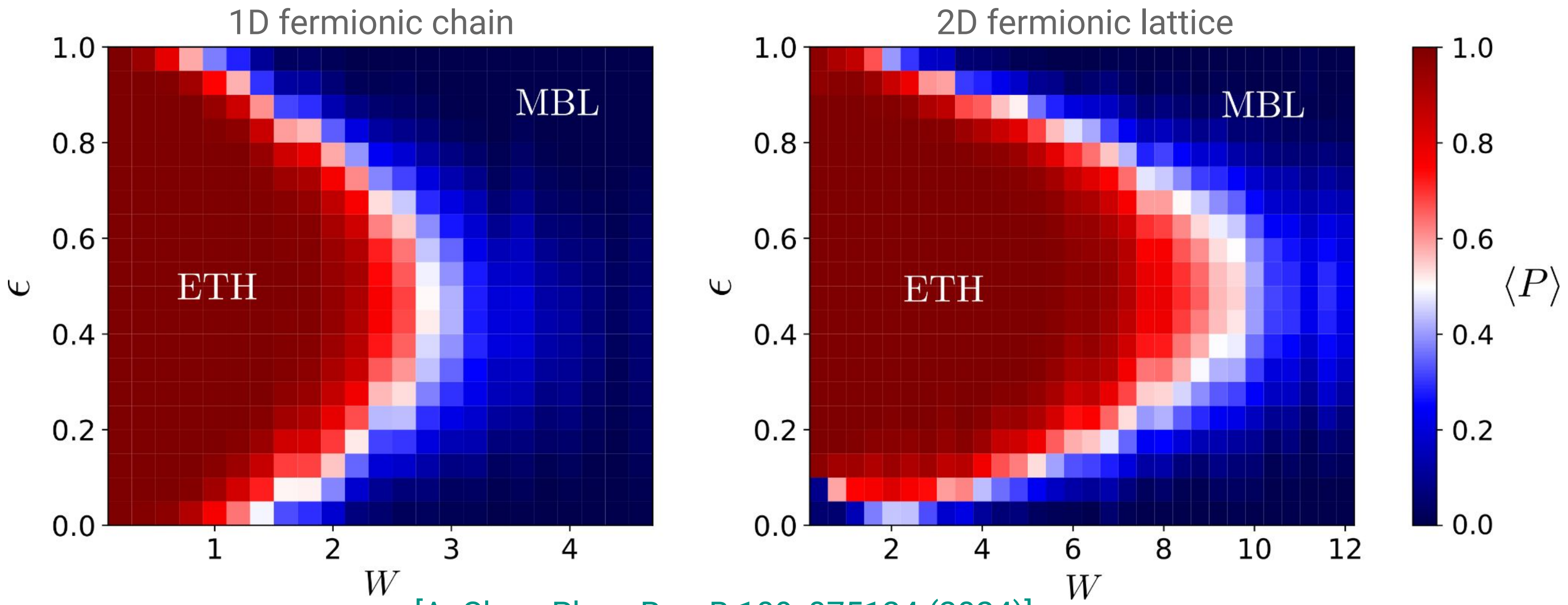
Many-body mobility edges revealed by convolutional neural networks



[A. Chen, Phys. Rev. B 109, 075124 (2024)]

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Recent applications of ML in CMP

Supervised/unsupervised learning (i.e. learning from big data sets)

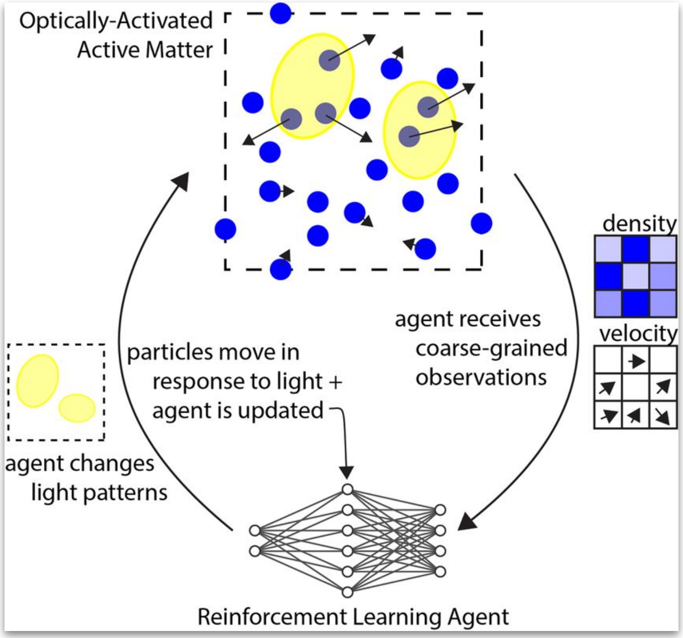
- Quantum state tomography
- ab initio calculations
- Phase classification -> this work

Reinforcement learning (i.e. learning by trial and error)

- Quantum device control
- Active matter control

Neural network architecture

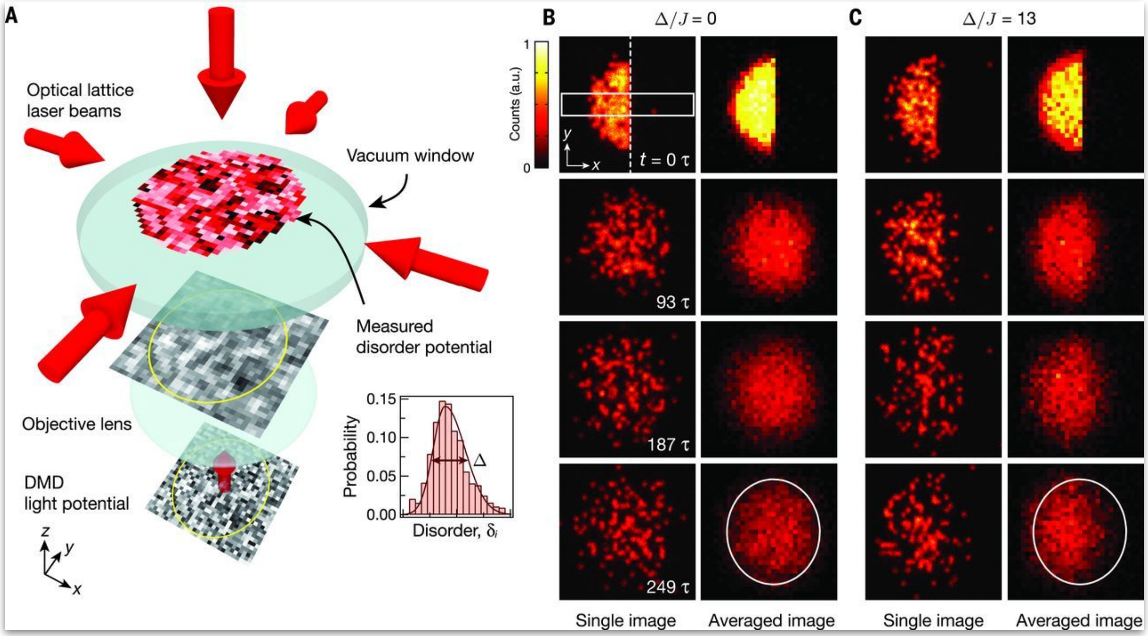
- Neural network as variational ansatz



Many-body localization

MBL = localization of many-body wavefunctions in Fock space

-> breaks eigenstate thermalization hypothesis (ETH) -> quantum memory?



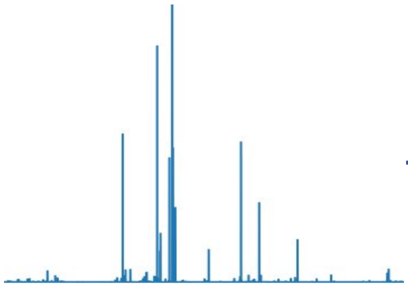
MBL in 2D optical lattice: Initial condition is partially preserved over long times.

Machine learning for MBL

It is hard to study the ETH-MBL phase transition…

- Computationally expensive
  - Degrees of freedom grow exponentially with system size
  - Conventional methods require multiple system sizes
- Strong finite-size effect at the transition -> No consensus on the scaling theory

Supervised learning presents an alternative approach to study the ETH-MBL phase transition.



Many-body wavefunction

Input → Neural network → Predict → Probability of the wavefunction being delocalized

Supervised learning: Prepare training data

Our systems: Repulsive, spinless fermions on 1D and 2D lattices with random on-site potentials

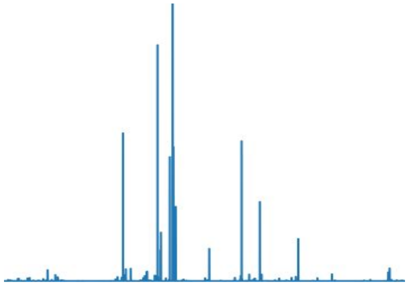
$$H = \sum_{\langle i,j \rangle} \left[-t \left(c_i^\dagger c_j + c_j^\dagger c_i \right) + V \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right) \right] + \sum_{i=1}^{N} u_i \left(n_i - \frac{1}{2} \right)$$

$u_i \in$ [-W/2, W/2]
W = disorder strength

50 disorder realizations at small W $\xrightarrow{\text{ED}}$

$\xrightarrow{\text{Label}}$ “1”

50 disorder realizations at large W $\xrightarrow{\text{ED}}$



$\xrightarrow{\text{Label}}$ “0”

Labeled training data

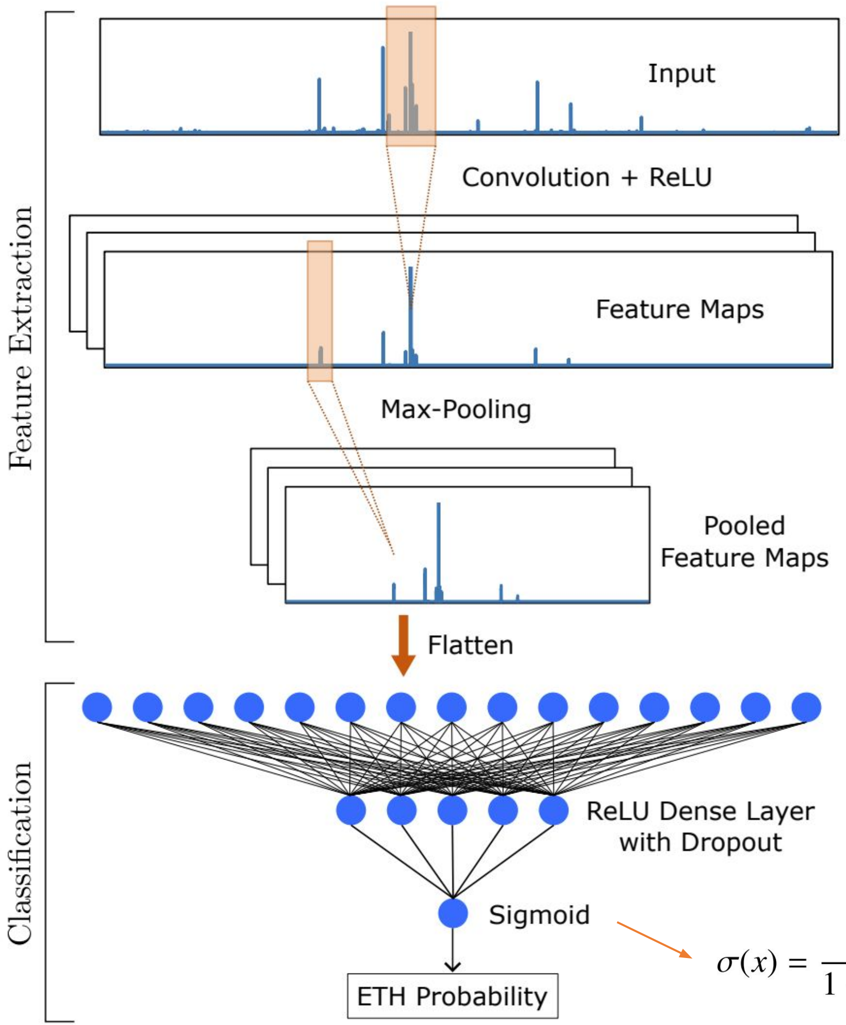
Neural network architecture

Deep NN =
Layers of linear maps

$$f(v) = Av + b$$

and nonlinear activation functions

$$\mathrm{ReLU}(x) = \max(0, x)$$



$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

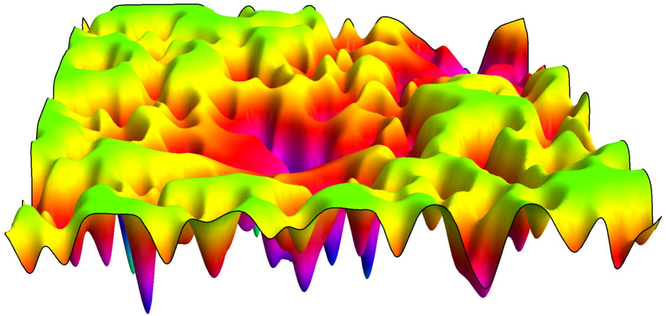
Figure from Wales, Annu. Rev. Phys. Chem. 69(1), 401 (2018)

Supervised learning: Training

Training in supervised learning = optimize the neural-network parameters (weights and biases) through gradient descent to minimize the loss function

$$\text{Loss} = -(\underbrace{y}_{\text{label}} \log(\underbrace{P}_{\text{prediction}}) + (1 - y)\log(1 - P))$$

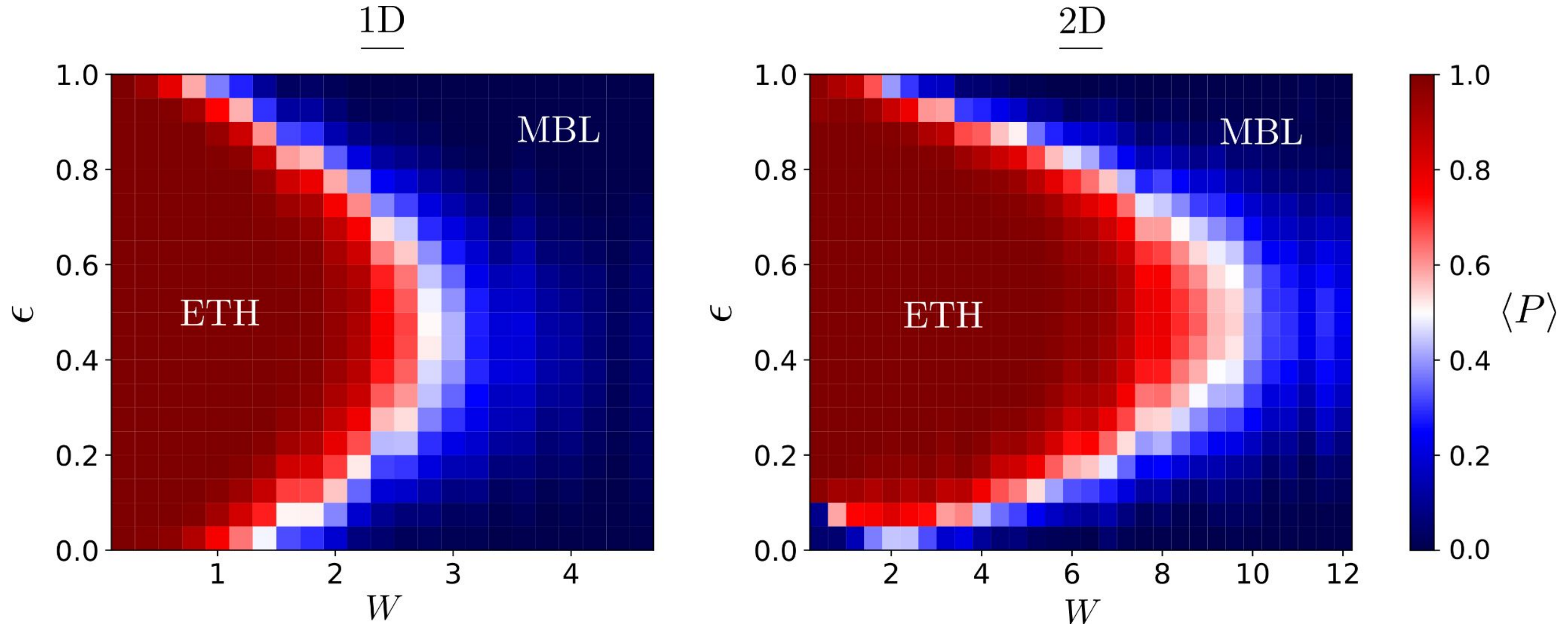
It's not easy – think of finding the ground state of a spin glass system through gradient descent.



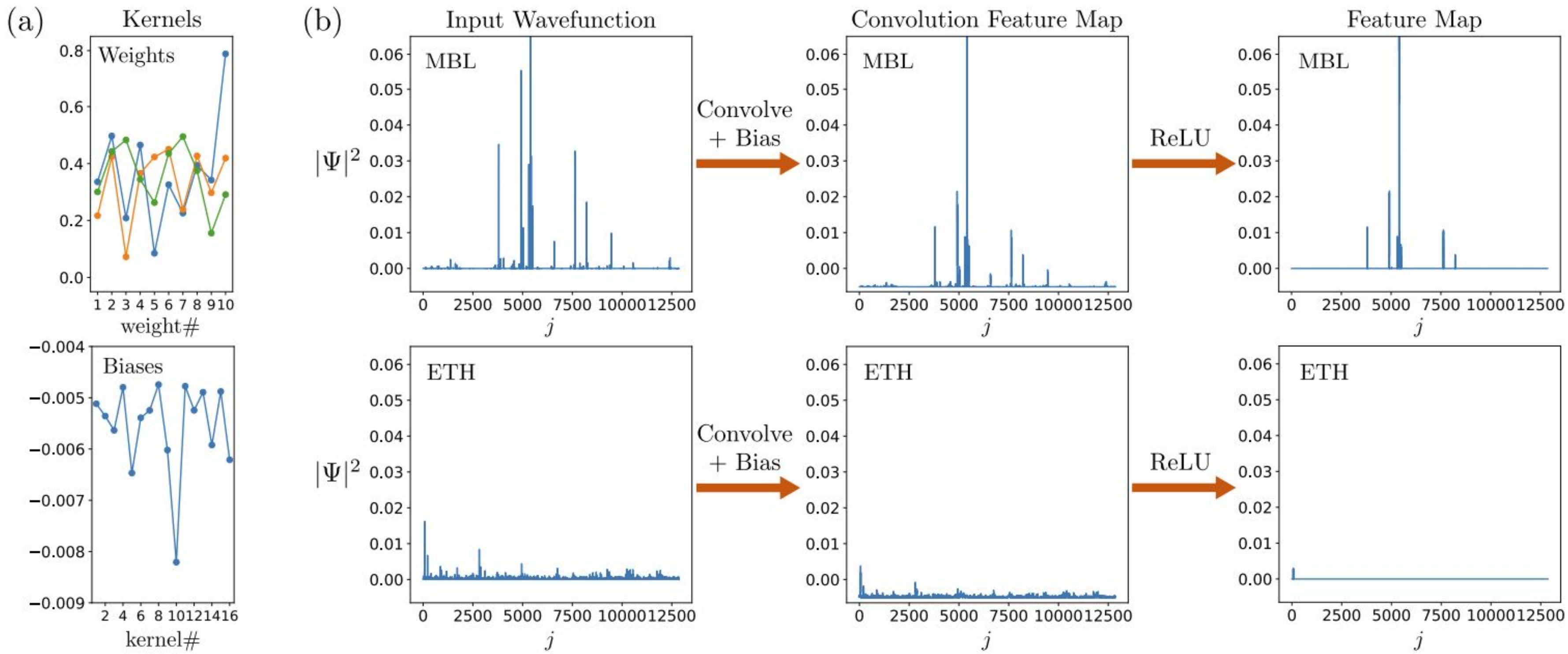
Successful training requires careful tuning of *hyperparameters* (learning rate, # neurons, etc).

Result: Energy-resolved phase diagrams

At small and large W, our trained CNNs correctly classify over 99.95% of the wavefunctions.
-> Use CNNs predictions in the intermediate region to generate phase diagrams



Result: What's in the black box?



Conclusion

- Using labelled data, we trained CNNs to classify many-body wavefunctions as delocalized (ETH) or localized (MBL).
- Using CNN’s predictions, we generated phase diagrams of finite-sized 1D and 2D disordered many-body systems.
- To extrapolate to the thermodynamic limit, we need to consider more system sizes and model the scaling behavior, providing another angle to characterize the elusive MBL transition.