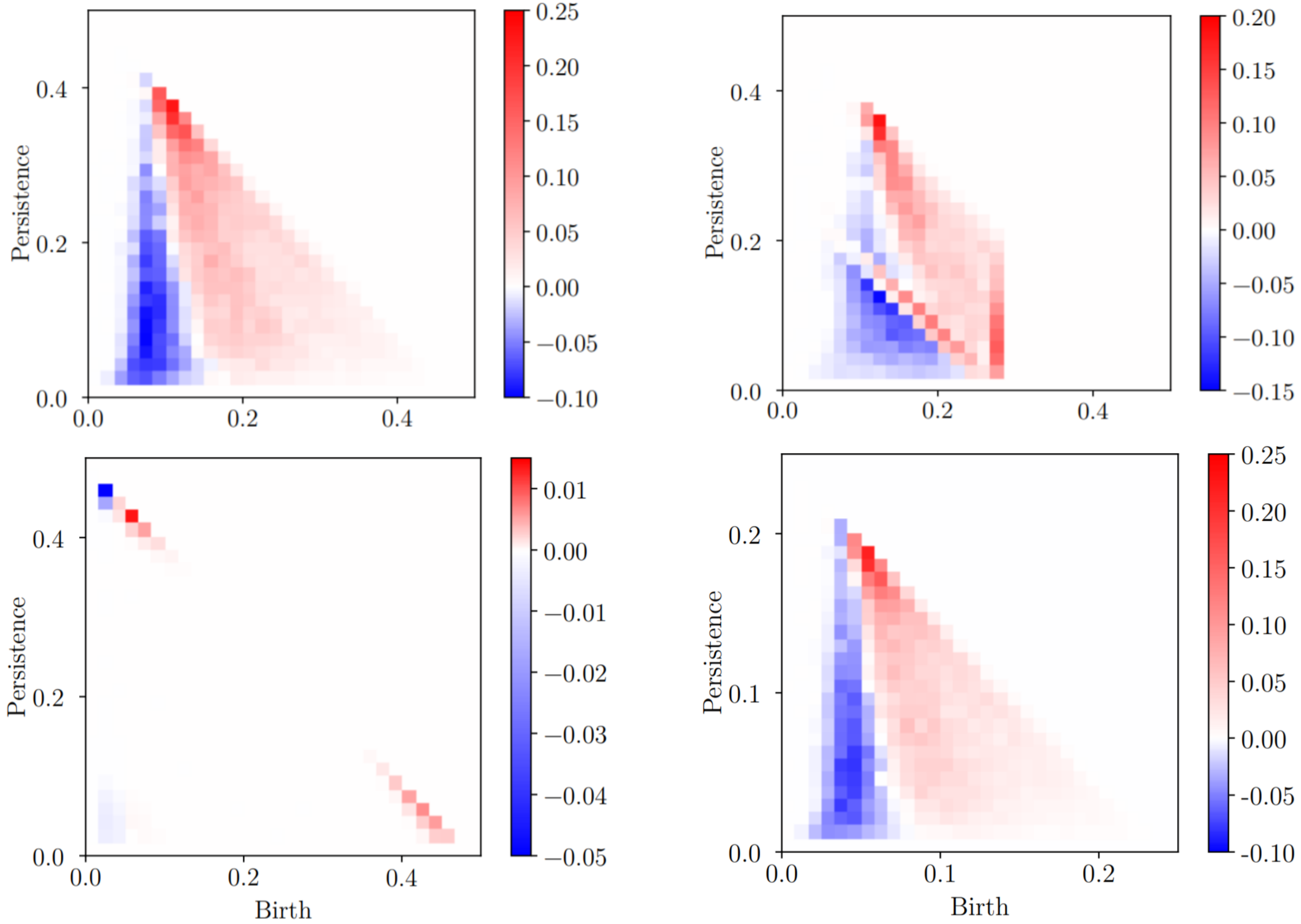
Findings

- For each phase transition we obtained an accurate determination of the critical temperature and exponent of correlation length using the k-nearest neighbours approach
- The previously proposed logistic regression approach fails in general to latch onto the phase transition
- However, the logistic regression does allow us to interpret which features are important in distinguishing phases

Logistic Regression Coefficients

Classical

Constrained



Nematic 2nd order

Nematic BKT

Current/Future Work

- This work is summarised in arXiv:2109.10960
- Extend to more complex models: e.g. lattice gauge theories
- Investigate what other TDA machinery can tell us:
  - Vineyards
  - Representative (co)cycles
  - Directed Persistence
- Persistent homology as a feature engineering preprocessing step for deep learning approaches