Extracting Critical Exponent by Finite-Size Scaling with Convolutional Neural Networks

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Machine learning has been successfully applied to identify phases and phase transitions in condensed matter systems. However, quantitative characterization of the critical fluctuations near phase transitions is lacking. In this study we extract the critical behavior of a quantum Hall plateau transition with a convolutional neural network. We introduce a finite-size scaling approach and show that the localization length critical exponent learned by the neural network is consistent with the value obtained by conventional approaches. We illustrate the physics behind the approach by a cross-examination of the inverse participation ratios.

Introduction.− Recent studies have established machine learning as an effective tool to identify phases and phase transitions. The prototypical two-dimensional Ising model has been studied, e.g., by the restricted Boltzmann machine (RBM) [1][3], the feed-forward sigmoid neural network [2], the convolutional neural network (CNN) [4][5], the principal component analysis [6], and the supporting vector machine [7]. Machine learning methods have also been applied to study the Potts model [8], the Ashkin-Teller model [9], the transverse-field Ising model [10][11], the Kitaev toric codes [12][17], the Hubbard model [12][15], and disordered electron systems [18][20] among others. The wide success in the identification of phases and the location of the phase transitions is possibly rooted in ideas like renormalization group [21][23]. Connections of neural network states and tensor network states have also been explored [24][27].

One of the advantages of machine learning is that one can provide raw low-level data, such as spin configurations, energy spectrum, or wave functions, so that only elementary knowledge in physics is required. With sufficiently large data sets, higher-level features can be recognized by various deep learning architectures [28] and then be used to distinguish phases. Nevertheless, quantitative understanding of the critical behavior and, hence, the identification of universality classes have been missing in the past studies.

To explore the critical behavior of the Anderson transition in disordered electronic systems, e.g., one can calculate different conventional quantities, such as the Lyapunov exponent [29], the inverse participation ratio (IPR) [30], the Thouless number [31], and the Chern number [32]. Most of these physical quantities cannot easily be cast into a neural network representation with low-level inputs like eigenenergies or eigenstates. The exception is the IPR, which measures the occupation of a wave function in real space. Fig. 1(a) illustrated that the IPR of a normalized eigenstate |ψ⟩ = ∑ₖ cₖ|k⟩, defined as

$$\text{IPR} = \sum_i |c_i|^4,$$

(1)

can be mapped to a single artificial neuron with the square of the local electron density |c_i|^4 as input. The weights for the inputs are all unity and a step-function activation can be used to semi-quantitatively distinguish the conducting states from the localized states. One expects that for a d-dimensional lattice with linear size L, the IPR of a conducting state tends to $L^{-d}$, while that of a localized state is a finite constant.

At the Anderson transition, there are strong fluctuations in the local density of states. The simple concept of the IPR can be generalized to the whole multifractality spectrum at the critical point to characterize infinitely many relevant operators [33][35]. Such a generalization developed by insightful physicists is not expected to be learned by a machine simply from large-scale data sets. But with cleverly designed algorithms, can machine display intelligence in the study of critical exponent?

In this Letter, we combine the conventional wisdom and the novel machine learning techniques to study the critical behavior of the quantum Hall plateau transition in a two-dimensional disordered electron system. The approach can be thought of as a generalization of the IPR study based on a CNN architecture. The learning is guided by a trial-and-error labelling scheme, which detects the cutoff in the length scale by finite system size. A localization length critical exponent $\nu = 2.22 \pm 0.04$ can be extracted from the finite-size scaling of the characteristic energy scale where the localization length is comparable to the system size. A comparison of the IPR results and the CNN study provides insights on how machine detects the critical fluctuations and identifies the relevant scales.

Model and Method.− We consider the disordered Hofstadter model on a square lattice with Hamiltonian

$$H_0 = -\sum_{\langle i,j \rangle} \{ e^{i\theta_{ij}} c_i^\dagger c_j + h.c. \} + \sum_i \epsilon_i c_i^\dagger c_i,$$

(2)

where the quantized flux per plaquette is 1/3. We project the on-site disorder to the lowest of the three magnetic subbands and suppress the kinetic energy such that the corresponding pure system is a Chern insulator with Chern number 1 and a perfectly flat band. The on-site random potential $\epsilon_i$ is distributed uniformly in [-0.5, 0.5]. In this model, extended states only exist at the band center $E_c = 0$. When the Fermi energy sweeps across the band center, the system exhibits a localization-delocalization-localization transition. The detail of the model and its critical behavior obtained by Thouless number calculation are available in Ref. [50]. For each system

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of the characteristic width of the density of the conducting states \([22]\). Without such Chern number or conductance calculation, we do not \textit{a priori} know which states are localized and which states are conducting. In fact, this is the loophole in the CNN training described above. To pursue a supervised learning, we need to label the states; this requires the knowledge of the conducting or the localized nature of the wave functions. However, explicitly acquiring such information by conventional approaches and supplying it to the CNN would defy the necessity of machine learning in the first place. To circumvent the difficulty, we introduce a trial-and-error method to identify the characteristic width for conducting states. We label the eigenstates within \(-E_m < E < E_m\) as conducting states, as illustrated in Fig. \(1\)\(b\), and vary \(E_m\) to study the CNN performance, according to the postulated idea sketched in Fig. \(1\)\(c\). In the vicinity of the critical energy \(E_c\), the localization length \(\xi\) diverges with critical exponent \(\nu\). The finite system size \(L\) provides a cutoff to the length scale. Close to \(E_c\), when \(\xi\) is greater than \(L\), the eigenstates are conducting. Otherwise, they are localized. We will show that the resulting performance curve can be used to extract the characteristic energy scale and hence \(\nu\).

\textbf{Results.} We start with a 12 \times 12 lattice and diagonalize the system with different disorder realizations and randomly select 35,000 wave functions for training. We then feed the square of the local electron density to the CNN and obtained the optimal CNN parameters. The performance of the CNN \(P(E_m)\), as we vary \(E_m\), is obtained by testing an independent set of 35,000 wave functions. Figure \(2\) plots \(P(E_m)\) as a function of \(E_m\), which has an asymmetric V-shape. We select four \(E_m\) and plot the corresponding density of conducting states, according to the CNN predictions. For small \(E_m\), \(P(E_m)\) decreases linearly and, correspondingly, the CNN cannot predict better than assuming all states are localized. When \(E_m\) is large enough, \(P(E_m)\) bends up. The CNN is no longer blind and starts to realize that the predictions can be more accurate if some states near the origin are recognized as conducting, as the labels suggest. With further growing \(E_m\), the CNN finds more and more conducting states and for \(E_m > 0.5\), it identifies almost all states as conducting.

The general trend of the increasing number of conducting states as \(E_m\) increases is reasonable. But to understand what determines \(P(E_m)\) and why it has a V-shape, we need to understand the fluctuations of the features recognized by neural networks. The precise features that are extracted by the CNN are numerous and difficult to describe, but it suffices to analyze the fluctuations of the IPR, which has an artificial neuron representation. Figure \(3\)\(a\) plots the mean value of IPR with its standard deviation as function of \(E\). IPR\((E)\) saturates at small \(E\), where \(\xi\) is greater than \(L\), and increases with \(E\), as the wave function becomes more and more localized. The insets show typical distributions of the IPRs at the center, in one tail, and in between. While they are suppressed in the tail by the decreasing \(\xi\) due to localization, the fluctuations of the IPRs increase toward the critical energy at the center until the...
finite-size cutoff starts to interfere. The fluctuating features extracted by the CNN necessarily lead to a confusion, or an imperfection $P(E_m) < 1$, in the classification. As illustrated in Fig. 3(b), we divide the conducting and localized states in the labels by $E_m$, while the machine classifies the states by the values of the features. If we assume that some feature $F$ is fluctuating in the colored region, the two red areas contain the states that are labelled as conducting but classified as localized, or vice versa. A cross-examination of the machine-learning results and the IPRs supports the interpretation. Figure 3(c) plots IPR($E$) as a function of $E$ with the following coloring scheme: The states with more than 80% probability of being conducting (localized) are represented by green dots (purple diamonds); the rest by red triangles are states with less certain classifications. The probabilities are given by the logistic output of the CNN with $E_m = 0.205$, represented by the vertical line in Fig. 3(c). We also include a horizontal line IPR = 0.027 (for illustrative purpose only) to further separate the plot area into four regions. The green (purple) points, for which the CNN-recognized features largely agree to the labels, are distributed mainly in the lower left (upper right) regions. The red points, for which fluctuations lead to confusion between the features and the labels, appear in all four regions in similar numbers. In agreement with Fig. 3(b), they dominate in the upper left and lower right regions, but are outnumbered in the other two regions. We emphasize that the IPR is not the feature that is recognized by the CNN, but we believe that it is generic enough to exemplify the fluctuations in the features that are recognized.

The trial-and-error labelling scheme we apply resembles the confusion scheme in Ref. [2]. However, there is a significant difference. The confusion scheme was introduced to study the location of a phase transition, which we know exactly in the present model. Instead, there is essentially only one phase, i.e. the localized phase (extended states exist only at $E = 0$), and the labelling scheme is introduced to detect the size cutoff in a finite system. So we observe the V-shape performance curve, not the W-shape curve in Ref. [2]. As $E_m$ increase, $P(E_m)$ first decreases because of the increasing inconsistent labels. For sufficiently large $E_m$, $P(E_m)$ increases as fluctuations diminish in the band tail. In fact, the physics learned is incorrect in the latter case: the CNN mistakenly identifies most localized states as conducting ones. In other words, high performance is, by no means, connecting to the recognition of the correct physics. The effectiveness of the present approach is expected to be insensitive to the detail of the CNN architecture, because the scaling behavior depends on where the finite size starts to influence, not how good the performance is. Nevertheless, observing the worst performance at the valley of the curve being significantly larger than 50% is an assuring evidence that the CNN is extracting non-trivial features.

Figure 4 plots $P(E_m)$ as a function of $E_m$ for $L = 9, 12, 15, 18, 21, \text{ and } 24$. The minimum of the asymmetric V-shape curves $P(E_m^{\text{min}})$ increases as $L$ increases, while the corresponding $E_m^{\text{min}}$ approaches 0. Interestingly, $P(E_m^{\text{min}})$ can be fit to a straight line that extrapolates to 100% accuracy at $E_m = 0$. This is consistent with the fact that in the
small system sizes, \( \nu \) is also in different models, it is more plausible to accept that for up to \( L = 72 \) [40]. While one may argue against the universality of the critical exponent in different models, it is more plausible to accept that for small system sizes, \( \nu = 2.35 \pm 0.03 \) [34, 35, 41] is universally observed in various models of the quantum Hall plateau transition. The exponent we obtained in the current study is, therefore, consistent with the early numerical studies within the similar size range.

Compared to the conventional approaches, the CNN study only requires the general knowledge of phase transitions and critical behavior, not that of the specific physics quantities such as the Thouless number and the Chern number, both related to electronic conductance. In fact, we do not and cannot describe what specific features the CNN extracted, even though in many ways we can think them as the generalizations of the IPR. In this sense, the machine displays intelligence, at least with human guidance. Such an approach certainly saves our efforts on understanding the model and the related physics in the beginning, but it comes with a cost. The CNN study is more numerically intensive than the conventional approaches, including the Chern number calculation, for the same system size. This is consistent with the necessary ingredients behind the rise of deep learning: capable hardware and large-scale data sets. Limited by our computational resources, the purpose of the present study is to demonstrate the practicability of extracting critical exponents with machine learning, not to push it to larger systems for higher precision.

**Conclusion.**—We feed the local density of the wave functions of a disordered lattice model for the quantum Hall plateau transition to a deep CNN. With trial-and-error labelling for the conducting properties of the states, the network can learn to classify the states with high but not perfect accuracy. The imperfect classification is closely related to the critical fluctuations, which can be suppressed by the finite system size. This allows us to quantify the range of the critical regime, which can be used to extract the localization length critical exponent to be \( \nu = 2.22 \pm 0.04 \). The combination of the finite-size scaling method and machine learning is expected to be applicable to generic phase transitions.

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**FIG. 4.** (Color online.) The performance curves for systems of size \( L = 9, 12, 15, 18, 21, \) and 24. The minima of the curves can be extrapolated to \( P(E_m) = 1 \) at \( E_m = 0 \) in the thermodynamic limit. The inset shows that the locations of the minima for various \( L \) can be fit by a power law \( E_m^{\min}(L) \sim L^{-1/\nu} \) with exponent \( \nu = 2.22 \pm 0.04 \).

Earlier numerical studies of the lattice model found \( \nu = 2.4 \pm 0.1 \) [36, 37]. However, recent numerical works on the Chalker-Cottington network model found a surprisingly larger \( \nu \approx 2.6 \) [38, 39], after slowly decaying corrections to scaling with increasing system size have been taken into account. The revisit of the lattice model with the Chern number calculation found no evidence of \( \nu > 2.5 \) for up to \( L = 72 \) [40]. While one may argue against the universality of the critical exponent in different models, it is more plausible to accept that for small system sizes, \( \nu = 2.35 \pm 0.03 \) [34, 35, 41] is universally observed in various models of the quantum Hall plateau transition. The exponent we obtained in the current study is, therefore, consistent with the early numerical studies within the similar size range.

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