Machine learning topological phases in real space

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We develop a supervised machine learning algorithm that is able to learn topological phases for finite systems in real space. The algorithm employs diagonalization in real space together with any supervised learning algorithm to learn topological phases through an eigenvector-ensembling procedure. We employ our method to successfully recover topological phase diagrams of Su-Schrieffer-Heeger models from data in real space using decision trees and show how entropy-based criteria can be used to retrieve topological information from local features. Our results demonstrate that learning topological phases in real space may be a viable alternative to momentum space computations, specially in cases when computing topological invariants in momentum space is impossible or unfeasible (e.g. disordered systems).

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I. INTRODUCTION

The quest for innovative materials that harness exotic quantum properties has lured physicists into the realm of topological insulators and topological states of matter \[1\]-\[23\]. These materials feature previously unthought of traits like bulk insulation coupled with metallic conductance at the surface and the splitting of currents according to spin orientation. Adding to that, these properties are protected by non-trivial topology that render them robust to many sources of perturbation like thermal noise. Such characteristics make them promising candidates to being the cornerstone of 21st century technologies like spintronics and quantum computing.

These new topological states of matter have been studied in several contexts in condensed matter physics including superconductors \[2\]-\[4\], ultracold atoms \[5\]-\[10\], photonic crystals \[11\] and photonic quantum walks \[20\]-\[21\]. Among these, the Su-Schrieffer-Heeger (SSH) model \[20\] has attracted particular theoretical interest due to its simplicity and generality.

The SSH model is the simplest tight-binding model that exhibits a topological phase transition. As such, it can be viewed as the Drosophila of the field, providing a simple framework for testing new techniques. It has found several interesting applications in the modelling of systems with non-trivial topology like optical lattices \[27\] and the polyacetylene molecule \[28\].

The model describes the movement of free electrons along a dimerized chain whose basic units consist of two distinct atoms. This movement, usually called "hopping" in the literature, can be made either between the atoms of a unit cell or between cells, and the allowed hopping rules for a given system completely determine its Hamiltonian. This is because the kinetic energies of the electrons are parameterized by a vector of real numbers \( \mathbf{t} \) that also encodes hopping terms, thus allowing for a compact mathematical description of a Hamiltonian in terms of creation/annihilation operators as

\[
\hat{H}(\mathbf{t}) = \Psi^\dagger H(\mathbf{t})\Psi
\]  

where the column vector

\[
\Psi = \left( c_A^1, c_B^1, \ldots, c_A^N, c_B^N \right)^T
\]

contains annihilation operators \( c_p^{A(B)} \) that erase electrons at atom A (B) and lattice site \( p \) and similarly the row vector

\[
\Psi^\dagger = \left( c_A^1, c_B^1, \ldots, c_A^N, c_B^N \right)
\]

contains creation operators \( c_p^{A(B)} \) that produce electrons at atom A (B) and lattice site \( p \). Please note that \( N \) is twice the number of unit cells in the chain and therefore an even integer.

The convenience of equation (1) is that all information about a system such as its eigenstates and eigenenergies can be recovered from the \( N \times N \) matrix \( H(\mathbf{t}) \). We can thus think of the vectors \( \mathbf{t} \) in parameter space as very compact representations of SSH models: each point in \( \mathbf{t} \)-space can be mapped to a \( N \times N \) matrix \( H(\mathbf{t}) \) whose eigenstates and eigenenergies can then be computed, as is usually done in quantum mechanics. As an example, a general matrix \( H(\mathbf{t}) \) describing a SSH system with hoppings between nearest and second nearest neighbors is given by

\[
H(t_1, t_2, T_1, T_2) = \begin{pmatrix}
0 & t_1 & 0 & T_1 & 0 & \cdots \\
0 & 0 & 0 & 0 & t_2 & 0 & T_2 & \cdots \\
T_1 & 0 & 0 & 0 & 0 & t_1 & 0 & \cdots \\
0 & 0 & 0 & 0 & t_2 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\]  

Knowing the vector \( \mathbf{t} = (t_1, t_2, T_1, T_2) \) corresponding to a particular system described by equation (2) should suffice to compute any of its physical properties, including its topological phase. Figure 1 depicts a SSH system described by equation (2).

The reason why topological materials garnered so much interest in recent years is that their physical properties are topologically robust. This means that these properties are stable under continuous (i.e., adiabatic) mathematical operations performed on the system’s underlying wave functions. This topological robustness is expressed theoretically in terms of a topological invariant that characterizes different phases of a system. In the particular case of the SSH model, the topological invariant used to classify its possible topological phases is the winding number.

The winding number is a topological property of any closed, oriented curve that measures how many times it winds around a point that does not belong to itself. It can be any integer and is usually chosen to be positive when the curve winds in counterclockwise motion with respect to the reference point (equivalently, when a closed, oriented curve winds in clockwise motion around a reference point its winding number is negative). Figure 2 shows several closed, oriented curves and their winding numbers computed with respect to a given point.

An interesting property of topological invariants like the winding number is that they are global properties of geometric objects: for each of the curves in figure 2 for example the winding number is a property of the whole curve that cannot be defined locally for each of its points.
For a SSH Hamiltonian like the one in eq. (1), the winding number is usually computed in momentum space via

$$W = \frac{1}{4\pi i} \int_0^{2\pi} dk Tr(\sigma_3 H(k)^{-1}\partial_k H(k)), \quad (3)$$

where $H(k)$ is the kernel of the Hamiltonian in momentum space and $\sigma_3$ is the chiral operator. This can be done for several Hamiltonians by varying the parameter $t$, resulting in phase diagrams in parameter space like the ones shown in figure 3.

Many recent papers have explored the possibility of treating the general problem of determining phase transition boundaries of physical systems as machine learning tasks [29]-[37]. In the particular case of topological phase transitions, the usual approach for supervised learning is to generate a data set $(H_1(k), W_1), \ldots, (H_n(k), W_n)$ whose inputs are representations of Hamiltonians in momentum space $H_i(k)$ and targets are their corresponding winding numbers $W_i$. Our paper extends this task to the case of learning topological phase transition curves from input data in real space.

Our motivation for this is that momentum space computations such as eq. (3) are only possible for systems with translational symmetry, which many physical systems of current interest (e.g. disordered systems) do not have. Moreover, since real space and momentum space eigenvectors are related by Fourier transforms, momentum space eigenvectors are essentially delocalized and therefore so is any information recovered from them. We argue here that a data-driven approach based on real space offers a viable alternative to momentum space computations that addresses these shortcomings.

Our reasoning goes as follows. First, while the topological invariants that characterize distinct phases are computed in momentum space, the topological properties of a Hamiltonian are the same regardless of the basis in functional space used to represent it. Thus, information about the topological phase of a given Hamiltonian should still be available when it is represented in real space. Second, even though the topological properties of a Hamiltonian are global, meaning that in general they cannot be said to be localized at a particular lattice site, in parameter space topology is indeed a local property: knowing the vector $t$ associated with a Hamiltonian completely determines its topological phase.

In a data-driven approach, locality is often exploited by means of a local constancy hypothesis. Mathematically, this policy prescribes the value of a function $W(t')$ at points where it is unknown in a vicinity of a data point $t$ as approximately equal to its known value $W(t)$,

$$W(t + \epsilon) \approx W(t). \quad (4)$$

That such a policy will usually be successful in classifying topological phases in parameter space can be better visualized in figure 3 where we draw phase diagrams for SSH models with first-neighbor (figure 3(a) and first- and second-neighbor (figure 3(b)) hoppings. In 3(a) for example, it is clear that knowing a particular Hamiltonian $H(t_1, t_2)$ with winding $W = 0$ (that is, in one of the red regions) means that there is a small neighborhood around $(t_1, t_2)$ in which all Hamiltonians belong to the same topological phase. Were we able to collect data on the topological phases of several Hamiltonians in parameter space, the problem of learning phase boundaries in a supervised setting would reduce to a standard problem of curve estimation which could then be tackled with conventional machine learning algorithms like $k$-nearest neighbors, decision trees or support vector machines. Whether employing the same strategy in the much higher-dimensional real space will be successful or not is the subject of this work.

From the discussion above, it becomes clear that phase diagrams in parameter space like those in figure 3 simply depict lower-dimensional representations of data from a much higher-dimensional space (i.e., the real lattice space). The problem of learning useful, lower-dimensional representations of complex data coming from a higher-dimensional space is at the heart and soul of machine learning. It is therefore a natural pursuit to try to develop machine learning algorithms (supervised and unsupervised) that can effectively learn useful properties of materials (here, their topological phase diagrams) from raw data (real space configurations). In the next section we present a supervised learning algorithm that performs this task.

II. MACHINE LEARNING ALGORITHM

In this section we detail a supervised learning algorithm for classification of topological phases of Hamiltonians using data from real space. As we implemented it in this paper, it consists of five steps:

1) Generating Hamiltonians and winding numbers,

2) Creating training/validation/test sets,
Figure 3. Phase diagrams. a) Eq. (1) with first-neighbor hoppings $t_1$ and $t_2$. The red regions with $W = 0$ are trivial, while the blue regions with $W = 1$ are topologically non-trivial. b) Eq. (1) with first ($t_1$ and $t_2$) and second ($T_1$ and $T_2$) nearest-neighbor hoppings. Here we set $t_1 = t_2 = 1$ and renamed the variables $T_1 \rightarrow t_1$, $T_2 \rightarrow t_2$ for convenience. The orange region ($W = 0$) is trivial while the others are topologically non-trivial.

3) Training on eigenvectors in real space: having split the Hamiltonians in training, validation and test sets, we compute the eigenstates of each Hamiltonian in real space. Since each Hamiltonian $H_i$ is represented by a $N \times N$ matrix, each one will generate $N$ eigenvectors $v_i^{(1)}, v_i^{(2)}, ..., v_i^{(N)}$. Our supervised learning algorithm of choice will take as input an eigenvector $v_i^{(j)}$ in real space and be trained to predict the winding $W_i$ of its corresponding Hamiltonian $H_i$. Therefore, our dataset will consist of eigenvector-winding pairs $(v_i^{(j)}, W_i)$. Importantly, we randomly shuffle the eigenvectors of all Hamiltonians in the training set so as not to expose the classifier to many examples of the same phase in sequence. In algorithms such as neural networks not performing this shuffling may have detrimental effects in performance.

4) Eigenvector ensembling: given that each Hamiltonian has $N$ eigenvectors, in order to predict a Hamiltonian’s phase we need to take into account how our system classified each one of its eigenvectors. A simple way to do this is to perform a majority vote. As an example, assume...
the possible classes (i.e., topological phases) are $W_1, W_2, ..., W_M$ and let $I_k$ be the indicator function of class $W_k$, that is

$$I_k(W_i) = \delta_{kl}. \quad (5)$$

Suppose our classifier labels the eigenstates $v_i^{(1)}, v_i^{(2)}, ..., v_i^{(N)}$ of $H_i$ as $W_i^{(1)}, W_i^{(2)}, ..., W_i^{(N)}$ respectively. Then the phase of $H_i$ will be labeled as $W_{i_{\text{max}}}$, 

$$i_{\text{max}} = \arg \max_{k=1, ..., M} \sum_{j=1}^{N} I_k(W_i^{(j)}) \quad (6)$$

which simply expresses that the most frequent class among the eigenvectors of a given Hamiltonian is chosen to be its class.

5) **Bootstrapping:** the eigenvector ensembling procedure described in the previous step can be viewed as estimating the probabilities that a single eigenvector will classify its parent Hamiltonian in each class: these will be equal to the fractions of a parent Hamiltonian’s eigenvectors that are classified in each class. Evidently, a different training set may lead to different estimates for these probabilities. In our paper, these estimates are refined using a bootstrapping procedure. This is to say that we repeat steps (1)-(4) $n_{\text{exp}}$ times, at each round sampling a new training set from our grid in $t$-space. The final estimated probabilities can then be arrived at by averaging the probabilities obtained in each experient.

A few comments are due before we proceed to the numerical experiments section. First, one may wonder why we chose to use the eigenvectors of the Hamiltonians instead of the Hamiltonians themselves as input data. Indeed (assuming our Hamiltonians are real matrices), it is tempting to write the Hamiltonians as vectors in $\mathbb{R}^{N^2}$ and use them directly as inputs to a learning algorithm. This in fact would probably be the first idea occurring to anyone trying to solve this problem. Nevertheless, after a little more thought it is easy to see that using the eigenvectors instead is a better idea. In fact, we can write a Hamiltonian matrix as a vector in $\mathbb{R}^{N^2}$ using row-major ordering as

$$H_i = \left(h_i^{(1,1)}, ..., h_i^{(1,N)}, ..., h_i^{(N,1)}, ..., h_i^{(N,N)} \right). \quad (7)$$

If instead we choose to use the eigenvectors, each data point will have the form

$$v_i^{(j)} = \left(v_i^{(j,1)}, ..., v_i^{(j,N)} \right) \quad (8)$$

Equation $(7)$ expresses $H_i$ as a vector sum of $N^2$ terms, while $(8)$ expresses $v_i^{(j)}$ as a vector sum of $N$ terms only. While at first sight the advantage of using $(8)$ instead of $(7)$ may not be apparent, it becomes quite clear when we consider how we shall feed a learning algorithm with these two types of data. Suppose for example we generate $T$ Hamiltonians, each of them a $N \times N$ matrix. In the case of equation $(7)$ we will have $T$ data points in a $N^2$-dimensional space, while in the case of equation $(8)$ we will have $NT$ data points in a $N$-dimensional space. Using eigenvectors instead of Hamiltonians thus amounts to a considerable reduction in the dimensionality of the problem with the added benefit of getting more data points to train on.

Another important point to note is that the eigenvector ensembling step is an example of ensemble learning: while classifying a single eigenvector may not yield good results, as long as these weak classifiers perform better than random guess it is usually the case that their ensemble performs much better. This is the same reasoning behind algorithms like random forests where an ensemble of decision trees (the weak learners) combine to yield a stronger learner.

Similarly, the bootstrap in step 5 is another example of ensemble learning with an interesting nuance: deciding the class of a Hamiltonian by averaging the learned probabilities for each class across several experiments might lead to a different result from simply counting the number of times a Hamiltonian was assigned to each class across the same experiments. This is a common problem in designing functional voting systems. The first method will choose for a Hamiltonian the most voted class across all experiments (similar to a popular majority system), whilst the second will choose the class that won most experiments (akin to the American electoral college). That these two methods might lead to different results is demonstrated time and again by the American presidential elections. In our paper, we average class probabilities for each Hamiltonian across all experiments, meaning that we stick to the popular majority system.

Finally, in the training stage (step 3 above) we are free to train any supervised learning algorithm on the eigenvectors of the training Hamiltonians. While this does not imply that all supervised learning algorithms will perform equally well, it does give us extra flexibility when using eigenvector ensembling. In particular in our paper we evaluate our procedure using decision trees. The choice of a simple algorithm like decision trees is meant to emphasize that for this kind of task it may be preferable to choose shallow, visualizable algorithms over deep, hard-to-visualize ones like deep neural networks which also demand much more hyperparameter tweaking. Perhaps given the recent fever around neural networks, supervised learning algorithms like tree-based methods have been little explored in the literature for this task, which further justifies our choice.

The other reason we chose decision trees is that they allow us to quantify the importance of each feature in learning the existing pattern in our data through entropy-
based criteria. For the problem at hand, this means that we will be able to pinpoint which lattice sites were most relevant in determining the topological phase of a Hamiltonian.

III. NUMERICAL EXPERIMENTS

In this section we present results for the numerical experiments we performed with the algorithm outlined in the previous section. We start with the results from the simplest case, the SSH model with nearest-neighbor hopping (3(a)), then we analyze the SSH model with first and second nearest-neighbor hoppings (3(b)).

In each experiment our goal is to recover the known phase diagrams in 2D parameter space, figures 3(a) and 3(b) from data in the much higher dimensional real space (100D - in both experiments lattices have 50 unit cells, yielding 100 × 100 Hamiltonian matrices). This task is particularly hard near phase boundaries, where numerical computation of winding numbers can become unstable. For this reason, when sampling our training set we only consider those Hamiltonians in the grid whose numerically computed winding numbers differ from the allowed values (0 = ϵ < 2} × \([-2, 2]\) in the \(t_1-t_2\) plane. This task is considerably more difficult than the previous one due to the higher number of classes (the winding numbers are now \(-1, 0, 1, 2\)) and also the fact that some of the labels encompass disconnected regions. Just as we did in the previous case, we can visualize how a typical experiment unfolds as seen from 2D parameter space. Figure 4 depicts a typical run of the experiment. In 4(a) we show a typical grid split into train/val/test sets as seen in parameter space. Figure 4(b) shows a scatter plot of winding number labels in parameter space for the training set. Figure 4(c) shows a phase prediction grid with eigenvector ensamblying results for this single experiment.

The bootstrap allows us to collect several statistics to evaluate performance. In particular, we report mean eigenvector accuracy on training data (98.2%), validation data (96.2%) and test data (77.7%). Mean Hamiltonian accuracies from eigenvector ensamblying substantially improve these numbers as expected. These were 100% for training data, 100% for validation data and 99.1% for test data.

Another advantage of bootstrapping is that we can average results from different experiments to arrive at an even more reliable prediction grid. In this experiment, Hamiltonian accuracies for train, validation and test data all go to 100% when we perform eigenvector ensamblying after bootstrapping.

In figure 6(a) we show a heatmap of class probabilities averaged across all 100 experiments. The heatmap expresses the percentage of eigenvectors that voted for the topological phase (\(W = 1\)) for every Hamiltonian in the grid. It can thus be seen that it faithfully portrays the underlying phase diagram of figure 3(a) with clear phase transition lines where both phases are equally likely.

A. Experiment 1: Decision Tree-learning a SSH model with nearest-neighbor hopping

In this experiment our grid consists of 6561 Hamiltonians uniformly distributed in the closed square \([-2, 2] \times \([-2, 2]\) in the \(t_1-t_2\) plane. Our test set in this experiment contains 1005 Hamiltonians (approx. 15.3% of all data) under the criterium that their numerically computed winding numbers differ from the allowed values (0 or 1 in this experiment) by more than \(\epsilon = 0.01\). Of the remaining 5556 Hamiltonians, 556 are randomly assigned to the training set (approx. 8.5%) and 5000 (approx 76.2%) are used for validation at each experiment. These proportions between training and validation sets are such that approximately 10% of Hamiltonians from out of the test set are used to train. Our algorithm of choice for this experiment was a simple decision tree model as implemented in the Python Scikit-Learn library.

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B. Experiment 2: Random Forest-learning a SSH model with first and second nearest-neighbor hoppings

In our second experiment we try to recover the phase diagram of figure 3(b) using a grid of 6561 Hamiltonians uniformly distributed in the closed square \([-2, 2] \times \([-2, 2]\) in the \(t_1-t_2\) plane. This task is considerably more difficult than the previous one due to the higher number of classes (the winding numbers are now \(-1,0,1,2\)) and also the fact that some of the labels encompass disconnected regions. For this reason, instead of using a single decision tree, we upgrade our model to a random forest with 50 trees. Following our rule that the test set consists of Hamiltonians whose numerically computed winding numbers differ from the allowed values by more than \(\epsilon = 0.01\), we end up with 1040 (15.8% of all data) test Hamiltonians. The remaining Hamiltonians are randomly split in half between training and validation sets at each experiment, giving us 2761 (42.1%) training Hamiltonians and 2760 (42.1%) validation Hamiltonians.

Just as we did in the previous case, we can visualize how a typical experiment unfolds as seen from 2D parameter space. This is shown in figure 5.

The average eigenvector accuracies across 100 repetitions of this experiment were 99.9% for training eigenvectors, 97.3% for validation eigenvectors and 67.8% for test eigenvectors. The average Hamiltonian accuracies result-
Figure 4. Visualization of a typical experiment from III A as seen from 2D parameter space. (a) Train/val/test split. (b) Distribution of winding numbers in the training set. (c) Phase prediction grid learned from real space.

### IV. TOPOLOGICAL LOCALIZATION

In the previous section we have shown the feasibility of learning topological phases from raw data in real space. In this section we examine how the algorithm was able to recover a global property of the Hamiltonians (their topological phase) from local features (eigenvector components on each lattice site).

We can view this learning task as trying to estimate a phase transition curve in 2D parameter space from 100D eigenvectors in real space. As we have already pointed out, the topological phase of a Hamiltonian is a local property in parameter space. Evidently, the diagonalization process transfers this locality to real space through the maps $v^{(j):} : \mathbb{R}^2 \rightarrow \mathbb{R}^{100}$, 

\[
(t_1, t_2) \rightarrow \left( v^{(j,1)}(t_1, t_2), \ldots, v^{(j,100)}(t_1, t_2) \right) = v^{(j)}(t_1, t_2)
\]

where $j = 1, \ldots, 100$ indexes the eigenvectors of the Hamiltonian $H(t_1, t_2)$. Thus, at least in principle, learning topological phases from local features should be possible. However, there is a practical qualm.

Although it may seem from figures 4(b) and 5(b) that we have used a large number of data points for this learning task, it is important to note that the decision trees have taken inputs from 100D space. In 100D space, our dataset will actually be very sparse. The difficulty arising from machine learning problems in high dimensional spaces is commonly referred to as the curse of dimensionality. It essentially expresses the fact that the amount of data needed to ensure a machine learning algorithm will generalize well out of its training set grows exponentially with the dimension of feature space.

Equation 9 itself gives us a hint to the solution for this issue. Indeed, it states very clearly that our learn-
The (normalized) relevance of a feature is given by how much it is able to reduce a loss function (e.g., entropy or Gini impurity). By averaging feature importances across 100 repetitions of both experiment 1 (III A) and experiment 2 (III B) we should be able to test whether some lattice sites were consistently more relevant than others in learning to classify topological phases from data in real space.

The bar plot in figure 7(a) shows how informative each feature was in learning topological phases for experiment 1. By sorting features in decreasing order of relevance and computing partial relevance sums as shown in figure 7(b) it is possible to visualize how each feature enhances the capability of learning the underlying pattern in the data. From figure 7(b) we see that only 6 features (1, 2, 4, 51, 52, 54) contribute more than 70% of total reduction in Gini impurity. Figure 7(a) on the other hand confirms that each of the 94 remaining features are much less relevant than those.

In figure 8 similar bar plots are shown for experiment 2. The much smoother curve in figure 8(b) than in 7(b) cajoles us into believing that topological information is much less localized for the SSH model with first and second neighbors than for the nearest neighbor model. Nevertheless, figure 8(a) still indicates that some features (e.g., 1, 2, 99, 100) were significantly more relevant than others in classifying topological phases from real space.

It is often the case in machine learning that parsimony leads to more robust and reliable results. This principle alone compels us to rerun both experiments 1 and 2 using only the most relevant features to check whether simpler models are still capable of learning topological phases in each case. But there is yet another, more physical, motivation: the fact that we have used periodic boundary conditions. Intuitively we expect that the use of periodic boundary conditions should eliminate border effects and even out feature importances. This seems to be in contradiction to the results shown in figures 7 and 8.

In our rerun of experiment 1, we use only features (1, 2, 4, 51, 52, 54) to train the algorithm. These features form the two sharp peaks seen in picture 7(a) and the information gain from adding further features to this subset clearly tapers off as seen from 7(b). Our choice is thus an application of the elbow method so often used in machine learning. Again, the experiment is repeated 100 times to smooth out results. Mean eigenvector accuracies were 97.1% for training data, 94.5% for validation data and 77.8% for test data. Mean Hamiltonian accuracies were 100% for training data, 97.9% for validation data and 78.2% for test data.
acies obtained from eigenvector ensembling were 98.8\% for training data, 98.5\% for validation data and 98.7\% for test data. Performing eigenvector ensembling on bootstrapped averages of eigenvector predictions across all 100 experiments slightly improve Hamiltonian accuracies to 99.1\% for training data, 98.5\% for validation data and 99.9\% for test data.

Choosing a smaller subset of features to rerun experiment 2 is a harder task as a consequence of its cumulative importance curve (figure 8(b)) being much smoother than that of experiment 1 (figure 7(b)). Thus applying a visual criterium such as the elbow method becomes a much more ambiguous task. Nevertheless, we can still distinguish three peaks in figure 8(a) and the underlying signal clearly exhibits a mirror symmetry with respect to its middle point (in reality, given that we have used periodic boundary conditions, the two peaks at the borders are actually part of a single peak). Using these observations as a guiding principle, we rerun experiment 2 with features (1, 2, 3, 4, 5, 6, 47, 49, 50, 51, 52, 54, 95, 96, 97, 98, 99, 100). This choice of features clearly abides to our policy: every feature chosen is accompanied by its mirror-symmetric partner. Taken together, these features account for more than 30\% of reduction in Gini impurity.

Mean eigenvector accuracies for our rerun of experiment 2 were 99.9\% for training data, 96.0\% for validation data and 63.7\% for test data. Eigenvector ensembling yields mean Hamiltonian accuracies of 100\% for training data, 99.6\% for validation data and 90.4\% for test data. Hamiltonian accuracies for bootstrapped eigenvector ensembling are slighty higher at 100\% for training data, 100\% for validation data and 91.3\% for test data.

V. CONCLUSION

Given the increasing complexity of systems studied in condensed matter physics and the rising demand for materials with unusual and robust properties to power future technological progress, it is only expected that data-driven approaches to physics will grow in demand. Our work represents a small step in this direction, as we have demonstrated the viability of applying a fully data-driven approach to the search for new topological materials bypassing the use of data in momentum space.

One advantage of using data from real space is that it enables us to learn which lattice sites carry more information about the topological phase of a system. We demonstrated this in section IV. Given that feature importances are usually measured in terms of quantities that have actual physical meaning like entropy, the results presented here suggest a new road for theoretical investigation. Whether there is a true physical meaning to the entropy-based topological localization discussed here or not is left for speculation.

We expect the eigenvector ensembling procedure employed in this paper to have further applications in sim-

Figure 6. Probability heatmaps learned from real space. Heatmaps were averaged across all 100 experiments in both cases. (a) The heatmap for experiment [III A] can be viewed as estimating the probability that a Hamiltonian in the grid has winding number equal to 1. (b) The probability heatmap for experiment [III B] is a superposition of individual heatmaps for each winding number.
ilar physics problems. The reason for our expectation is
that most of physics is based on eigenvector decomposition,
and statistical physics itself can be seen as an
application of similar ensembling principles. It is therefore
reasonable to assume that similar data-driven physics
problems could benefit from this technique.

Finally, we should point out some immediate possibili-
ties that arise from this work. The most straightforward
one is the application of the same algorithm to disor-
dered systems. But perhaps a more provocative endeav-
our would be the development of a similar unsupervised
learning algorithm that performs topological phase seg-
mentation in real space. The development of such an
algorithm could greatly hasten the discovery of new topo-
logical materials.

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Figure 7. Normalized feature importances measured by Gini impurity for experiment 1. (a) Feature importances for each lattice site. (b) Cumulative feature importances. Both pictures show that most of the relevant topological information used by the decision trees was located on the two peaks at features (1,2) and (51, 52). Taken together, features (1, 51, 52, 2, 4, 54) account for more than 70% of relevant topological information.
Figure 8. Normalized feature importances measured by Gini impurity for experiment 2. (a) Feature importances for each lattice site. (b) Cumulative feature importances. Note the three clearly defined peaks near features (1,2), (51,52) and (99,100) and the mirror symmetry exhibited by the signal with respect to its middle point. Features (1, 2, 3, 4, 5, 6, 47, 49, 50, 51, 52, 54, 95, 96, 97, 98, 99, 100) account for more than 30% of the relevant topological information used by the trees.