Replicating Phase Transitions in Vicsek Model

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CS146: Modern Computational Statistics

December 21, 2018

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Introduction

My Capstone research topic is the collective motion of self-organizing particles. Part of my work was to replicate the Vicsek model (Vicsek, Czirók, Ben-Jacob, Cohen, & Shochet, 1995). Prior to this final project, I already collected some data from my simulations. In the original paper, the authors used tools in statistical physics such as finite size scaling, combined with line-fitting to estimate critical parameters for phase transitions in the model. Thus, my goal for this final project is to infer those parameters using a Bayesian approach in the hope of reproducing their results.

1 The Problem

1.1 Summary of the Vicsek model

The Vicsek model was originally developed to investigate self-organizing biological systems such as bird flocks. In this agent-based model, all units (particles) move synchronously at discrete times steps basing on local interaction rules. Two distinct features of this model is (a) all units have the same magnitude of velocity and (b) each unit's direction of motion is determined by the average direction of its neighbors within some fixed radius (vision), with some added perturbations.

A formal definition of the Vicsek model is included in the Appendix for reference. For the purpose of this paper, it is important to define the following terms:

System size L The linear size of the simulation field where particles interact. This is a control parameter.

Noise η The magnitude of random angular perturbations added to each particle's motion. When $\eta = 0$, all particles move deterministically. When η is at its maximum (2π), particles' motions are fully random. This is a control parameter.

Order parameter ϕ A statistic calculated from the system's global state, reflecting the degree to which particles are aligned with one another. It is defined as the magnitude of the (vector) average normalized velocity

$$\phi = \frac{1}{N}\left|\sum_{i=1}^{N} \frac{\mathbf{v}_i}{v_i}\right|$$

where $\frac{\mathbf{v}_i}{v_i}$, a unit vector, is the normalized vector velocity for particle i, and N is the total number of particles in the system. A completely disordered state has $\phi = 0$ and the maximum order is $\phi = 1$ (see Figure 1, adopted from Vicsek et al. (1995)).

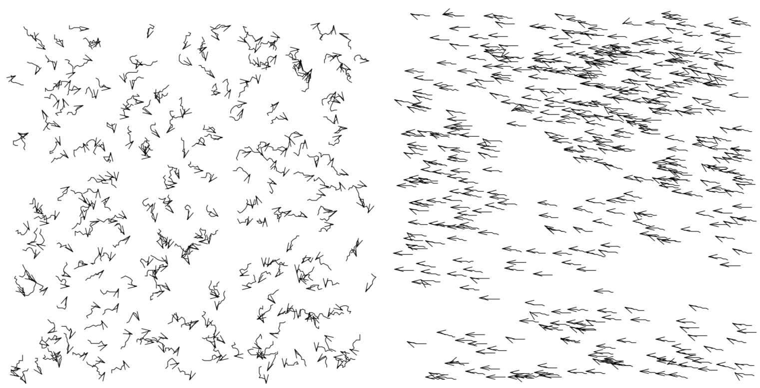

Figure 1. The state on the left has a low order and the state on the right has $\phi \approx 1$.

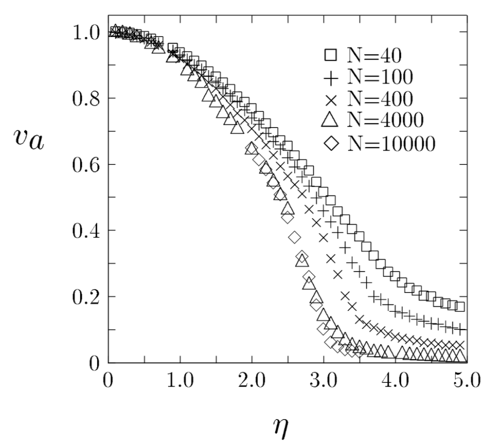

Figure 2. Transition from ordered to disordered phase with increasing η. The number of particles N is proportional to the squared system size L^2 due to fixed density. On the y-axis, $v_a = \phi$ is the order parameter defined by average velocity.

1.2 Phase transitions in the Vicsek model

In Vicsek et al. (1995), a phase transition in order parameter with respect to increasing noise is observed (Figure 2). This behavior is analogous to the continuous phase transition in equilibrium systems, such as ferromagnetic interactions where temperature is the noise and magnetization is the order parameter. Therefore, the authors assume the following behavior

$$\phi \sim [\eta_c(\infty) - \eta]^\beta$$

where $\eta_c(\infty)$ is the critical noise in theoretical thermodynamic limit (as system size L approaches ∞) and β is the critical exponent. When η exceeds the critical point—that is, when $\eta_c(\infty) - \eta < 0$, the system is in a disordered state ($\phi = 0$). While the value of $\eta_c(\infty)$ depends on density and other parameters, β is believed to be universal. There has been prior empirical determination of this critical exponent through simulations: $\beta = 0.45 \pm 0.07$ in Vicsek et al. (1995); $\beta = 0.42 \pm 0.03$ in Czirók, Stanley, and Vicsek (1997); $\beta = 0.45 \pm 0.03$ and $\beta = 0.42 \pm 0.04$ in Baglietto and Albano (2008).

In practice, the phase transition behaviors are affected by simulation size as can be seen in Figure 2. Since we cannot simulate systems of infinite size, we account for these effects using finite-size scaling theory

$$\phi = \begin{cases} \left(\frac{\eta_c(L)-\eta}{\eta_c(L)}\right)^\beta & \eta < \eta_c(L) \\ 0 & \eta \geq \eta_c(L) \end{cases} \tag{1}$$

where $\eta_c(L)$ is the effective critical noise for a system of finite size L, which is itself described by

$$\eta_c(L) = \eta_c(\infty) + kL^{-1/\nu} \tag{2}$$

where k is a scaling constant and ν is the correlation length critical exponent.

2 Model[1] and Assumptions

My modeling goal is to infer the parameters $\eta_c(\infty)$, β and ν, check the plausibility of the model against data (see Figure 3), and compare my critical exponents with those in the literature[2].

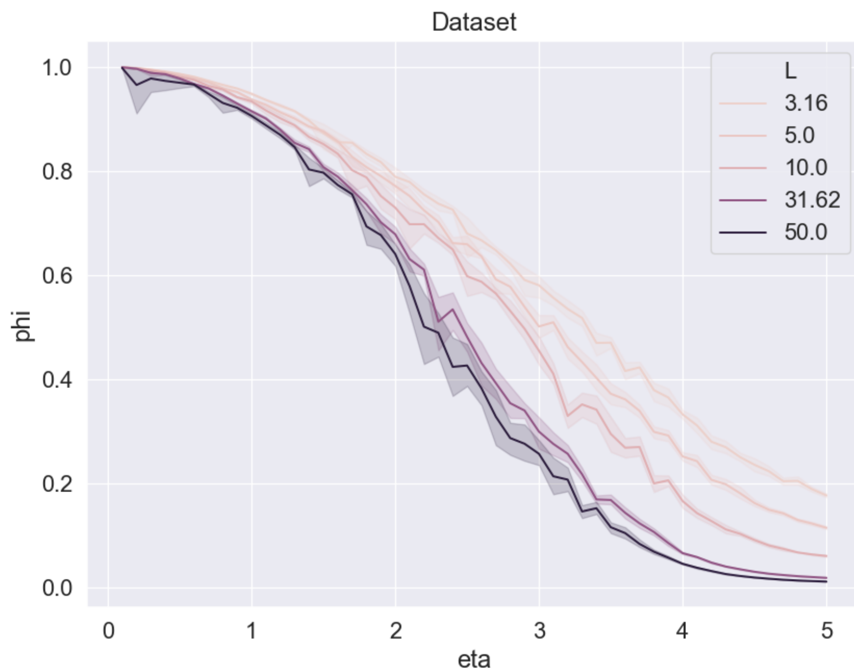

Figure 3. Visualization of the dataset for this modeling task—a replication of Figure 2.

2.1 Model structure

The graphical model in Figure 4 describes the relationship among variables in my model. The observed variables are L, η, and ϕ and unobserved variables are β, ν, $\eta_c(\infty)$, k and σ. More specifically, L and η are control parameters in the sense that during my simulation experiments, I

[1]From now on I will refer to the statistical model as simply "model" and the self-organization model as "Vicsek model".

[2]I had said in my original proposal that I also wanted to compare with the critical noise estimated in the Vicsek paper. However, I found out that this is not possible as my data was generated under a different density (which leads to a different critical noise), and I do not have the computational resource to run simulations with the same density as Vicsek in a reasonable amount of time.

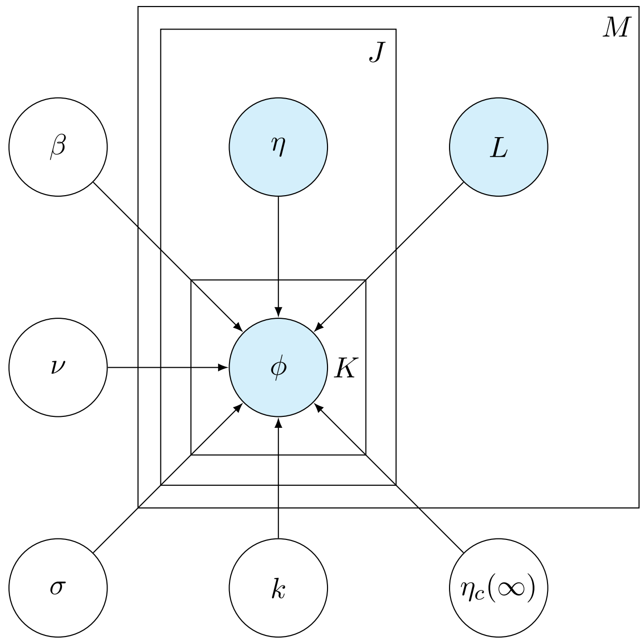

Figure 4. Graphical model. Observed variables are in blue.

varied those parameters to observe the response quantity ϕ. I used $M = 5$ different values for L ($\{3.16, 5, 10, 31.6, 50\}$), and $J = 50$ different values for η ($\{0.1, 0.2, ..., 5.0\}$). For each unique set of L and η, I repeated $K = 10$ trials. These are reflected in the plate notations.

The model assumes the following generative process:

1. For each $m \in \{1, 2, ..., M\}$: the variables L_m, $\eta_c(\infty)$, k and ν together determine $\eta_c(L_m)$ through Eq. (2), where $\eta_c(L_m)$ is the effective critical noise for a system of finite size L_m.

2. For each $j \in \{1, 2, ..., J\}$: the variables η_j, $\eta_c(L_m)$, and β determine ϕ_0 through Eq. (1), where ϕ_0 stands for the "true" order parameter obtained through theoretical calculations.

3. For each trial $k \in \{1, 2, ..., K\}$: the observed order parameter ϕ is drawn from a normal distribution centered around ϕ_0 with standard deviation σ, which accounts for both sampling and observation error.

Note that the intermediate quantities $\eta_c(L)$ and ϕ_0, though useful in describing the model, can be eliminated from the likelihood function (and also the graphical model). Thus the final likelihood is

$$\phi \sim \mathcal{N}\left(\left(\frac{\max\{0, \eta_c(\infty) + kL^{-1/\nu} - \eta\}}{\eta_c(\infty) + kL^{-1/\nu}}\right)^{\beta}, \sigma\right)$$

where the max operation accounts for both cases in Eq. (1).

2.2 Choice of priors

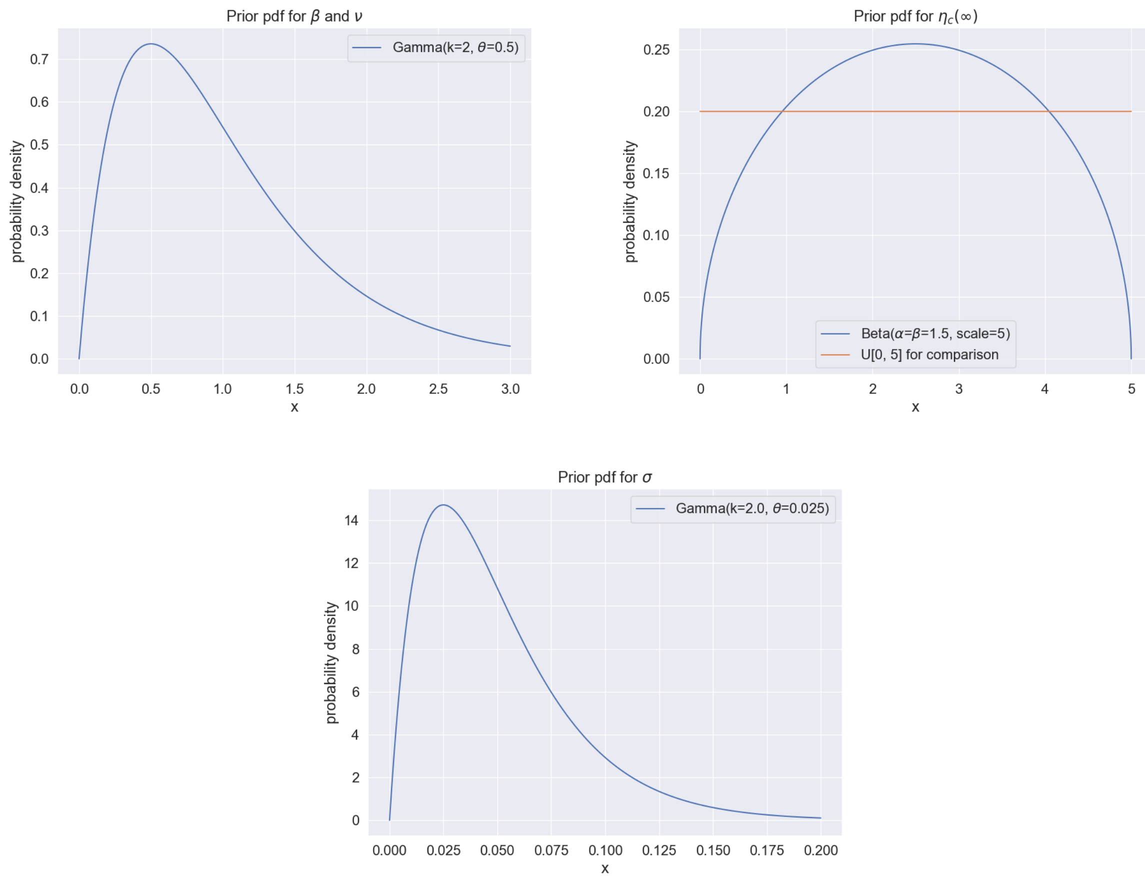

Figure 5. Visualization of priors distributions.

***k*:** From Eq. (2), we know that k must be positive, since $\eta_c(L)$ should always be larger than $\eta_c(\infty)$. However, we do not have prior knowledge for its scale. Therefore, I use an uninformative uniform prior over all positive real.

$\boldsymbol{\beta, \nu}$: These critical exponents must be positive for correct scaling direction (e.g. decaying rather than blowing up). Inspecting tables of values of critical exponents from Wikipedia and Baglietto and Albano (2008), we see that they never exceed 3. Therefore, I used a gamma prior with shape $k = 2$ and scale $\theta = 0.5$.

$\boldsymbol{\eta_c(\infty)}$: From Figure 2, we see that the phase transition occurs between $\eta = 0$ to $\eta = 5$ and the critical point is more likely to lie in the middle than at the ends of the η spectrum.

Therefore, I used a scaled beta distribution ($\alpha = \beta = 1.5$, $scale = 5$) as the prior.

$\boldsymbol{\sigma}$: Since σ accounts for errors associated with the observation of ϕ values, and ϕ is bounded by 0 and 1, I chose a gamma distribution with a small scale ($k = 2$, $\theta = 0.025$) as the prior.

2.3 Generating fake data

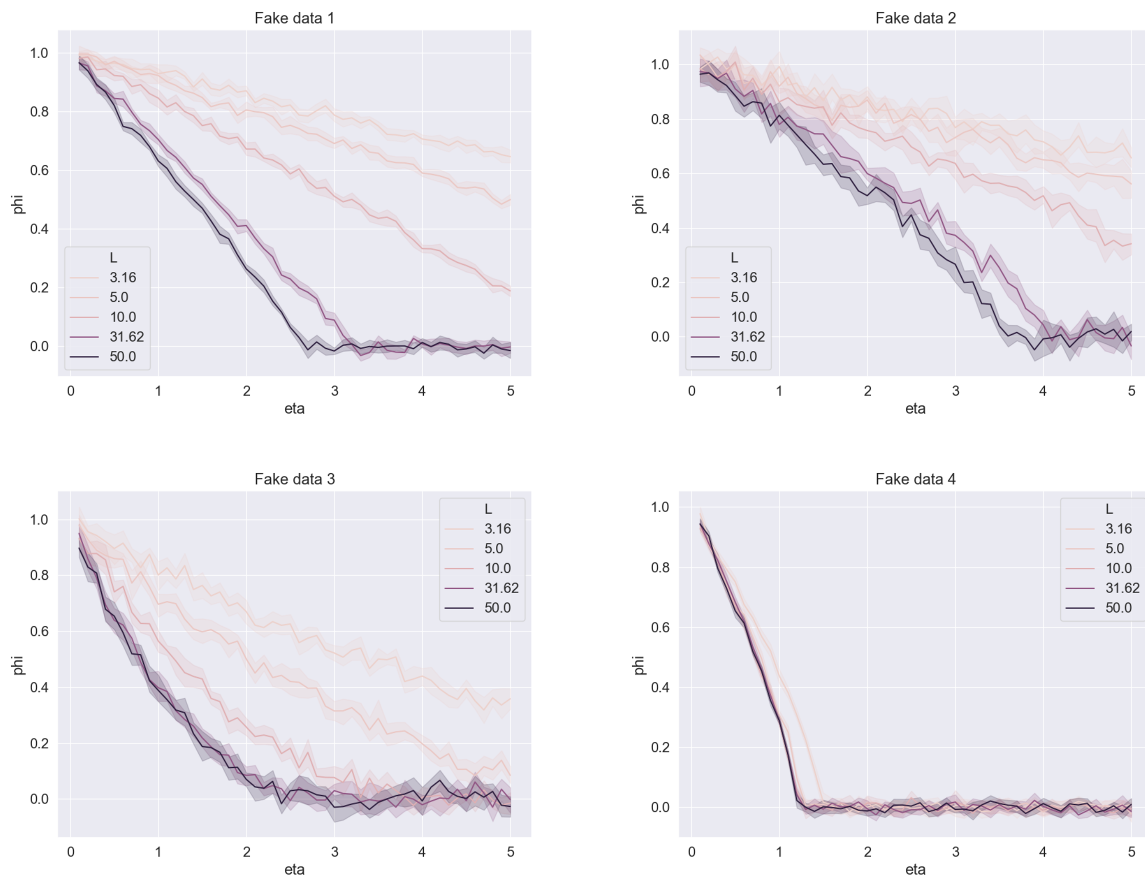

Figure 6. Visualization of fake datasets generated from the chosen priors.

Inspired by one of the videos we watched for a class preparation, I sampled from the priors and generated a few sets of fake data to test whether the model and the prior choices are reasonable. Indeed, all the fake datasets in Figure 6 look like plausible phase transitions that could occur in some physical systems.

3 Inference and Prediction

Running the model with PyStan, I obtained the following statistics:

	mean	sd	n_{eff}	$\hat{R}$
k	4.26	0.2	212	1.03
$\eta_c(\infty)$	1.87	0.26	194	1.03
β	0.61	4.3e-3	539	1.01
ν	4.16	0.48	194	1.03
σ	0.06	9.4e-4	1226	1.0

The values of $\hat{R}$ are in a reasonable range. The effective sample size n_{eff}, though not ideal (the lowest around 200), is roughly acceptable.

In Figure 7, we see that each parameter is unimodally distributed. Some pairs are strongly correlated, which are justified. For example, since the likelihood function contains the sum $\eta_c(\infty) + kL^{-1/\nu}$, it is reasonable to expect $\eta_c(\infty)$ and k to be negatively correlated to compensate each other.

To visualize the parameters we inferred, I plotted the data and the curves reconstructed from posterior samples together in Figure 8. The brown curve ($L = \infty$) on the left is the inferred phase transition behavior in the theoretical thermodynamic limit. Note that confidence intervals *were* plotted[3] for the solid curves as well, and we cannot see them because they are very small.

Although the inferred curves scale in a similar manner as the actual data with increasing L, they do not completely capture the change in curvature in the observed data. The inferred curves tend to be sharp around the critical point (where order parameter drops to zero) whereas in the actual data it is smoothed out. It is well established that theoretical phase transition in infinite size systems has sharp *singularities* around critical points and smoothing effects occur in finite size systems. Therefore this discrepancy between inferred curves and actual data is likely due to the fact that Eq. (1) and (2) do not account for the smoothing effects.

In Figure 9, I generated some predictions. For each L, I took three random posterior samples, and plotted a predicted observation for each of them. I selected two plots to include here

[3] I took each sample (out of 4000) from Stan, calculated ϕ for each pair of L and η using parameters in the posterior sample. Thus each point on the solid curve is made from 4000 samples. However, since the standard deviation is very low, the confidence interval cannot be seen.

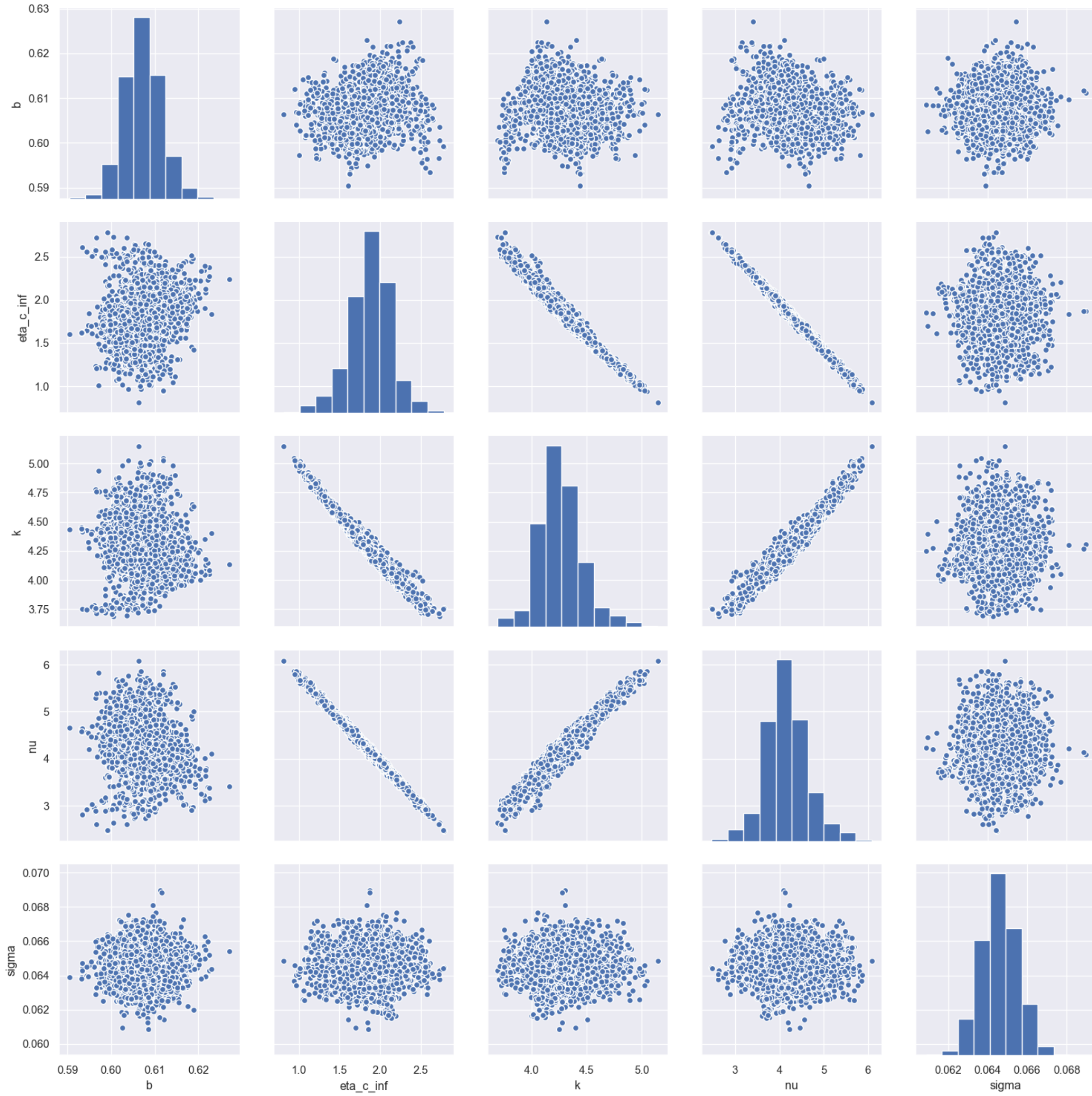

Figure 7. Pairwise distribution plots of posterior samples.

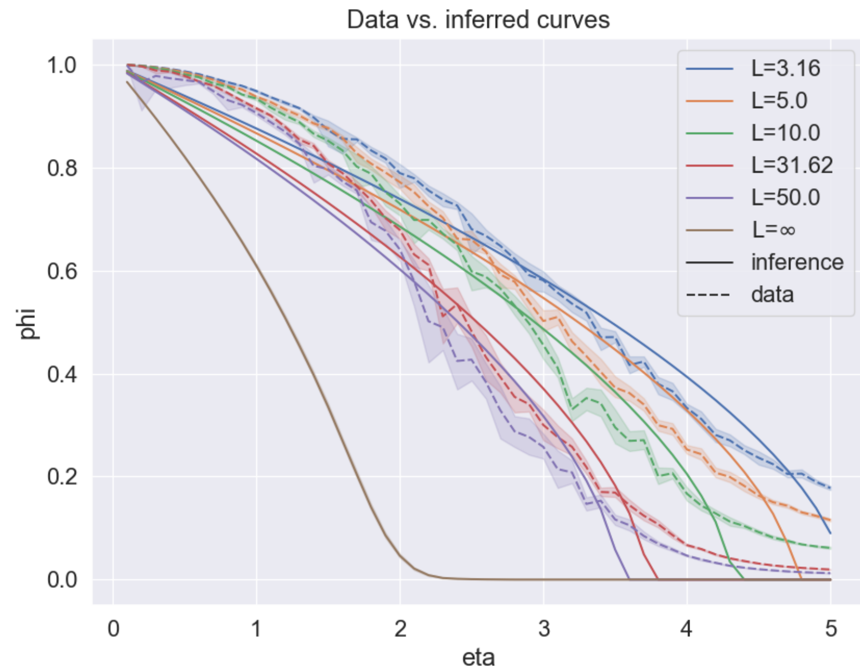

Figure 8. Data and reconstructed curves from inferred parameters.

and the rest (for other values of L) can be found in the Jupyter Notebook. We can see that in the prediction curves, the error margins are slightly larger than the actual data. This might be due to (a) the model overestimated σ to compensate for the poor fit in curvature (b) though my model assumed constant σ across different values of L and η, this might not be true as we can see that the errors in real data tend to be larger in the middle (during the phase transition) than at extreme values of η. They might also be greater for systems of larger size L, which can be harder to converge.

It is also important to recognize that although the predictions contain negative values of ϕ (especially with $L = 50$ and η between 4 and 5), in reality, the order parameter cannot be negative. This reveals a limitation of the model, that it assumes $\phi \sim \mathcal{N}(0, \sigma)$ during the disordered phase (i.e., when $\eta > \eta_c$), which leads to some negative ϕ values.

To summarize, the model performed well in characterizing the scaling behavior of $\eta_c(L)$ as L increases. It does not capture the smoothing effect of the actual data around critical points of phase transition. The mean of the inferred parameter β is 0.61, which deviates from those in the

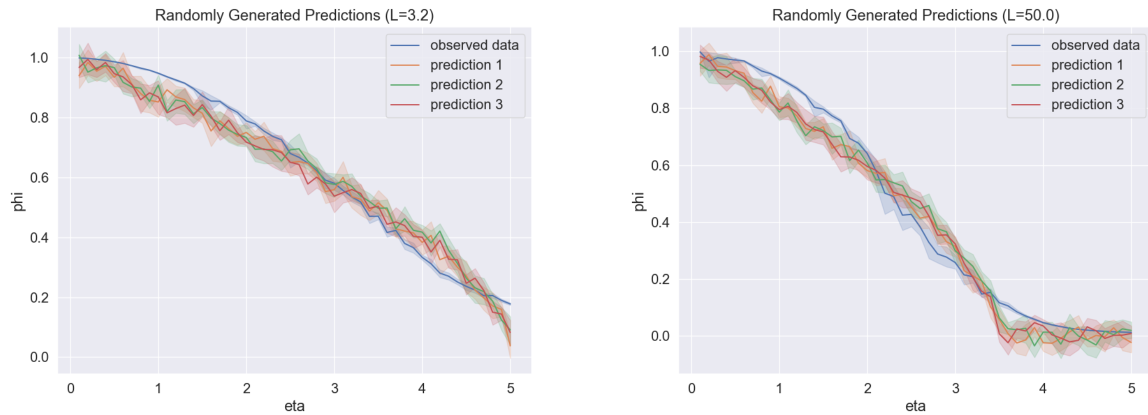

Figure 9. Three predictions for each $L \in \{3.2, 50.0\}$

literature (between 0.42 and 0.45), but is still qualitatively reasonable–for example, it is smaller than 1, meaning that it captures the correct concavity of the phase transition curves. To further improve the model, one needs to (a) address the question of how to characterize the smoothing effects in finite size phase transitions (b) obtain better data, especially from simulations of larger L and perhaps for longer run time to make sure the systems converge.

References

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Appendix

Formal Description of the Vicsek Model

Consider n particles moving in a two-dimensional square arena of linear size L with periodic boundary conditions. The position of a particle at time $t+1$ is updated by

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} + \mathbf{v}^{(t+1)}\Delta t \tag{3}$$

where we set $\Delta t = 1$, and $\mathbf{v}^{(t+1)}$ is the particle's velocity at time $t+1$, which is given by

$$\mathbf{v}^{(t+1)} = v_0(\cos\theta^{(t+1)}, \sin\theta^{(t+1)}) \tag{4}$$

Here v_0 is the magnitude of the velocity, which is constant among all particles across time. The direction of the velocity, θ, is given by

$$\theta^{(t+1)} = \arg\left\{\sum_{k\in\mathcal{S}^{(t)}} \mathbf{v}_k^{(t)}\right\} + \delta\theta \tag{5}$$

where $\mathcal{S}^{(t)}$ represents the set of particles, at time t, lie in the neighborhood with a radius of r_0. The term $\sum_{k\in\mathcal{S}^{(t)}} \mathbf{v}_k^{(t)}$ represents the average (vector) velocity of neighboring particles. The term $\delta\theta$ represents a (usually small) random angular noise added to $\theta^{(t+1)}$ and is an uncorrelated random process drawn from $U[-\frac{\eta}{2}, \frac{\eta}{2}]$.