Neural network topological snake models for locating general phase diagrams

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Machine learning for locating phase diagram has received intensive research interest in recent years. However, its application in automatically locating phase diagram is limited to single closed phase boundary. In this paper, in order to locate phase diagrams with multiple phases and complex boundaries, we introduce (i) a network-shaped and topologically fixed snake model and (ii) a topologically transformable snake model, both driven by discriminative cooperative networks. The phase diagrams of quantum and classical spin-1 model are obtained. Our method is flexible to determine the phase diagram with just snapshots of configurations from the cold-atom or other experiments.

Introduction.— In recent years, machine learning has been providing new ideas and method in various fields of physics due to its powerful fitting, expressive and predictive capabilities, etc [1]. In particular, physicists are beginning to use the latest machine learning tools to study a long-standing task in physics, namely the study of phases and phase diagrams of matter [2]. In the early stage, a large number of lattice classical spin models [3–8], and topological quantum systems [9, 10], which achieve proof of concept by using supervised machine learning, although the method requires prior knowledge of the problem.

At the same time, unsupervised machine learning, such as, principal component analysis [11–13], t-distributed stochastic neighbor embedding [2], diffusion map [14–17] are also applied to the study of phase transitions. Their characteristics can be obtained by various artificially defined quantities, such as the Carinski-Harabaz index [18] for topological or ordered-disordered phase transitions. More developments in this direction can be found in review article [1].

An unsupervised method, the confusion method was proposed in 2017 [19], to determine the true phase transition point by successively guessing it while measuring the performance curve of the neural network, and then determine the true critical point based on the peak position of “W”-shape of the performance curve. This confusion method has been applied to classical and quantum phase transitions [19–21]. It has also been applied to determine phase diagrams from the cold-atom experimental data [22].

By resorting to the snake model, also known as the active contour model developed by Kass [23], Liu et al. propose a discriminate cooperative networks (DCN) for detecting phase transition in the two-dimensional parameter space while avoiding the very time-consuming and violent search for parameters [24]. This work has only one snake, which can only bracket one target phase surrounded by another phase.

Actually, physicists wish to explore more general and complex phase diagrams, in an unsupervised manner, to determine the boundaries between the phases of superfluid, insulator, superconductivity, spin liquid, topological phases, supersolid and so on [25, 26]. In this paper, with the help of the tools in computer vision field, we introduce two types of snake models based on the neural network, (i) network-shaped snake model, which is topology-preserved. (ii) a topologically transformable snake.

First of all, inspired by the topology-preserving networks developed by M. Buten for image segmentation [27], we propose to combine network-shaped snakes and neural networks to determine phase diagrams with multiple phases by inputting the configurations of lattice models. The network snake is a generalization of a simple snake, which has multiple subsnakes connected by nodes, and each subsnake is similar to a simple snake in that it has many vertexes. In our neural-network based network snake model, the sub-snakes of the network snake converge to the real phase transition boundaries and the nodes converge to the intersection of several different phases. Secondly, beyond topological preserved models, we also introduce topological transformations [28], i.e., topological (T) snake, and combine it with the neural network. The T-snake inherits the characteristics of the simple snake, but the topological transformation occurs during the evolution when some condition is satisfied. After topological transformations, such as splitting, the subsnakes eventually converge to the true phase transition boundaries.

With the topological preserved and topological flexibility with neural network, the phase diagram of physical systems are obtained. The first example is the Blume-Capel (BC) model of nearest-neighbor interactions on a square lattice [29], which has three very typical phases, the ferromagnetic phase, the subferromagnetic phase and the disordered phase. Our network-snake model is just good enough to give the boundary between these three phases. Another application is to determine the Halden phase of the quantum spin-1.
In above equation, the derivative and the fourth derivative of $C$ contains the Euler-Lagrange equations containing the second and forth terms and $E_{int}$, which only depends on the parameters $\varepsilon s$ and Eq. (6) can be simplified as

$$\beta_n(C^A_{n-1} - C^A_{n}) - \beta_n(C^A_{n-1} - C^A_{n-2}) + F_C^A(C^A) = 0,$$

$$\beta_n(C^B_{n-1} - C^B_{n}) - \beta_n(C^B_{n-1} - C^B_{n-2}) + F_C^B(C^B) = 0,$$

$$\beta_n(C^C_{n-1} - C^C_{n}) - \beta_n(C^C_{n-1} - C^C_{n-2}) + F_C^C(C^C) = 0,$$

where $\beta_n$ is another parameter to be controlled and $F_C$ is the external force as in Eq. (6).

In Fig. 2, we use the network-shaped snake model without DCN to test an image, which has three color blocks (black, gray, and white) and a total of three boundaries between them. In Fig. 2(a), network-shaped snakes are initialized to deviate from the true boundaries. The image gradient forces on each node are also

\[ F_{\text{img}} = \alpha(s) |C'(s)|^2 + \beta(s) |C''(s)|^2. \]  

(3)

In equation, $C''(s)$ and $C''''(s)$ are the second derivative and the forth derivative of $C(s)$ with respect to $s$. The parameters $\alpha(s)$ and $\beta(s)$ are adjustable and control the continuity and smooth of the curve.

In order to get the best position of the snake, we need the minimum value for the total energy. One can assume some trial contour $C_{\text{trial}}(s) = C(s) + \delta(s)$ which differs from the true contour by $\varepsilon \delta(s)$, where $\varepsilon$ is a small quantity and $\delta(s)$ is an arbitrary function, and then solve the equation $dE(\varepsilon, C, C', C'')/d\varepsilon = 0$. Eventually, one obtains the Euler-Lagrange equations containing the second order derivatives

$$\frac{\partial E}{\partial C} - \frac{d}{ds} \left( \frac{\partial E}{\partial C'} \right) + \frac{d^2}{ds^2} \left( \frac{\partial E}{\partial C''} \right) = 0 \]  

(4)

where $C, C', C''$ are considered as independent parameters and Eq. (4) can be simplified as

$$\frac{\partial E_{\text{img}}}{\partial C} - \alpha C'' + \beta C'''' = 0. \]  

(5)

In the language of mechanics, the motion of the nodes $C_i$ on the snake is driven by both external $F_i^{\text{ext}}$ and internal force $F_i^{\text{int}}$, where $F_i^{\text{int}} = -\alpha C'' + \beta C''''$, and $F_i^{\text{ext}} = \delta E_{\text{img}}/\partial C_i$. When the sum of the two forces is zero, namely, and the balance between them leads to the following equation as a matrix

$$AC + F^{\text{ext}}(C) = 0, \]  

(6)

where $A$ is a pentagonal banded matrix (see the appendix), which only depends on the parameters $\alpha$ and $\beta$. The solution can be obtained as [23, 27]

\[ C_i = (A + \gamma I)^{-1} [\gamma C(t-1) + \kappa F^{\text{ext}}(C(t-1))]. \]  

(7)

where $I$ is the identity matrix and $\kappa$ is an additional parameter in order to control the weight between internal and image energy and $t$ is the iteration time, $\gamma$ is coefficient of damping forces.

Network-shaped snakes without DCN.— The early snake models were closed contours or semi-closed contours, but they were usually set one by one in the image. The biggest difficulty is that the topological shape is restricted. To overcome the limitation of topology, as shown in Fig. 1, the network snake has been designed as several sub-snakes connected by a common node labeled as $C_n^A, C_n^B, or C_n^C$ with $\rho(C) = 3$ in red. Each sub-snake also vertexes with $\rho(C) = 1, 2$ in purple, blue colors, the updating of the sub-snakes obeys Eq. (7). The difficulty is how to control the movement of the common node (red symbol) during the energy minimization process. The derivatives approximated by finite differences are not defined for nodes with a degree $\rho(C) > 2$, because the required neighboring nodes are either not available or exist multiple times [27]. The position of the common node needs to be solved iteratively using the equations below,

$$\beta_n(C^A_{n-1} - C^A_n) = \beta_n(C^A_{n-1} - C^A_{n-2}) + F_C^A(C^A) = 0,$$

$$\beta_n(C^B_{n-1} - C^B_n) = \beta_n(C^B_{n-1} - C^B_{n-2}) + F_C^B(C^B) = 0,$$

$$\beta_n(C^C_{n-1} - C^C_n) = \beta_n(C^C_{n-1} - C^C_{n-2}) + F_C^C(C^C) = 0,$$

where $\beta_n$ is another parameter to be controlled and $F_C$ is the external force as in Eq. (6).
given by the arrows. After many times of the evolutions, sub-snakes closest to the real boundary are displayed in Fig. 2(b). The lengths of the arrows are relatively short. In Fig. 2(c), at each step of the iteration, the internal energies of the three snakes are also measured. In the first 20,000 iterations, the internal energies of 2 snakes are decreasing more slowly and the other one is increasing slowly. Suddenly, around 21607 iterations, the increasing or decreasing trend becomes dramatic. This exact number of iteration steps is determined by taking the derivative of the internal energy of the three snakes, and the number of steps versus the derivative are shown in Fig. 2(d).

**Network-shaped snakes with DCN**— Here we focus on the basic formula of the network-shaped snake model with DCN, and other details can be found in Ref. [24]. As shown in Fig. 3 (a), the network is divided into a guessing network $G$ and a learning network $N$. The $G$ absorbs the guessed phase boundary parameter $\lambda$, labeled by the positions of the yellow triangles, around the parameter $\lambda_g$ labeled by the blue nodes. The $G$ outputs two neurons through the sigmoid function to determine the probabilities that the system belongs to the phase $A$ or $B$, defined as

$$G_{A,B}(\lambda) = \text{sigmoid}[s_{A,B}(\lambda - \lambda_g)/\sigma],$$

(9)

where $s_{A,B} = -, +, +$. The network $N$ is a fully-connected network that absorbs the configurations/wave functions $d(\lambda)$ of the models and output their classifications.

The cost function between $N$ and $G$ is defined as

$$C(N, G) = -\log N G - \log(1 - N)(1 - G).$$

(10)

The dynamics of both networks can be defined as

$$\Delta \lambda_g = -\alpha_{\lambda} \partial C / \partial \lambda_g, \quad \Delta \sigma = -\alpha_{\sigma} \partial C / \partial \sigma$$

and

$$\Delta W_{ij} = -\alpha_{W} \partial C / \partial W_{ij},$$

where $\alpha_{\lambda}, \alpha_{\sigma}$ and $\alpha_{W}$ are the learning rates [24].

To construct the network-shaped snake with DCN, we build three simple snakes, and each one has its own DCN. It is important to note that they have a common vertex, i.e., the node, whose position needs to be solved sequentially according to Eq. (8). During the iterative process, the snakes may overtake or deviate from the best position. However, we can finally determine the best positions by comparing the loss function of the three snakes throughout the iterations.

**Blume-Capel model.**— To test our algorithm, we choose the most commonly used in statistical mechanics, the BC model, whose spins $S_i$ only takes three values 0 and $\pm 1$. Its Hamiltonian on the square lattice is defined as

$$H = -J_x \sum_{\langle i,j \rangle_x} S_i S_j - J_y \sum_{\langle i,j \rangle_y} S_i S_j + D \sum_i S_i^2 - h \sum_i S_i,$$

(11)

where $\langle i,j \rangle$ represents summation over only the nearest neighboring pair of spins along two directions and the exchange interactions between sites denote as $J_x$ and $J_y$. The cost function between $N$ and $G$ is defined as

$$C(N, G) = -\log N G - \log(1 - N)(1 - G).$$

(10)
$J_y$ respectively. $D$ is a single-spin anisotropy parameter and $h$ is an external magnetic field.

The phase diagram of the BC model is very rich. Here we focus on three typical phases, the ferromagnetic, superantiferromagnetic and paramagnetic phases. Their configurations in a 4-site cell are $++-00$, $++'-++'-00$ respectively. The input to the neural network is the average of the configurations under each parameter. In Fig. 3 (c), the thin lines indicate the initialized snake and the red line indicates selected snake, consistent with the phase boundary. In Fig. 3 (d), the loss functions are shown. When the number of iteration steps is 65, the values of the three loss functions are smaller.

**Topological snakes and the spin-1 chain.**— Simple snakes [24] have to change the topological features when they encounter a phase diagram with two target phases whose boundaries need to be determined. Here, we are first apply the T-snake model [28] to solve such problem.

This method introduces an affine cell decomposition in medical images [28, 31]. We first divide the phase diagram into a number of triangular cells and record the intersection of the initial (updated) snakes and these cells. As soon as the intersection meets certain conditions, then the snake splits.

Figure 4(a) shows a snake that meets the splitting conditions. In the area marked in black, the two curved segments of the snake are very close together. Eventually, the snake splits from one close contour to two closed contours as shown in Fig. 4(b). Figure 4(c) shows the zoomed-in shape of the shaded area before the split, with the six intersections marked. In Fig. 4(d), the condition is illustrated. Once the intersection 2 and 5 meet in a side of a triangular cell, then 1 and 4 are linked, and similarly, 3 and 6 are connected.

Spin-1 antiferromagnetic Heisenberg chain is choosen as an example [30], whose Hamiltons is

$$H = J \sum_i S_i S_{i+1} + \sum_i \left[ D (S_i^z)^2 - B S_i^z \right], \tag{12}$$

where $B$ and $D$ are the magnetic field and anisotropy parameter. The phase diagram of this model contains a Haldane phase in the plane $B$ versus $D$ [24].

In order to illustrate how to detect of two closed phase boundaries with a single snake, we artificially flip the original phase diagram along the axis $D/J = 0.6$ and keeping the old one as shown in Fig. 5. The two blue areas, i.e., Haldane phases, are the separated target phases.

In Fig. 5, we firstly initialize a snake marked by the red dots, which is an oval shape and almost encloses the target phases. Then the snake updates according to the dynamics of both networks $\mathcal{N}$ and $\mathcal{G}$. During evolution, the snake began to become thinner, as in the segments near sites 38, 27, and 16 marked by red numbers in black circles. Eventually, the snake’s intersections around the red numbers 18 satisfy the split condition. One snake topologically transforms into two new ones. Then, the new snakes are evolved to stay at the Haldane phase boundary respectively, marked with white lines and circles.

Furthermore, some detailed parameters are given. The number of nodes for the initial snake is fixed to be 50, and then the number of nodes is modified to 30 for each new snake. The three basic parameters of the initial snake model are tuned to $\alpha = 0.02$, $\beta = 0.02$, and $\gamma = 0.25$ and $\beta$ increases to 0.4 after splitting. The network $\mathcal{N}$ consists of 80 input neurons, 80 hidden neurons, and 2 output neurons.

**Conclusion.**— In summary, to locate more general phase diagrams, we introduce two snake models with fixed topology and flexible topology. In addition to the internal force of the snake, the driving external force of the snake is the cross entropy of the discriminative cooperative network instead of the conventional image force. For the topologically flexible snake model, after splitting, each subsnake evolves completely independently and finally converges to the phase boundaries. For a topologically fixed snake, each snake is always fighting with each other to reach the best position during the up-
dating. We finally select the appropriate boundaries by the loss function.

In the field of machine vision, this method can segment the contours of very complex targets, including roads, cells, etc [27]. In physics, our approach is very promising to further promote the application of machine learning in determine phase diagrams of the experimental cold-atom systems [22]. This method may be able to determine to other interesting phase diagrams, such as those of water, CO$_2$ [32, 33] under different values of pressure and temperature, even the phase diagram from high-energy physics [34], which need to be further tested later.

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Appendix: solution of the matrix

In Eq. (7), the pentadiagonal banded matrix $A$ is defined as

$$A = \begin{bmatrix} a_0 & b_0 & a_1 & \cdots & a_{N-2} & b_{N-1} \\ b_0 & c_1 & b_1 & a_1 & \cdots & a_{N-3} & b_{N-2} \\ a_1 & b_2 & c_2 & b_2 & a_2 & \cdots & a_{N-4} & b_{N-3} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\ a_{N-2} & b_{N-4} & c_{N-3} & b_{N-4} & a_{N-3} & \cdots & a_2 & b_1 \\ b_{N-1} & a_{N-1} & b_{N-2} & c_{N-2} & b_{N-2} & a_{N-2} & \cdots & a_1 \\ b_{N-1} & a_{N-1} & b_{N-2} & c_{N-2} & b_{N-2} & a_{N-2} & \cdots & a_1 \end{bmatrix},$$

where the values of $a_i$, $b_i$, $c_i$ are as follows

$$a_i = \beta, b_i = -4\beta - \alpha, c_i = 6\beta + 2\alpha. \quad (14)$$

Eq. (13) defines the $A$-matrix for a periodic boundary or a ring snake. If the snake has an open boundary fixed at both ends, the matrix $A$ has to be modified. In addition, the common node $C_n$ of the three snakes in this paper needs to modify $A$ according to Eq. (8).

The solution Eq. (7) is obtained in the following way.

Similar to Newton’s second law, we assume that the contour $C(s, t)$ satisfies the following equation

$$\mu \frac{\partial^2 C(s, t)}{\partial t^2} = F_{\text{dum}}(C(s, t)) + F_{\text{int}}(C(s, t)) + F_{\text{ext}}(C(s, t)),$$

where $F_{\text{dum}}(C(s, t))$ is a damping force, $\mu$ is an inertia mass. The time $t$ is introduced so that this static problem becomes a dynamic equation. The inertia term on the left side is omitted as the acceleration would put the contour to exceed the real boundary. Therefore one gets

$$-F_{\text{dum}} = \gamma \frac{\partial C(s, t)}{\partial t} = F_{\text{int}}(C(s, t)) + F_{\text{ext}}(C(s, t)). \quad (16)$$

Let $\Delta t = 1$, the discrete active contour of dynamics obeys

$$\gamma[C(t) - C(t - 1)] = -AC(t) + \kappa F_{\text{ext}}(C(t - 1)). \quad (17)$$

Then the following solution is obtained,

$$C_t = (A + \gamma I)^{-1}\gamma[C(t) - C(t - 1) + \kappa F_{\text{ext}}(C(t - 1))], \quad (18)$$

where $I$ is the identity matrix and $\kappa$ is an additional parameter in order to control the weight between internal and image energy.