Identifying quantum phase transitions using artificial neural networks on experimental data

Benno S. Rem\textsuperscript{1,2}, Niklas Käming\textsuperscript{1}*, Matthias Tarnowski\textsuperscript{1,2}, Luca Asteria\textsuperscript{1}, Nick Fläschner\textsuperscript{1}, Christoph Becker\textsuperscript{1,3}, Klaus Sengstock\textsuperscript{1,2,3*} and Christof Weitenberg\textsuperscript{1,2}

Machine-learning techniques such as artificial neural networks are currently revolutionizing many technological areas and have also proven successful in quantum physics applications\textsuperscript{4–6}. Here, we employ an artificial neural network and deep-learning techniques to identify quantum phase transitions from single-shot experimental momentum-space density images of ultracold quantum gases and obtain results that were not feasible with conventional methods. We map out the complete two-dimensional topological phase diagram of the Haldane model\textsuperscript{5–7} and provide an improved characterization of the superfluid-to-Mott-insulator transition in an inhomogeneous Bose–Hubbard system\textsuperscript{8–10}. Our work points the way to unravel complex phase diagrams of general experimental systems, where the Hamiltonian and the order parameters might not be known.

Ultracold quantum gases have been established as a formidable experimental platform to study quantum many-body systems in a well-controlled environment\textsuperscript{11,12}. Important breakthroughs include the realization of paradigmatic condensed-matter models such as the Mott insulator transition or topological quantum matter. While these systems offer complementary observables compared to solid-state systems, finding proper observables for quantum phases remains a key challenge, in particular in exotic systems such as non-local topological order or many-body localization. Here we explore a new approach building on modern machine-learning techniques\textsuperscript{13,14}. Inspired by the success of convolutional neural networks in image recognition, we feed such a network with single images of momentum-space density, which are a standard experimental output of quantum gas experiments (Fig. 1). We train it on large datasets of labelled images taken far away from the phase transition and apply the trained network to test data across the phase transition. The network is able to identify the correct position of the phase transition in parameter space from single experimental images. This is a crucial advance for optimizing experimental parameters, because the phase can now be determined from single images for direct decisions in the laboratory, and points towards future fully automated quantum simulators. We expect these techniques to be valuable also for in situ snapshots as captured by quantum gas microscopes\textsuperscript{14,15}. Similar approaches were previously applied to numerical simulations of various physical models\textsuperscript{15,16–22} and recently to scanning tunnelling microscopy data\textsuperscript{23}. Neural networks are also opening new avenues in other areas of quantum physics, such as the representation of quantum many-body states\textsuperscript{24–26} or the optimization of complex systems\textsuperscript{24–26}.

We demonstrate the power of artificial neural networks on two physical examples, namely the topological phase transition in the Haldane model and the superfluid-to-Mott-insulator transition in the Bose–Hubbard model, both realized employing cold atoms in optical lattices. We show that we can perform tasks that were not possible with conventional techniques, such as the determination of non-local topological order from a single-shot image—a problem for which there is no physical model—and a localization of the superfluid-to-Mott-insulator transition, superior to the usual determination via interference contrast. Our examples show that machine learning can help in the identification of observables that were not previously obvious.

In a first set of experiments, we consider the Haldane model on the honeycomb lattice\textsuperscript{2}, a paradigmatic model for topological bands without a net magnetic flux possessing possible Chern numbers $C = -1, 0, 1$ (inset in Fig. 2b). The topological phase diagram is spanned by the Peierls phase $\Phi$ and the sublattice energy offset $\Delta_{AB}$, which quantify the breaking of time-reversal symmetry and inversion symmetry, respectively. The phase boundaries are given by $\Delta_{AB} = \pm \sqrt{\frac{3}{2}J} \sin(\Phi)$ (ref. \textsuperscript{2}). We realize a Haldane-like Hamiltonian as an effective Floquet Hamiltonian for ultracold fermionic atoms in a driven honeycomb optical lattice\textsuperscript{6,7,27,28}. In this Floquet realization, the inversion symmetry breaking is controlled via the shaking frequency $\omega$ and the time-reversal symmetry is controlled by the shaking phase $\Phi$ (see Methods). In the experiments, we adiabatically ramp up the shaking amplitude and then ramp the shaking frequency to populate the lowest band. After different waiting times in the Floquet system, we suddenly switch off all trapping potentials, such that the cloud expands during a certain time-of-flight and the momentum distribution is mapped onto the real-space density distribution, which we capture in an absorption image (Fig. 2a). These momentum-space images are directly fed into the convolutional neural network (see Methods for a description of the network architecture). The suitability of the momentum-space density is motivated by state tomography methods, which rely on such images and allow the full measurement of the Berry curvature\textsuperscript{29}. However, there is no physical model for how to extract the Chern number from single images and thus the Chern number is not obvious for the human eye\textsuperscript{2}.

We take data for varying shaking frequencies and shaking phases, thus mapping out the topological phase diagram. For training the network, we use data far away from the phase boundaries, where we can unambiguously label them with a Chern number $C = -1, 0$ or $+1$. We then use the trained network to classify the images in the transition region. The network outputs the probabilities for each class $P_C$ (Fig. 2b). Along a cut through the phase diagram for circular shaking ($\Phi = -90^\circ$), the network predicts a single Chern number with near unit certainty away from the phase transitions, even outside the training regions. Moreover, it shows a smooth crossover between

---

\textsuperscript{1}Institut für Laserphysik, Universität Hamburg, Hamburg, Germany. \textsuperscript{2}The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany. \textsuperscript{3}Zentrum für Optische Quantentechnologien, Universität Hamburg, Hamburg, Germany. \textsuperscript{*}e-mail: klaus.sengstock@physnet.uni-hamburg.de
two Chern numbers in a small transition region with a full width of 100–200 Hz, which is due to the inhomogeneity of the system.

We use the same trained network to map out the entire two-dimensional phase diagram using just a few images per parameter set. In Fig. 2c we plot the expectation value of the Chern number \( C = \sum_{C=\pm1} C \times P_C \) as a function of the shaking frequency and shaking phase. The network identifies the two lobes with Chern numbers \(-1\) and \(+1\), which are characteristic for the Haldane model, in quantitative agreement with a numerical calculation of the Floquet system (see Methods). The identification from single snapshots allows mapping out the full two-dimensional Haldane phase diagram.

**Fig. 1** | Using a neural network to identify physical phases from experimental images. Single images of the density of atoms in momentum space after time-of-flight (false-colour representation of a single-channel image) serve as input for a deep convolutional neural network with a variety of layers including convolutional filters and fully connected layers. The white line represents the sliding of the filters across the input image. The final softmax layer outputs the probability that the image belongs to one of the classes (here, Chern numbers \( C = -1, 0 \) or \(+1\)). The weights of the network are trained on many labelled images and the network can then classify an unknown single image with high confidence. This approach—originally developed for image recognition—works well for identifying physical quantum phases from experimental images.

**Fig. 2** | Mapping out a topological phase diagram using a neural network. a. Examples of single experimental images of ultracold fermionic atoms released from the driven optical lattice. The shaking phase is \( \phi = -90° \) and the shaking frequencies are \( \omega/2\pi = 5.0 \text{kHz (} C = 0 \), \( \omega/2\pi = 6.4 \text{kHz (} C = 1 \) and \( \omega/2\pi = 7.8 \text{kHz (} C = 0 \), respectively. The images are 151×151 pixels in size centred around zero momentum and include the full first Brillouin zone (white hexagon). b. Probability for the different Chern number classes as identified by the trained neural network. The network was trained for Floquet frequencies far away from the phase transitions (grey, thin short lines in c). The probability is averaged over the results for 47 individual images and the error bars denote Clopper–Pearson 68% confidence intervals using the Wald method. We identify the positions of the phase transitions at 6.124(3) kHz and 6.869(3) kHz by fitting an error function to the data and extracting the point of 50% probability. The dashed lines show the transitions as expected from an ab initio numerical calculation. The inset illustrates the tight-binding scheme of the Haldane model with the staggered fluxes through the subplaquettes. c. The Haldane-like phase diagram of the Floquet system obtained from 10,436 evaluated test images (3–7 images per parameter) using a neural network trained at the parameters indicated by the grey lines (in total 15,963 images for training and 3,992 images for validation of the network). The training regions cover only 3% of the phase diagram. The solid lines indicate the predicted phase transitions from our ab initio numerical calculation. d. The circles show the positions of the phase transitions for circular shaking (\( \phi = -90° \)) at varying lattice depths \( V \) identified by a network trained with the data at \( V = 7.4 E \text{\textsubscript{r}} \) (see Methods). The error bars denote the width of the error function fitted to the network output as in b. The lines show the predicted phase transitions from our ab initio numerical calculation with the red regions indicating the systematic uncertainty calculated for an error of 0.2° on the polarization of the lattice beams. Source data for b–d are provided in Supplementary Data 1–3.
a

Bragg peaks at multiples of the reciprocal lattice vector indicate the coherence in the system for small $U/6\gamma$. The visibility of the Bragg peaks is evaluated at the indicated boxes at constant distance from the centre to remove the influence from the density envelope. The condensate fraction is obtained from bimodal fits to the diffraction peaks\(^\text{a}\). Visibility, condensate fraction and the results from the trained network for the probability for the superfluid phase $P_{\text{SF}}$ as a function of $U/6\gamma$. The probability is averaged over the results for 31 individual images and the error bars denote Clopper–Pearson 68% confidence intervals using the Wald method. Visibility and condensate fraction drop smoothly, while the probability curve obtained from the network clearly defines a superfluid region, a Mott-insulating region and a transition region (red area, $4.3 < U/6\gamma < 10.9$) in agreement with the predictions for the transition at filling $n = 1$, $n = 2$ and $n = 3$ (black solid lines\(^{39}\) and dashed lines\(^{39}\), which occur in the inhomogeneous system. The network was trained with data far away from the phase transition (grey areas). The inset illustrates the hopping term and the on-site interaction term of the Hubbard model. Source data for $b$ are provided in Supplementary Data 4.

We note that this has been unfeasible with traditional methods. As a nice illustration of the robustness of the method, the network, which was trained at a lattice depth of $V = 7.4E_{\text{r}}$, (where $E_{\text{r}}$ is the recoil energy), also correctly predicts the topological phase transitions for other lattice depths (Fig. 2d) (see Methods for further cross-checks on the network performance). Furthermore, while experimental issues such as a significant population of the second band or the comparison of different phases within the micromotion of the Floquet system often cause difficulties in conventional data analysis\(^{35,36}\), the network is successfully trained to account for them, because they are also present in the training data.

As a second example, we study the Bose–Hubbard model, which is a paradigmatic model for strongly correlated many-body systems and a pioneering model for quantum simulations with ultracold atoms\(^{39,40}\). The Hamiltonian describes the competition between the kinetic energy quantified by the tunnel element $J$ and the interaction energy quantified by the on-site interaction $U$ (see inset to Fig. 3b). In a cold-atom realization, the parameters $J$ and $U$ can be tuned via the lattice depth $V$ (ref.\(^{14}\)). At a commensurate filling of $n$ atoms per site, the model hosts a quantum phase transition from a superfluid phase to a Mott insulating phase. In the presence of an external trap, different fillings are realized within the system, which can be described with a local density approximation and form a sequence of shells with commensurate densities in the Mott insulating regime, as directly observed with high-resolution in situ imaging\(^{41,42}\). In a mean field approximation, these transitions occur at $U/\gamma = 5.8$; $9.9$; $13.9$ for a filling of $n = 1$; $2$; $3$ (ref.\(^{14}\)). Here $\gamma$ is the number of nearest-neighbouring lattice sites, which is 6 for the two-dimensional triangular lattice considered here\(^{43}\). Two different correlated calculations for the triangular lattice predict the transition around $U/6\gamma = 4.43$–$4.9$; $7.53$–$8.3$; $10.6$–$11.9$ for $n = 1$; $2$; $3$ (refs.\(^{31,34}\)).

Here, we study the phase transition using the momentum distribution with its characteristic Bragg peaks indicating the coherence in the system\(^{35,36}\) (Fig. 3a). We feed the momentum-space images into a neural network and study its identification of the phase transition (see Fig. 3b). We train the neural network with data far in the superfluid regime ($1.3 < U/6\gamma < 2.2$) and far in the Mott insulator regime ($120 < U/6\gamma < 415$) using a total of 557 images. When the trained network is applied to classify the data from the intermediate lattice depths, we find two clear plateaux for the superfluid phase and the Mott insulating phase, as well as a well-defined transition region for $4.3 < U/6\gamma < 10.9$ (for $0.95 > P_{\text{SF}} > 0.05$), where the probability for the superfluid phase $P_{\text{SF}}$ decreases from 1 to 0. The transition region agrees with the parameter range, over which the successive Mott shells $n = 1$; $2$; $3$ are expected to form in the inhomogeneous system (see Fig. 3b). In the Supplementary Information, we calculate the fraction of particles in the superfluid phase of such an inhomogeneous system within a simplified model and discuss a possible relation to the outcome of the neural network. For our estimated particle numbers, we expect shells of $n = 1$, $n = 2$ and $n = 3$ to form. We have analysed and confirmed the robustness of the phase transition region to the choice of training regions.

For comparison, we also plot the visibility and the condensate fraction obtained from the same data, which are conventionally used to characterize the transition\(^{26,32}\). These quantities only drop smoothly as a function of $U/6\gamma$ with no clear indication of the location of the phase transition. While the visibility, which captures the short-range coherence of the system, remains finite deep into the Mott insulating region due to coherent particle–hole admixtures, the signal from the neural network reaches an unambiguous identification of the Mott insulating phase with $P_{\text{SF}} \approx 0$ for $U/6\gamma > 10.9$. Our analysis shows that the characterization of the superfluid-to-Mott-insulator transition in a Bose–Hubbard system from momentum-space images does enormously profit from machine-learning techniques, which yield a much smaller transition region as compared to the conventional analysis using either the visibility or the condensate fraction.

In conclusion, we have demonstrated the identification of phase transitions by applying machine-learning techniques to common experimental momentum-space images using the example of a Chern insulator and a Mott insulator. Except for the labelled training data, no further information was required for setting up the data analysis pipeline (that is, neither the data pre-processing nor the network architecture is based on prior knowledge about the system), which renders our approach to be very general. Our results point the way to unravel complex phase diagrams of experimental systems, where the Hamiltonian and the order parameters might not be known. Future directions include unsupervised machine-learning algorithms\(^{42,43}\) (that is, with unlabelled data and without pre-information about the number of phases). This approach might be useful, for example, for the experimental identification of interacting topological systems. Machine-learning approaches can also be used for reconstructing challenging many-body quantities, such as entanglement entropy, that are experimentally hard to access\(^{18}\). Furthermore, cold-atom systems are a promising platform for realizing quantum machine-learning ideas, which combine machine-learning techniques with the speed-up of quantum computers\(^{39}\).

**Online content**

Any methods, additional references, Nature Research reporting summaries, source data, statements of code and data availability and
associated accession codes are available at https://doi.org/10.1038/s41567-019-0554-0.

Received: 1 November 2018; Accepted: 13 May 2019; Published online: 1 July 2019

References

1. Carrasquilla, J. & Melko, R. G. Machine learning phases of matter. Nat. Phys. 13, 431–434 (2017).
2. van Nieuwenburg, E. P. L., Liu, Y.-H. & Huber, S. D. Learning phase transitions by confusion. Nat. Phys. 13, 435–439 (2017).
3. Carleo, G. & Troyer, M. Solving the quantum many-body problem with artificial neural networks. Science 355, 602–606 (2017).
4. Gao, X. & Duan, L.-M. Efficient representation of quantum many-body states with deep neural networks. Nat. Commun. 8, 662 (2017).
5. Haldane, F. D. M. Model for a quantum Hall effect without Landau levels: condensed-matter realization of the “parity anomaly”, Phys. Rev. Lett. 61, 2015–2018 (1988).
6. Jotzu, G. et al. Experimental realization of the topological Haldane model with ultracold fermions. Nature 515, 237–240 (2014).
7. Fläschner, N. et al. Experimental reconstruction of the Berry curvature in a Floquet Bloch band. Science 352, 1091–1094 (2016).
8. Fisher, M. P. A., Weichman, P. B., Grinstein, G. & Fisher, D. S. Boson localization and the superfluid-insulator transition. Phys. Rev. B 40, 546–570 (1989).
9. Jaksh, D., Bruder, C., Cirac, J. I., Gardiner, C. W. & Zoller, P. Cold bosonic atoms in optical lattices. Phys. Rev. Lett. 81, 3108–3111 (1998).
10. Greiner, M., Mandel, O., Esslinger, T., Hänisch, T. W. & Bloch, I. Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms. Nature 415, 39–44 (2002).
11. Lewenstein, M. et al. Ultracold atomic gases in optical lattices: mimicking condensed matter physics and beyond. Adv. Phys. 56, 243–379 (2007).
12. Bloch, I., Dalibard, J. & Zwerger, W. Many-body physics with ultracold gases. Rev. Mod. Phys. 80, 885–964 (2008).
13. LeCun, Y., Bengio, Y. & Hinton, G. Deep learning. Nature 521, 436–444 (2015).
14. Bakr, W. S. et al. Probing the superfluid-to-Mott insulator transition at the single-atom level. Science 329, 547–550 (2010).
15. Sherson, J. F. et al. Single-atom-resolved fluorescence imaging of an atomic Mott insulator. Nature 467, 68–72 (2010).
16. Ohtsuki, T. & Ohtsuki, T. Deep learning the quantum phase transitions in random two-dimensional electron systems. J. Phys. Soc. Jpn 85, 123706 (2016).
17. Ch‘ng, K., Carrasquilla, J., Melko, R. G. & Khatami, E. Machine learning phases of strongly correlated fermions. Phys. Rev. X 7, 031038 (2017).
18. Broecker, P., Carrasquilla, J., Melko, R. G. & Trebst, S. Machine learning quantum phases of matter beyond the fermion sign problem. Sci. Rep. 7, 8823 (2017).
19. Huembeli, P., Assaad, F. F. & Trebst, S. Quantum phase recognition via unsupervised machine learning. Preprint at https://arxiv.org/abs/1707.00663 (2017).
20. M. Tomoyose, B. and S. B. R. and M. T. and L. A. and C. B. and C. W. and A. K. and H. H. and M. O. and J. F. and P. S. acknowledge financial support from the European Commission (Marie Skłodowska Curie Fellowship INFOS, grant number 652837).
Methods

Experimental set-up and system preparation. The experiments are performed with ultracold atoms in optical lattices. For the Haldane model, we use spin-polarized fermionic $^{40}$K atoms (mass $m = 40$ a.m.u.) in a honeycomb optical lattice formed by three lattice beams of wavelength $\lambda = 1,804$ nm intersecting at an angle of 120°. By controlling the polarization of the lattice beams, we produce an energy offset between the A and B sublattices of $h \nu = 6.1$ kHz for the lattice depth of 7.4$E_r$ in units of the recoil energy $E_r = h^2/2m\lambda^2$ (ref. 1). The external trapping frequency of about 70 Hz is dominated by the finite size of the lattice beams. We shake the lattice by modulating the phases of the three interfering laser beams with $\omega_{\text{sh}} = \Delta \omega \pm (2\cos(\phi) + 3\sin(\omega t))$ and $\phi_0 = 0$, respectively. Here, $\omega_r/2\pi$ is the shaking frequency, $\Delta \omega$ is the shaking amplitude and $\phi$ is the shaking phase. The formula describes an elliptical forcing, which produces a Floquet system with new properties$^{40,41}$. For $\phi = 0$, 180°, the shaking is linear (under $\phi = 45°$ with respect to a reciprocal lattice vector), thus preserving time-reversal symmetry, and for $\phi = 90°$, the shaking is circular clockwise or anticlockwise, respectively, and maximally breaks time-reversal symmetry.

For the preparation of the Floquet bands, we start with a completely filled lowest band of the static lattice and perform ramps of the Floquet parameters. We first ramp up the shaking amplitude within 5 ms to 1 kHz at a shaking frequency of 4.5 kHz (far from the $C = \frac{\pi}{2}$ regimes) and then ramp the shaking frequency to the final value within 2 ms. Due to the closing of the bandgaps and the heating rates, the preparation cannot be fully adiabatic and leads to a population in the lowest band of typically 50–75%. We measure the population in the lowest band by ramping back onto the bare bands, performing adiabatic band mapping and counting the population in the first and second Brillouin zones (compare ref. 1). Supplementary Fig. 1 shows the fractional population in the lowest Floquet Bloch band for the different Floquet parameters as obtained by this procedure. As there is additional heating during the ramping back to the bare bands, the measurement gives a lower bound on the fractional population that is relevant to the measurements of the momentum density. The preparation works best for circular shaking ($\phi = \pm 90°$) with a population above 70%. We attribute this to the fact that the bandgap between the two Floquet bands is largest for circular shaking. The smaller population of the lowest band away from circular shaking might be the origin of the slightly larger deviation between the measured and the numerical phase diagram at these shaking phases. We choose varying waiting times in the Floquet system to ensure a sampling of the Floquet micromotion of the system. We image the cloud after an expansion of 21 ms time-of-flight.

For the Bose–Hubbard model, we use $^{87}$Rb atoms (mass $m = 87$ a.m.u.) in a triangular optical lattice of wavelength $\lambda = 830$ nm as described in ref. 7. For the preparation of the two-dimensional Bose–Hubbard system, we first ramp up the triangular lattice to a fixed depth of $3.0E_r$, thus creating a stack of decoupled two-dimensional systems. We then adiabatically ramp up the triangular lattice within 150 ms to prepare the system. The momentum-space density is imaged after a 21 ms time-of-flight. The Hubbard parameters $J$ and $U$ are obtained from a band structure calculation of the optical lattice potential. The inhomogeneous system has a mean harmonic trapping frequency of $\nu_\perp 2\pi = 90$ Hz. The determination of the visibility and the condensate fraction is described in ref. 12.

Network architecture and implementation. Motivated by their success in image recognition, we employ convolutional layers to identify physical phases by feature maps. See, for example, refs. 13–15 for an introduction to machine-learning techniques from a physics perspective. We have studied a variety of network architectures and found that convolutional neural networks have a better performance than shallow fully connected networks judged by the comparison of their predicted phase diagrams with the numerical prediction. Within the convolutional neural networks, we found the results to be quite robust to the choice of parameters such as the number of layers or the filter sizes. For the data presented in the main text, we used the architectures defined in Table 1. The code is implemented in Matlab 2017b using the build-in functionality for neuronal networks and is run on graphics processing units. We use the technique of data augmentation for training (such as shifting, flipping, rotating or scaling of images or adding noise), because flipping the images may change physical properties of the system (see discussion below). We ensure that the amount of training data is symmetric (for example, it contains the same number of images for $\phi = 90°$ and for $\phi = 90°$).

To train the networks on the Bose–Hubbard data, we choose an initial learning rate of 0.001. To improve the learning rates, the mini batch size is set to 90. As the dataset size for the Bose–Hubbard system is significantly smaller than that for the Haldane system, we decided to not split validation data and limit the training to 50 epochs, which achieves good results for our parameters. The data are shuffled every epoch and the other parameters are the default values.

To extract the transition point from the probability curve of the classes, we fit a heuristic error function and take the $P = 0.5$ value as the transition point. In the case of the Haldane system, we use the form $P(x) = \frac{1}{2} \left[ \text{erf} \left( \frac{x - \bar{x}}{\sigma} \right) - \text{erf} \left( \frac{x - \bar{x}}{\sigma} \right) \right]$ with the two transitions at $x_1$ and $x_2$ and the widths $\sigma_1$ and $\sigma_2$. In the case of the Bose–Hubbard system, we fit the error function as a function of $\log(1/U/6f)$, which is approximately linearly related to the lattice depth.

Discussion of network performance. We have carried out several cross-checks to gain some understanding of the neural network$^{16,17}$. Interpreting deep networks is still in its infancy and the networks often appear like a black box. We compared the networks of the two examples of the Bose–Hubbard system and the Haldane system and found that applying the network trained on one example to the data from the other example gives a definite result: the Haldane data are all identified.

### Table 1 | Network architectures

| Layer | Layer description |
|-------|-------------------|
| 1     | Image input 87x87x1 images with ‘zerocentre’ normalization |
| 2     | Convolution 8x5x5x1 convolutions with stride [2 2] and padding [0 0 0 0] |
| 3     | Batchnorm Batch normalization with 8 channels |
| 4     | ReLU RelU (rectified-linear unit layer) |
| 5     | Fully connected Fully connected layer with 3 neurons |
| 6     | ReLU RelU |
| 7     | Dropout 50% dropout |
| 8     | Fully connected Fully connected layer with 190 neurons |
| 9     | ReLU RelU |
| 10    | Dropout 50% dropout |
| 11    | Fully connected Fully connected layer with 3 neurons |
| 12    | Softmax Softmax |
| 13    | Classification output 8x8x7x1 images with ‘zerocentre’ normalization |
| 14    | Cross-channel normalization with 5 channels per element |
| 15    | RelU RelU |
| 16    | Dropout 50% dropout |
| 17    | Fully connected Fully connected layer with 2 neurons |
| 18    | Softmax Softmax |
| 19    | Cross-channel normalization with 6 channels per element |
| 20    | RelU RelU |

The table shows the layers of the network architectures used in this work. The network for the Haldane system consists of 13 layers; the network for the Bose–Hubbard system consists of 14 layers.
as a Mott insulator instead of a superfluid and the Bose–Hubbard data are all identified as topologically trivial ($C=0$). Identifying the data from the Bose–Hubbard system as topologically trivial is a correct classification and might point a way to using the networks for transfer learning.

To understand how the classification depends on the size of the image input, we repeat the training and analysis for cropped images and monitor the success probability for the validation data. In the case of the Haldane model, the training is successful down to cropping the input images to slightly less than one reciprocal lattice vector (see Supplementary Fig. 4). This might be surprising, because the images do then not contain the full Brillouin zone, which is in general required to define the Chern number from a momentum-resolved Bloch state tomography. However, for a specific realization, such as the Haldane-like model studied here, non-local information of the Chern number might be directly encoded in certain local momenta. Also in the case of the Bose–Hubbard system, the training is insensitive to the image size over a broad range (Supplementary Fig. 5).

As another cross-check, we apply the trained network for the Haldane model to images that were flipped along the horizontal axis, the vertical axis or both (Supplementary Fig. 6). Flipping the images amounts to flipping the momentum distribution. While the phase diagrams are distorted, the regions with non-trivial Chern number are still clearly identified. For a single flip, the Chern number inverts for the flip around the vertical axis, which transforms the $K$ point into the $K'$ point. For a discussion of the sign of the Chern number in such a Floquet realization of the Haldane model, see also the Supplementary Material of ref. 28. A flipping around both axes corresponds to an inversion in momentum space, which changes the sign of the breaking of time-reversal symmetry and therefore leads to a change of sign in the Chern number.

To gain some insight into why the neural network can identify the Chern number from the momentum-space images released from the driven lattices, one should consider the Bloch state tomography introduced in refs. 7,29. They rely on similar images, but require varying hold times in the static lattice before expansion for a full reconstruction of the state. While the Chern number can be obtained from a full state tomography by calculating the Berry curvature and integrating it over the first Brillouin zone, it is not obvious that this can be done unambiguously from the limited information of a single such image. Therefore, our results pave a way of analysing phase transitions in quantum gas experiments. Also note that the state tomography method a priori cannot distinguish between a pseudospin state on the northern or southern hemisphere of the Bloch sphere and this information usually requires an additional measurement of adiabatic band mapping. Supplementary Fig. 7 shows a selection of typical single images for the three classes. The class $C=0$ contains images for shaking frequency above and below the $C=\pm 1$ region and it is notable that the network successfully groups these two regions as one class. While the human eye can see some similarity in the images, it cannot extract the Chern number (including its sign), whereas the artificial neural network can extract it.

Data availability
Source data for Figs. 2 and 3 are available in the Supplementary information. All data files including onnx files of the trained networks are available from the corresponding author on request.

References
40. Struck, J. et al. Quantum simulation of frustrated classical magnetism in triangular optical lattices. Science 333, 996–999 (2011).
41. Eckardt, A. Colloquium: atomic quantum gases in periodically driven optical lattices. Rev. Mod. Phys. 89, 011004 (2017).
42. Asteria, L. et al. Measuring quantized circular dichroism in ultracold topological matter. Nat. Phys. 15, 449–454 (2019).
43. Nielsen, M. A. Neural Networks and Deep Learning (Determination Press, 2015).
44. Goodfellow, I., Bengio, Y. & Courville, A. Deep Learning (MIT Press, 2017).
45. Mehta, P. et al. A high-bias, low-variance introduction to Machine Learning for physicists. Phys. Rep. 810, 1–124 (2019).
46. Lin, H. W., Tegmark, M. & Rolnik, D. Why does deep and cheap learning work so well? J. Stat. Phys. 168, 1223–1247 (2017).
47. Montavon, G., Samek, W. & Müller, K.-R. Methods for interpreting and understanding deep neural networks. Digit. Signal Process. 73, 1–15 (2018).
48. Sun, N., Yi, J., Zhang, P., Shen, H. & Zhai, H. Deep learning topological invariants of band insulators. Phys. Rev. B 98, 085402 (2018).