Machine learning non-Hermitian topological phases

Brajesh Narayan
School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Awadhesh Narayan
Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India

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Non-Hermitian topological phases have gained widespread interest due to their unconventional properties, which have no Hermitian counterparts. In this work, we propose to use machine learning to identify and predict non-Hermitian topological phases, based on their winding number. We consider two examples – non-Hermitian Su-Schrieffer Heeger model in one dimension and non-Hermitian nodal line semimetal in three dimensions – to demonstrate the use of neural networks to accurately characterize the topological phases. We show that for the one dimensional model, a fully connected neural network gives an accuracy greater than 99.9%, and is robust to the introduction of disorder. For the three dimensional model, we find that a convolutional neural network accurately predicts the different topological phases.

Introduction– The Hermitian nature of the Hamiltonian is a central postulate of quantum mechanics [1]. However, the investigation of systems with departure from Hermiticity has a long history [2–8]. Study of such open systems has been widely applied in nuclear reactions, quantum optics, photonics and mesoscopic systems [9].

The interest in non-Hermitian systems has seen a resurgence with a vibrant interaction with the field of topological phases – this has resulted in a rapid flurry of activity on non-Hermitian topological phases [10–16]. These exhibit remarkable properties with no counterparts in Hermitian systems, such as exceptional points [17], non-Hermitian skin effects [18–21] and breakdown of bulk-boundary correspondence [22–26], to name just a few.

In addition to the rapid advancements in the theory of non-Hermitian topological phases, there have been several exciting developments in their experimental study. Photonic crystals [27–29], optical systems [30–31] and topolelectrical circuits [32] have been demonstrated to be versatile platforms to investigate non-Hermitian topological phases.

In recent years, machine learning techniques have been applied, with success, to a number of physical settings [33–35]. In particular, the study of different phases and phase transitions has been actively pursued in the last few years using machine learning methods [35–39]. Excitingly, these techniques have also been employed in identification and characterization of Hermitian topological phases of matter. These topological phases are novel phases of matter, which can not be classified by conventional Landau-Ginzburg symmetry breaking paradigm [40–42]. Neural networks have been successfully used to learn topological invariants [43–45]. Unsupervised machine learning has been demonstrated to be useful for identifying topological phases [46, 47]. Furthermore, real space formulations of the topological invariants have been studied using artificial neural networks [48, 49]. Recently, new insights into machine learning of topological quantum phase transitions have been gained [50].

In this contribution, we introduce machine learning for non-Hermitian topological phases. Using two different examples – non-Hermitian Su-Schrieffer-Heeger model in one dimension and non-Hermitian nodal line semimetal in three dimensions – we demonstrate that machine learning can be used for identifying non-Hermitian topological phases based on their winding number. We discover that for the one dimensional case, a fully connected neural network yields an excellent prediction accuracy of greater than 99.9%. We show that these predictions are robust upon introducing noise to the training data. On the other hand, for the three dimensional example, we find that the overall accuracy for the fully connected network is less than 50%. We demonstrate that use of a convolutional neural network gives an excellent performance for this higher dimensional case, yielding an accuracy exceeding 99.8%.

Su-Schrieffer-Heeger model– We begin our analysis by considering the Su-Schrieffer-Heeger model – the paradigmatic non-Hermitian model exhibiting topological phases [14, 51]. The Hamiltonian reads

\[ H(k) = (t_1 + t_2 \cos k)\sigma_x + (t_2 \sin k + i\gamma/2)\sigma_y, \]

where \( \sigma_i \) (\( i = x, y, z \)) are the Pauli matrices and \( k \) denotes the momentum. Here \( t_1 \) and \( t_2 \) are hopping strengths and a finite \( \gamma \) introduces a non-Hermiticity to the Hamiltonian. The non-Hermitian topological phase of this model is characterized by the winding number, \( W = 1 \), while the trivial phase has \( W = 0 \). The model features several interesting aspects including the non-Hermitian skin effect as well as a breakdown of the bulk-boundary correspondence.

We rewrite our Hamiltonian in the form \( H(k) = \]
h_x(k)σ_x + h_y(k)σ_y and use it as an input for our neural network at P different points. Here h_x = t_1 + t_2 \cos k, h_y = t_2 \sin k + iγ/2 and \( k = 2\pi n/P \) (\( n = 0, ..., P \)). The input data can also be written as \((P + 1) \times 2\) matrices of the form

\[
\begin{pmatrix}
h_x(0) & h_x(2\pi/P) & \cdots & h_x(2\pi) \\
h_y(0) & h_y(2\pi/P) & \cdots & h_y(2\pi)
\end{pmatrix}^T.
\]

The winding number, \( W \), is defined as

\[
W = -(i/2\pi) \int_0^{2\pi} U^*(k) \partial_k U(k) dk,
\]

where \( U(k) = h_x(k) + ih_y(k) \). For discretized data, the above winding number equation can be rewritten as

\[
W = (1/2\pi) \sum_{n=1}^{P} \Delta \Theta(n),
\]

where \( \Delta \Theta(n) = (\Theta(n) - \Theta(n-1)) \mod 2\pi \) and \( \Theta(n) = \arg[U(2\pi n/P)]\).

With this input, we constructed a fully connected, i.e., dense, neural network with two hidden layers. We used 100 neurons in the first hidden layer and 32 neurons for the second hidden layer. Rectified linear unit (ReLU) activation function was used for the hidden layers. To train our neural network we generated a training set with \( 1 \times 10^5 \) samples. For generating the training set, we set \( t_2 = 1, \gamma = 4/3 \) and \( t_1 \) was chosen randomly from the range \([-3,3]\). The network was trained with 2000 batches, with each batch having a size of 50. The training was performed 50 times, i.e., number of epochs is 50. The loss (or cost) with each epoch of training is shown in Fig. 1 (a). We note that the neural network converges rapidly, without any over-fitting.

After having trained the neural network on the training set, we use the network to predict the winding number on a test set which consisted of \( 1 \times 10^4 \) samples not seen by the network during the training. The predicted winding number, \( W_p \), is presented in Fig. 1 (b). We note that our trained neural networks yield winding numbers close to integer values and we also plot the output rounded off to the nearest integer, as is common practice \[44\]. We find that our trained neural networks show a very high accuracy of more than 99.9%. In particular, it is able to correctly predict the values of \( t_1 \) at which the topological phase transition from \( W = 1 \) to \( W = 0 \) takes place.

Our randomly sampled Hamiltonian does not include any noise. On the other hand, data collected from experiments would invariably show some degree of noise. To simulate this scenario, we artificially incorporated noise in our training data. To do so, we randomly changed the winding number from 0 to 1 and vice versa for a subset of the training set. We replaced the winding number by its incorrect value in 1%, 5% and 10% of the training data. The resulting predictions for the winding number and their rounded off value are shown in Fig. 2. Remarkably, the trained neural network is very robust and we obtain a very high accuracy greater than 99.8% in all these cases. This suggests that our neural network approach could be reliable even in the presence of noise in the input training data.

**Nodal line semimetal model**– We now consider a higher dimensional model to understand if the network is able to learn the winding number and phase transitions in a more general setting. The non-Hermitian continuum model for a nodal line semimetal reads [25]

\[
H = (m - B k^2)\sigma_x + (v_z k_z + i\gamma_z)\sigma_z,
\]

where \( k = \sqrt{k_x^2 + k_y^2 + k_z^2} \) and \( v_z \) is the Fermi velocity. The parameters \( m \) and \( B \) control the existence and radius

![FIG. 1. Fully connected neural network for the non-Hermitian Su-Schrieffer-Heeger model.](image-url)
We obtained very high accuracy of 99.95% or the fully connected network by changing its architecture.

To gain more insight into our convolutional neural network, whose schematic is shown in Fig. 3(c), we investigate the details of its learning. Our convolutional neural network consists of three hidden layers, two convolutional layers and one fully connected layer. The first layer in the network is a convolutional layer with 80 filters, hence 80 different convolutions are performed with respect to the input Hamiltonian.

\[ B^i(n) = f(A^i_{11}h_x(2\pi(n-1)/P) + A^i_{12}h_z(2\pi(n-1)/P) + A^i_{13}h_y(2\pi(n-1)/P) + A^i_{14}) \]

where \( A^i_{\alpha\beta} \) is a 2 \times 2 kernel, \( i = 1, \ldots, 80 \), \( n \in \mathbb{Z} \) & \( n = [-P+1, 0] \cup (0, P) \), \( \alpha, \beta = 1, 2 \) and \( f(x) \) is the activation function. The second layer is also a convolutional layer with 64 filters. Here the convolutions are performed using a 1 \times 1 kernel, \( C^i \). The output of this layer,

\[ D^i(n) = f\left( \sum_{i=1}^{N} C^i B^i(n) + C^0 \right) \]

is equivalent to the \( \Delta \Theta(n) \) of the winding number formula. In the third and the final hidden layer, which is fully connected, the network attempts to add all \( \Delta \Theta(n) \) to output the winding number. In the final layer, all the 20 neurons of the last hidden layer are mapped on to a single output neuron to yield the predicted winding number.
FIG. 3. Convolutional neural network for non-Hermitian nodal line semimetal model. (a) Computed and (b) predicted winding number as a function of $k_x$ and $k_y$, when $m = 0.4, \gamma_z = 0.2, v_z = B = 1$ and $k_z = 0$. Areas with winding numbers 0, -1/2 and -1 are shown in green, blue and red, respectively. We obtained an accuracy of 99.95%. In (b) the incorrect predictions are marked in magenta. These occur predominantly near the phase boundaries. (c) Schematic of our convolutional neural network with 2 convolutional layers, with 80 and 64 filters and kernel size of $2 \times 2$ and $1 \times 1$, followed by a fully connected layer with 20 neurons before the output layer, which was used to predict the winding numbers.

$$W_p = \sum_{q=1}^{20} F_q E_q + G.$$  \hspace{1cm} (8)

In the above, $E_n = f \left( \sum_{i=1}^{N} M_{qN} D(n) + N_q \right)$ with $q = 1, \ldots, 20$. The network successfully determines all the fitting parameters, $A_i, C_i, M_{qN}, N_q, F_q$ and $G$, during the training. With these insights, we can conclude that the network is capable of learning the winding number formula even in a higher dimensional case with co-existence of several different topological phases. This is a reliable and efficient approach to characterize non-Hermitian topological phases and the understanding gained from the scrutiny of its inner workings would be useful for formulating extensions to other systems, to study not just the winding number but also other intriguing properties such as exceptional points and non-Hermitian skin effects.

Summary and outlook– We demonstrated the use of machine learning to identify non-Hermitian topological phases, characterized by their winding numbers. For the one-dimensional non-Hermitian Su-Schrieffer-Heeger model, we trained a fully connected neural network to predict the different phases with an accuracy greater than 99.9%. For a three-dimensional non-Hermitian nodal line semimetal model, we constructed and trained a convolutional network to yield excellent accuracy in predictions of the topological phases. Our proposed methods could be potentially useful for machine learning of other non-Hermitian topological phases \[52\] \[59\], including those with disorder \[60\] \[61\]. Furthermore, we envisage that our methods could be applied for identification of non-Hermitian topological phases in future experiments.

Note added– After finalizing this work, we became aware of a complementary study by Zhang et al \[62\]. Where overlapping, our results are consistent with theirs.

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