University of Zurich[UZH]

Frank Schindler
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Probing many-body localization **with neural networks**

Titus Neupert
(U Zurich)

Nicolas Regnault
(ENS Paris)

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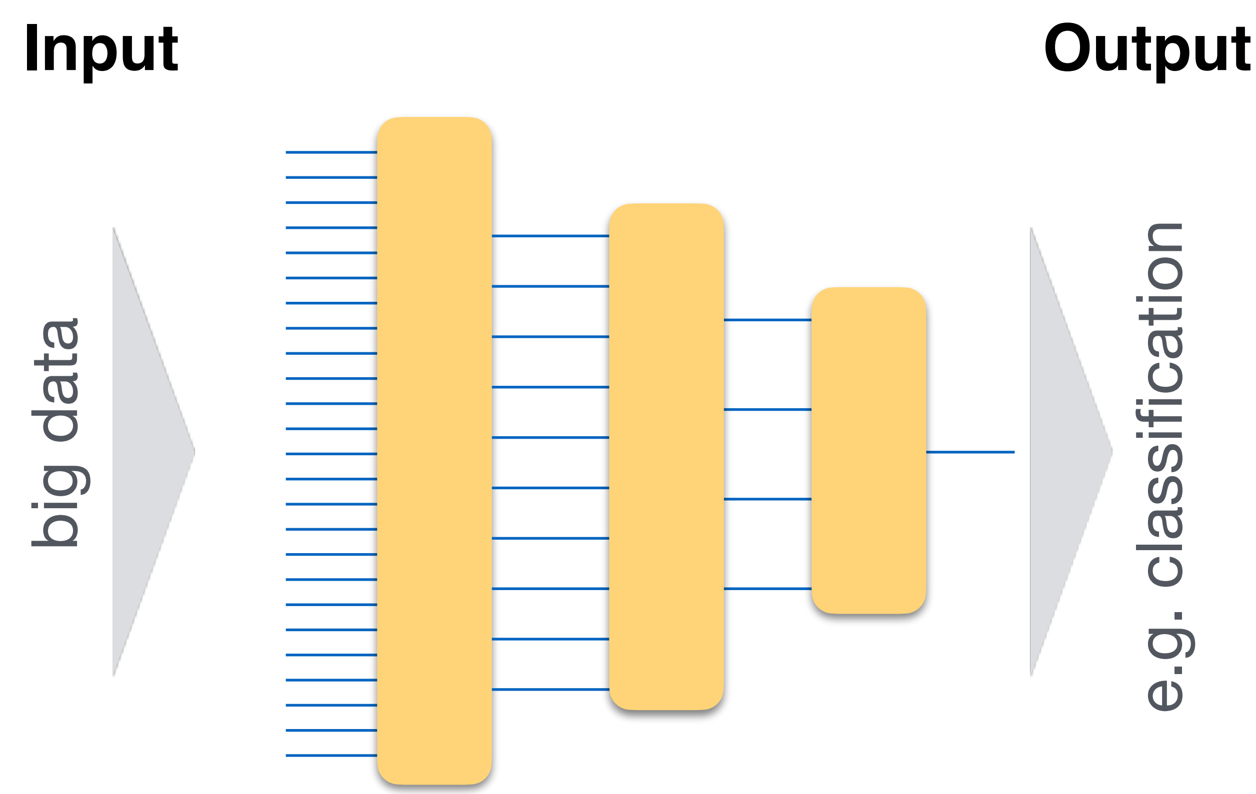
1) Intro to neural networks
2) Problem: Detection of MBL versus thermalization
3) Network architecture
4) Results on phase diagrams and structure of MBL states
5) Dreaming

Machine Learning/ Artificial Intelligence

Supervised learning

Train network with large amount of **labelled data** (input-output pairs): Reduce **cost function** (distance measure between network output and labels) via gradient descent.

Verify network performance on distinct test data set.



Unsupervised learning

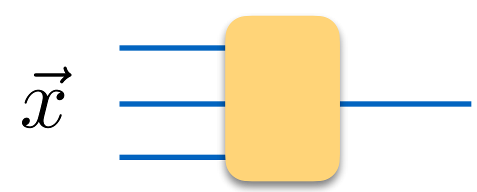
Use unlabelled data, network learns to cluster data/find structure/learn probability distribution of features

Holy grail of the field

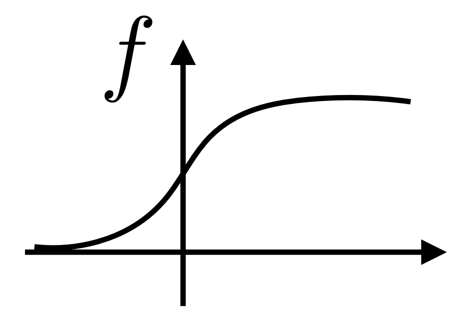
Supervised learning with Artificial Neural Networks

goal: learn complicated function $\hat{F}(\vec{x})$ with $\dim(\vec{x}) \gg 1$
from examples by finding $\min_F \mathrm{Error}[F, \hat{F}]$

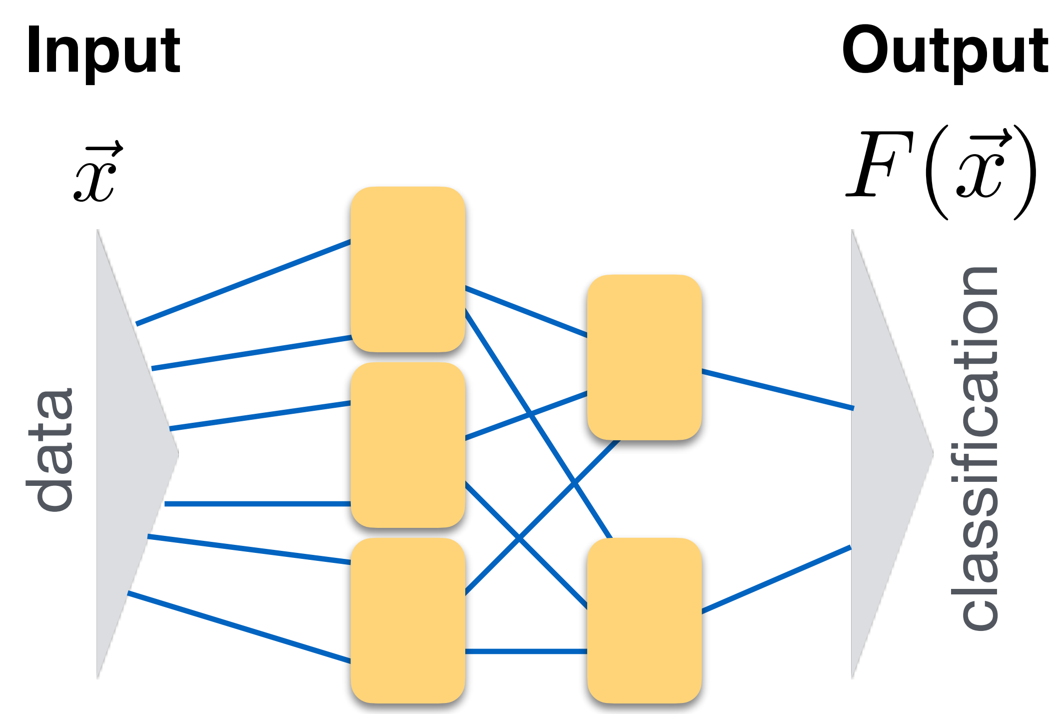
Individual neuron:
combination of linear map (weights + biases) and nonlinear activation function



$f(\vec{w} \cdot \vec{x} + b)$



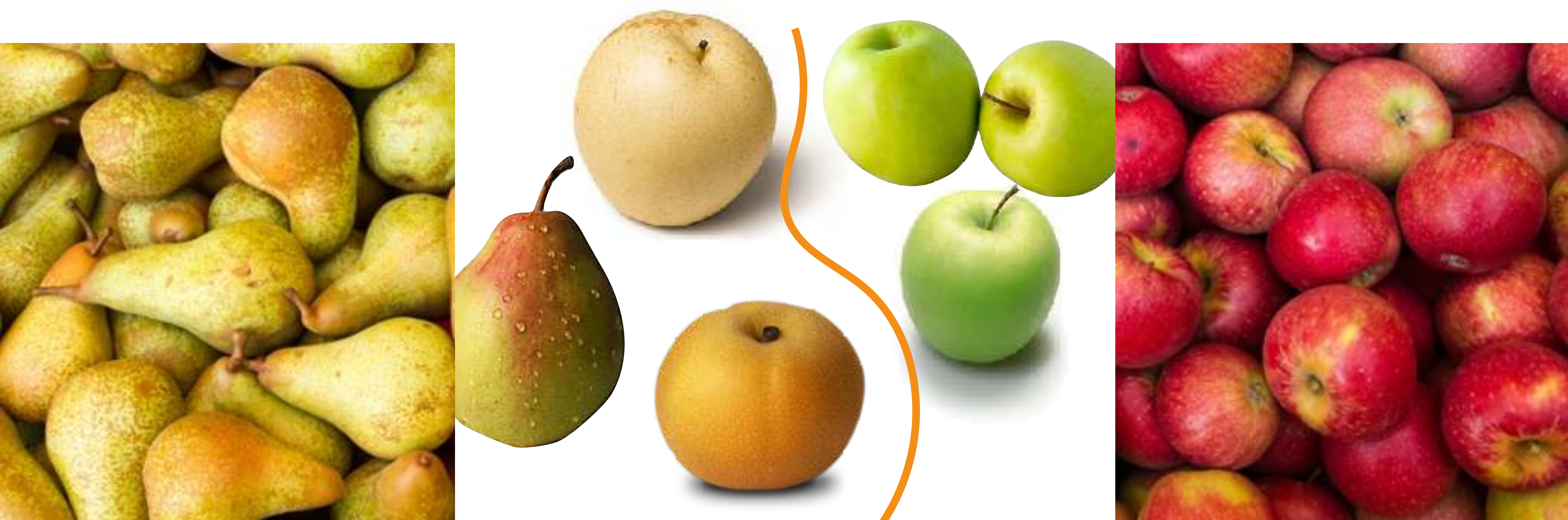
Deep network: many layers of neurons



Objective:
Classification of phases of matter using entanglement spectra

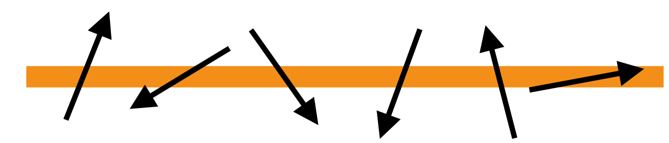
Supervised learning:
Train network with data deep in the respective phase

Determine phase boundary:
Apply network to states for which classification is less clear



Toy problem: Many-body localization

Standard model of MBL: spin-1/2 disordered Heisenberg chain, open boundary conditions



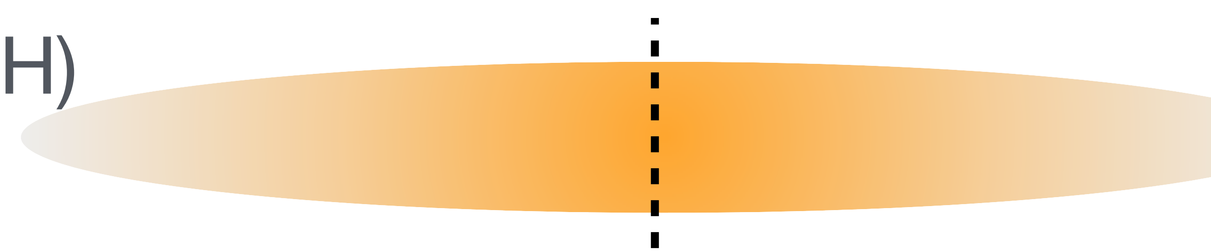
$$H = J \sum_{\mathsf{r}=1}^{N-1} \boldsymbol{S}_{\mathsf{r}} \cdot \boldsymbol{S}_{\mathsf{r}+1} + \sum_{\mathsf{r}=1}^{N} h_{\mathsf{r}} S_{\mathsf{r}}^{z}$$

$$J = 1$$

$$h_{\mathsf{r}} \in [-\bar{h}, \bar{h}]$$

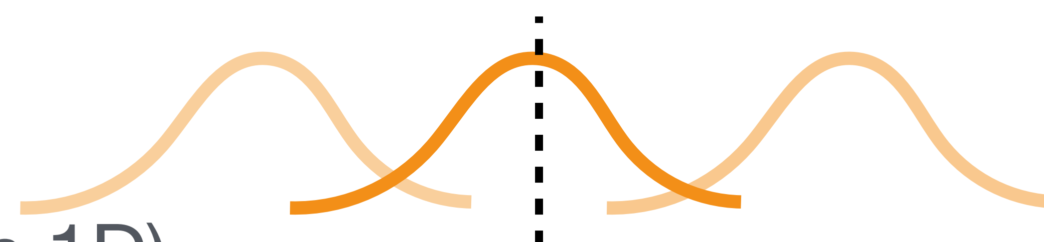
$\bar{h} \ll 1$ **thermalizing** regime (obeys ETH)

volume law entanglement



$\bar{h} \gg 1$ **many-body localized** regime

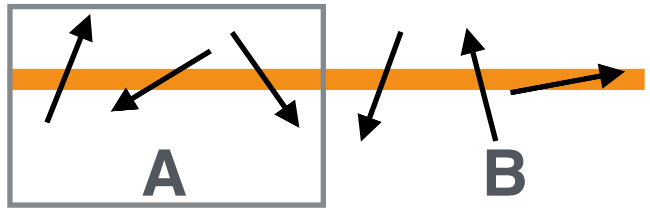
area law entanglement (constant in 1D)



Conventional classification methods

based on energy level spectrum or entanglement entropy/spectrum

$$\rho_A = \mathrm{Tr}_B \left|\Psi\right\rangle \left\langle\Psi\right| \equiv e^{-H_{\mathrm{e}}}$$



i) **Schmidt gap**: $\lambda_1(\rho_A) - \lambda_2(\rho_A)$ $\to 1$ for MBL (nearly pure)

$\ll 1$ for ETH

ii) Volume vs. area law **scaling** of $S(N_A)$ with N_A

iii) **Standard deviation** of $S(N_A)$ over many consecutive eigenstates

large near the transition where both MBL and ETH like states coexist

iii) **Level statistics** of either the entanglement spectrum or the energy spectrum follow distinct statistical distributions in each regime

Conventional classification methods

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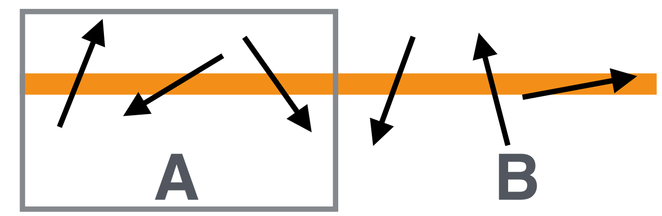


crude

i) **Schmidt gap**: $\lambda_1(\rho_A) - \lambda_2(\rho_A) \quad \to 1$ for MBL (nearly pure)

needs finite size scaling

ii) Volume vs. area law **scaling** of $S(N$

phase transition does not correspond to maximum

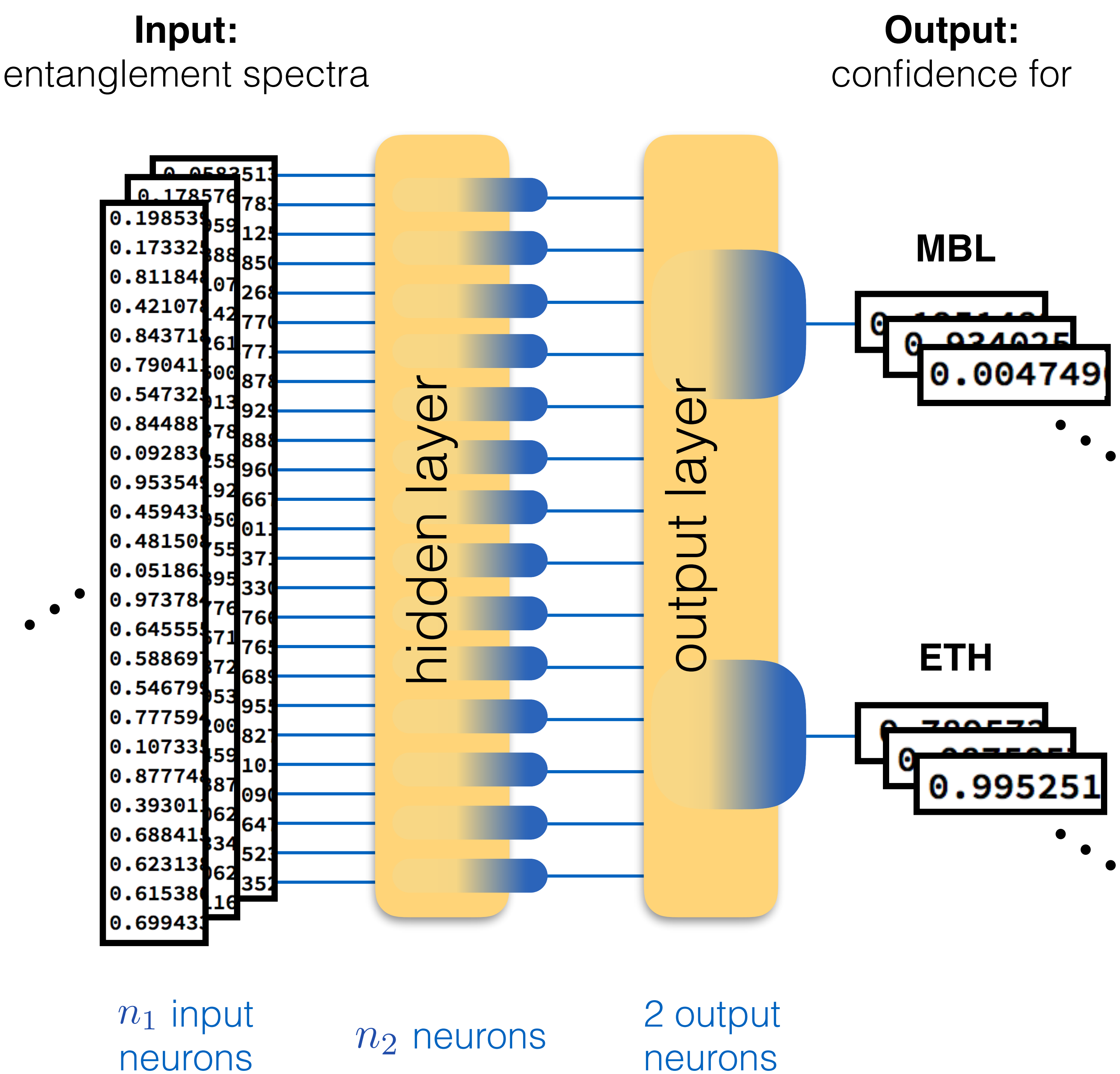
iii) **Standard deviation** of $S(N_A)$ o… es

large near the transition where both MBL and ETH like states coexist

iii) **Level statistics** of either the entanglement spectrum or the energy spectrum follow distinct statistical distributions in each regime

needs large systems

Structure of neural network



$$\mathrm{ReLu}_i(x) = x_i\,\theta(x_i)$$

$$\mathrm{Softmax}_i(x) = \frac{e^{-x_i}}{\sum_j e^{-x_j}}$$

Cost function and regularization

In training, we minimize the following functional for F via gradient descent:

Cross entropy

$$\mathrm{Error}[F,\hat{F}] = -\sum_{\vec{x}\in\mathrm{TD}}\sum_{i=1}^{2}\hat{F}_i(\vec{x})\log F_i(\vec{x}) + \mu\sum_{\vec{w}}|\vec{w}|^2 - \delta\sum_{\vec{x}\in\mathrm{TR}}\sum_{i=1}^{2}F_i(\vec{x})\log F_i(\vec{x})$$

labelled training data

classifying output neurons: 2 options, ETH or MBL

Weight decay

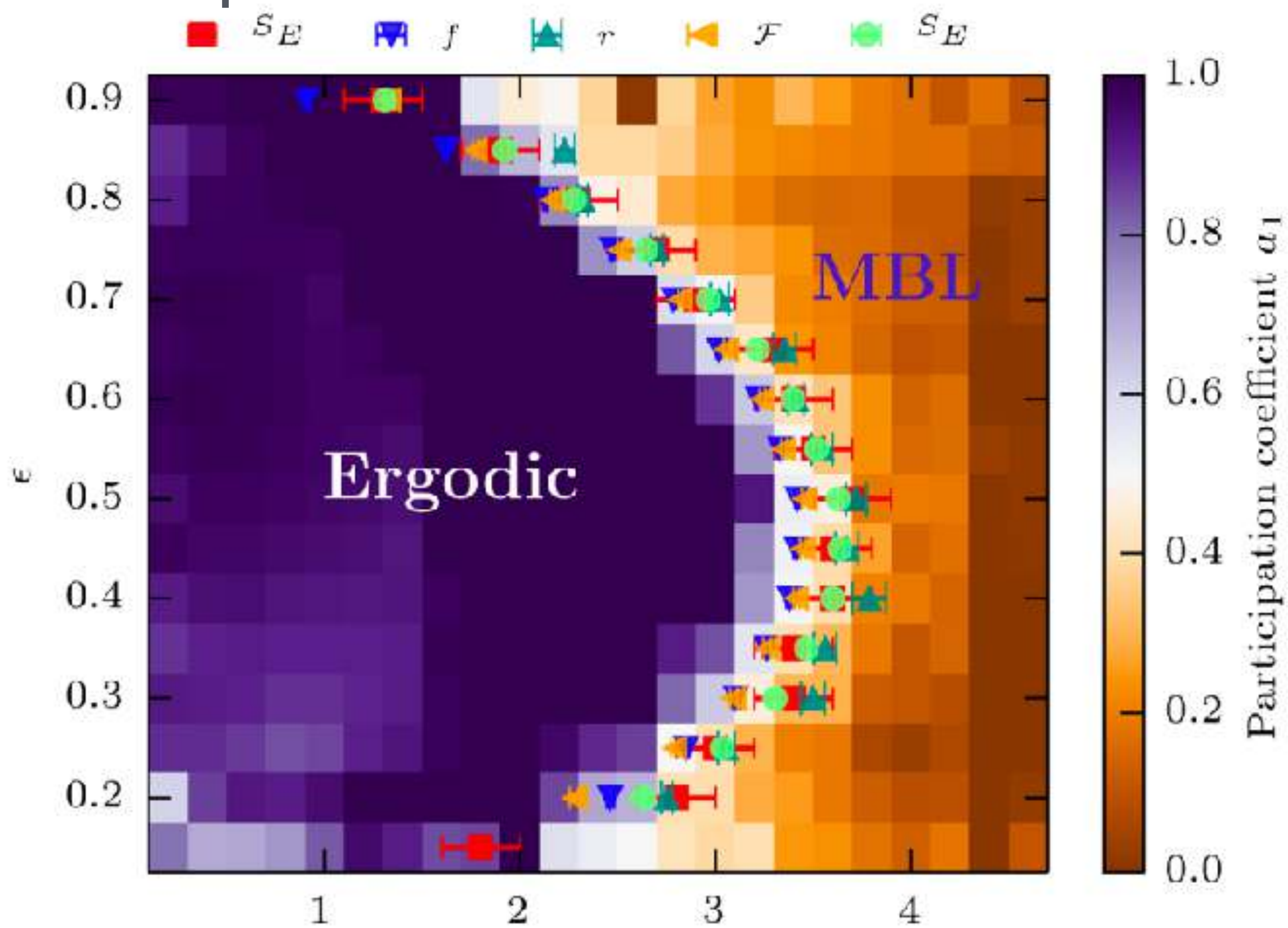
favors having only few nonzero weights/using as few neurons as possible

Confidence optimization

favors unlabelled data near phase transition to be classified confidently

random subset of spectra near transition

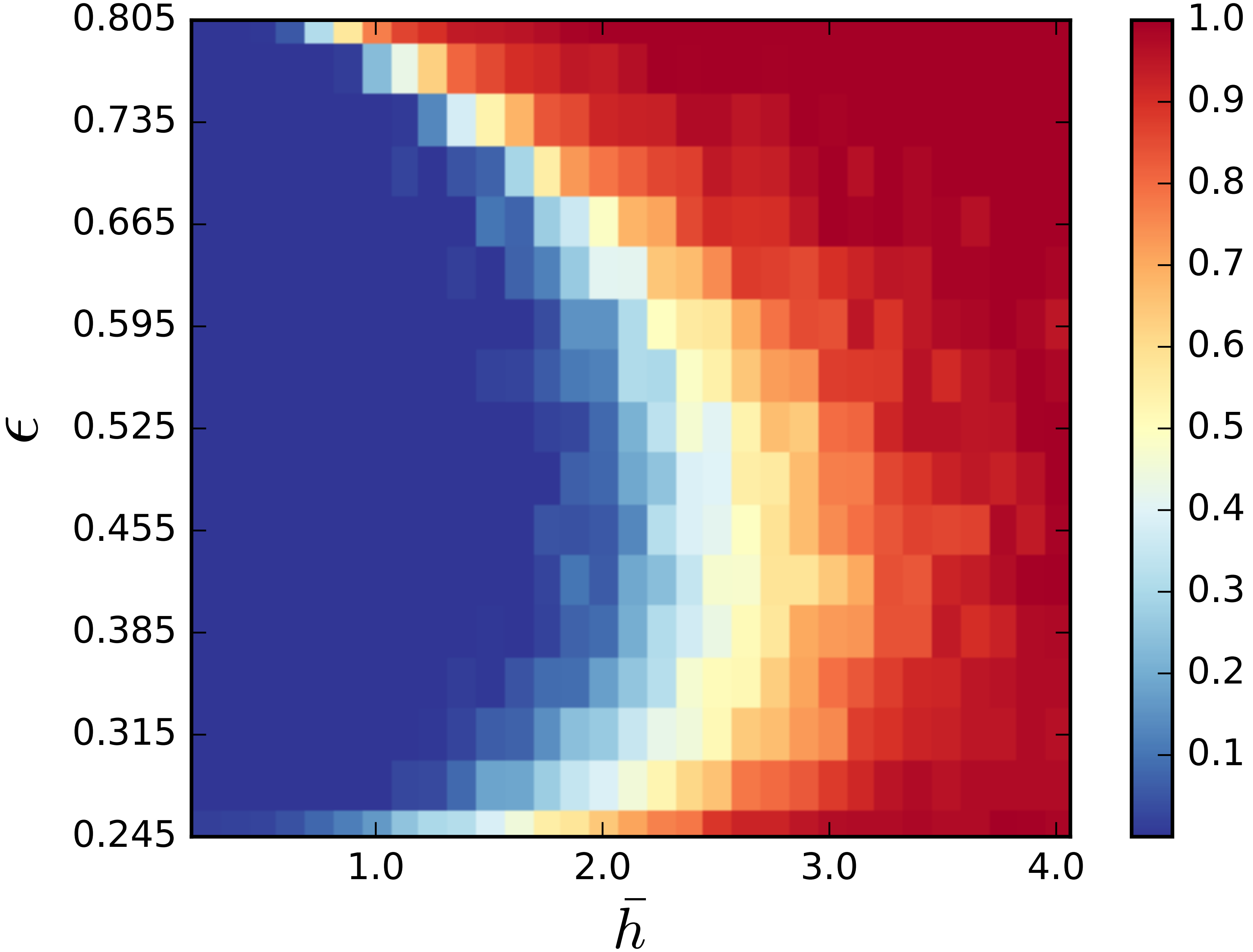
For comparison: Conventional methods



Volume law coefficient of the entanglement entropy

[Luitz et al., PRB 2015]

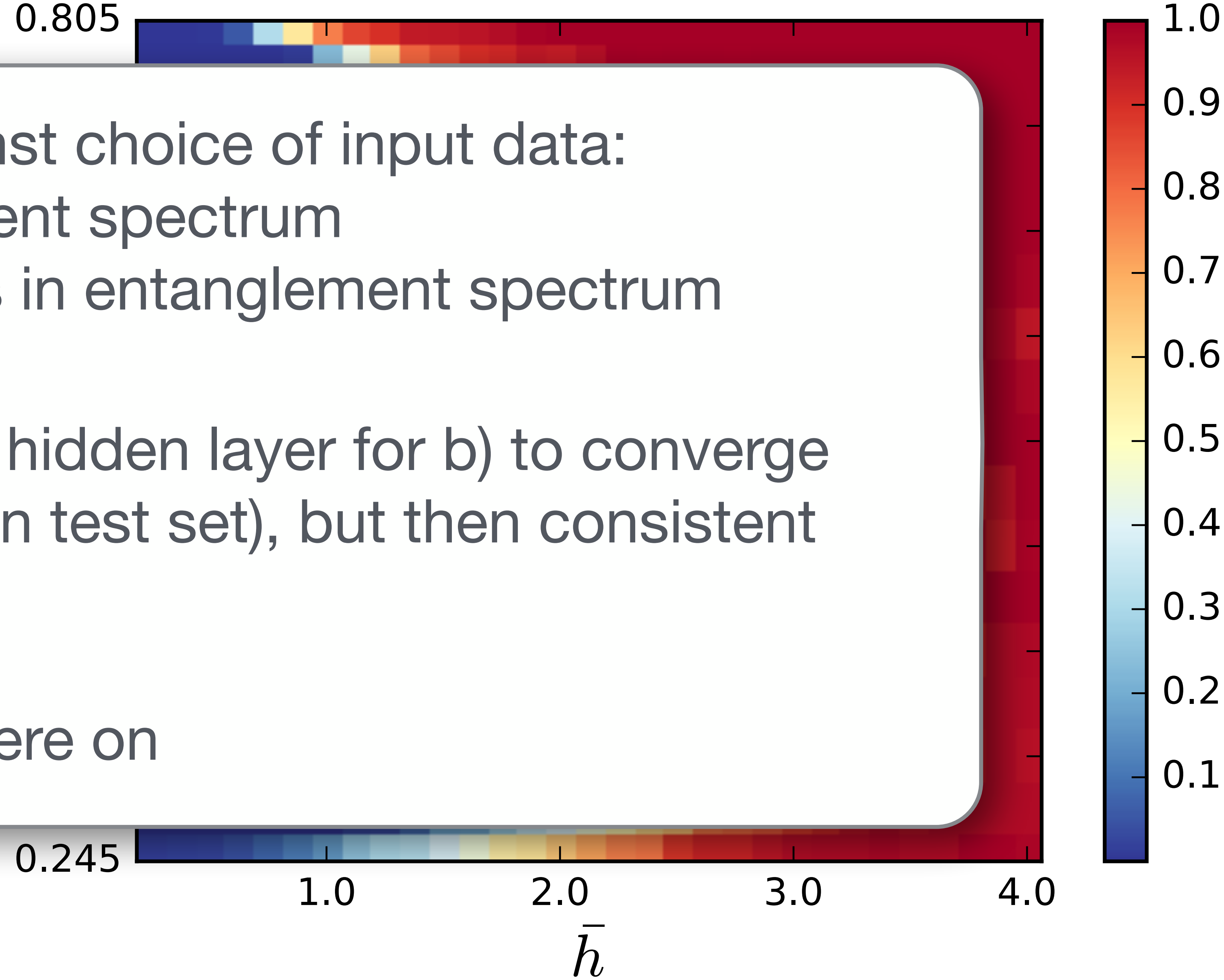
Results: Disorder-averaged phase diagram



Confidence for MBL averaged over disorder realization and eigenstates in energy window

- fewer disorder realizations (40)
- smaller system (N=16)

Results: Disorder-averaged phase diagram



Robust against choice of input data:
a) entanglement spectrum
b) differences in entanglement spectrum

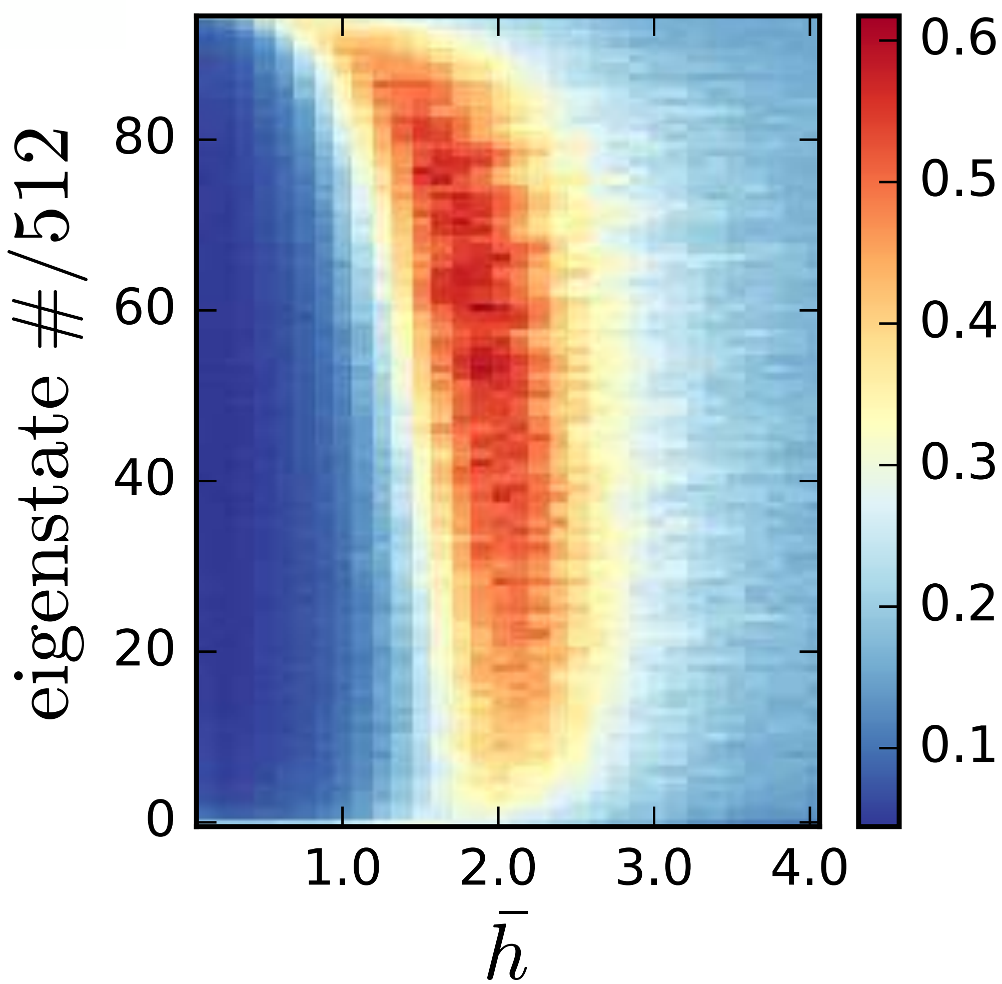
Need second hidden layer for b) to converge (yield 100% on test set), but then consistent results

Use a) from here on

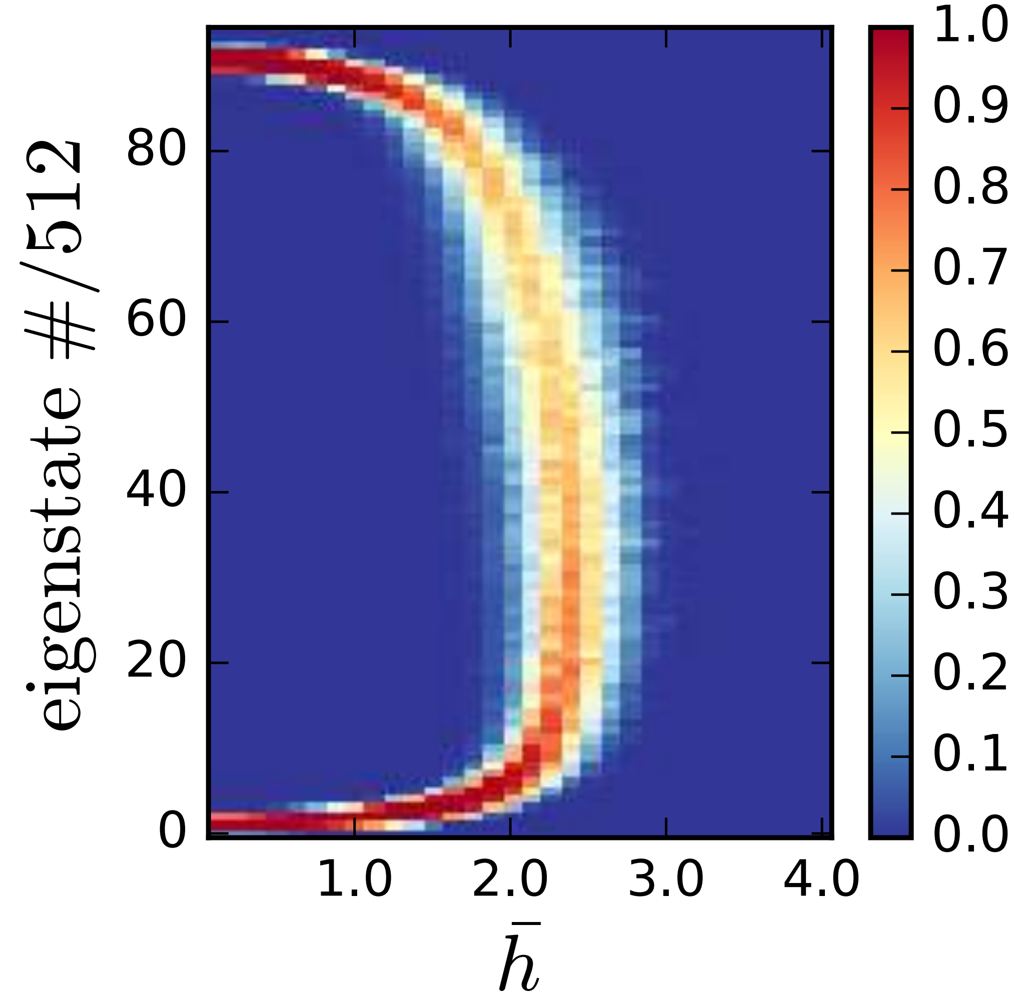
Confidence for MBL averaged over disorder realization and eigenstates in energy window

- fewer disorder realizations (40)
- smaller system (N=16)

Results: Transition in single disorder realization



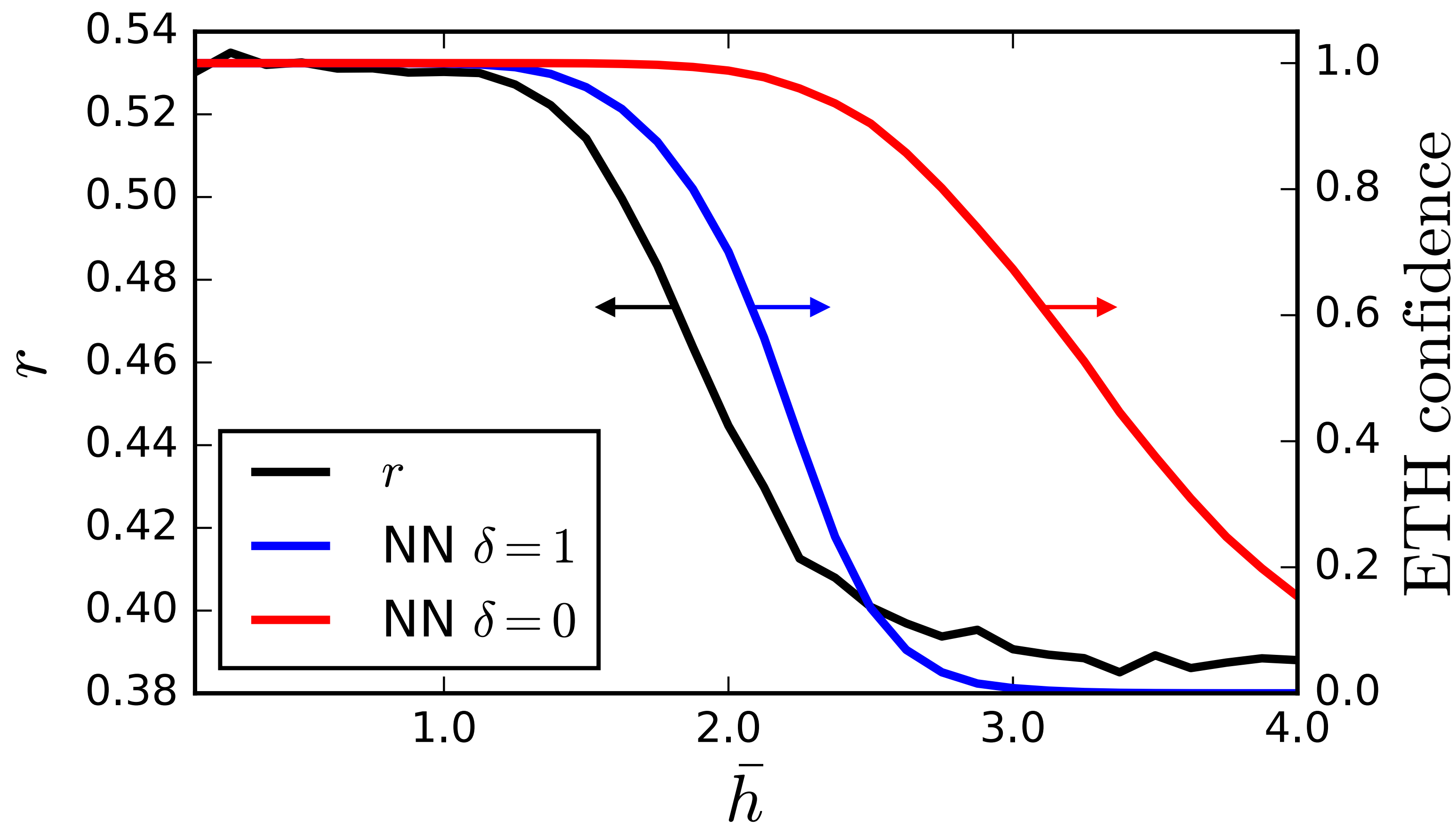
standard deviation of entanglement entropy over 512 consecutive eigenstates



fraction of uncertainly classified states (out of 512 consecutive states)

output >0.9 taken as certain

Results: **Comparison with energy level statistics**



blue: with confidence optimization

red: without confidence optimization

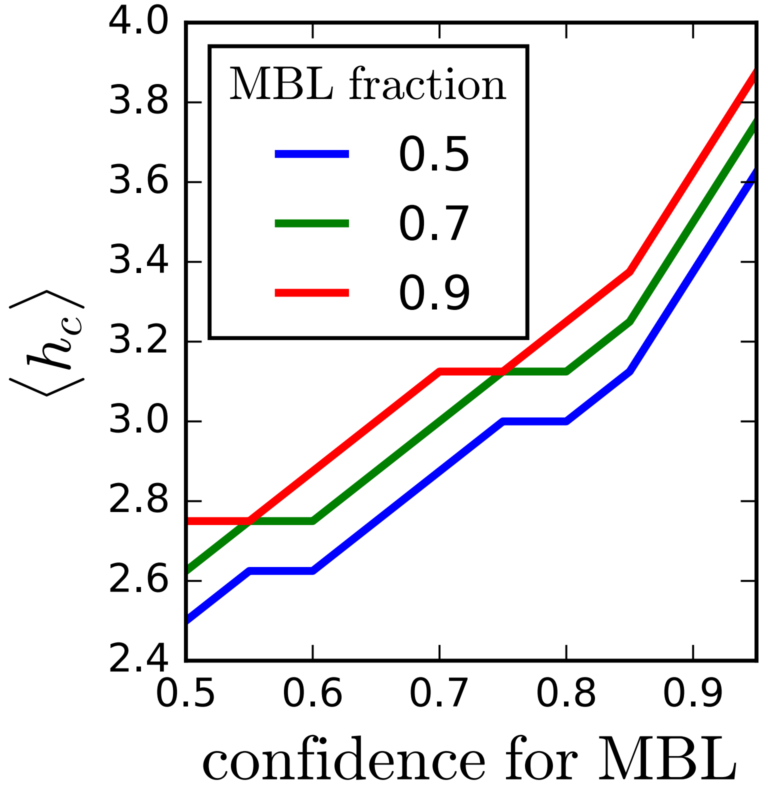
Ratio of adjacent gaps:

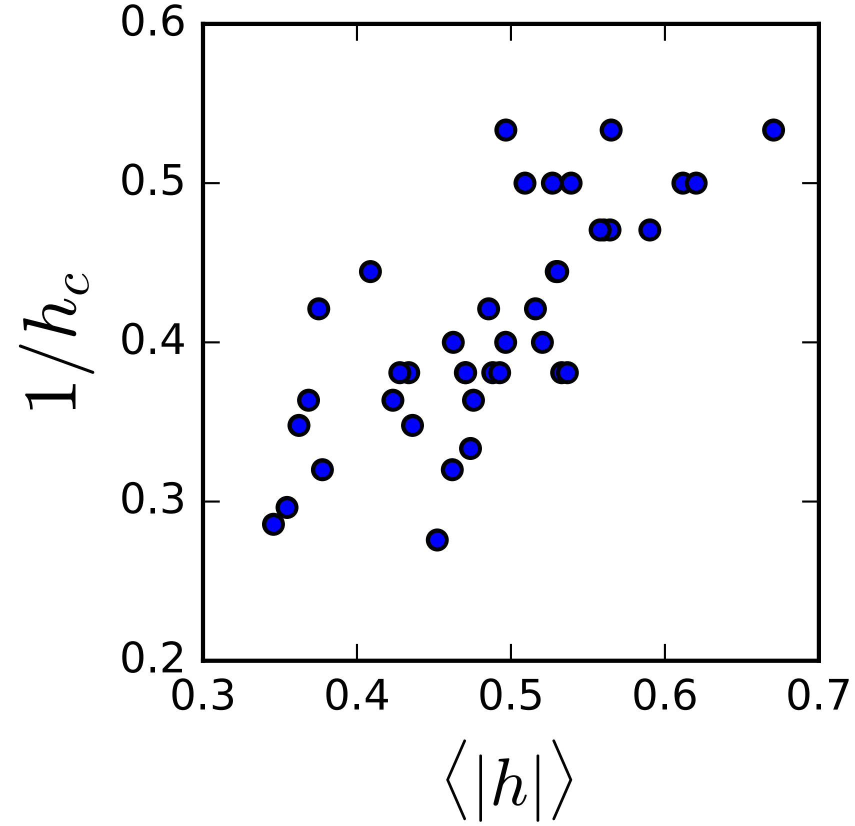
$$r_n = \frac{\min\left(E_n - E_{n-1}, E_{n+1} - E_n\right)}{\max\left(E_n - E_{n-1}, E_{n+1} - E_n\right)}$$

ETH: GOE statistics $r \sim 0.530$

MBL: Poisson statistics $r \sim 0.386$

Results: Determination of critical field





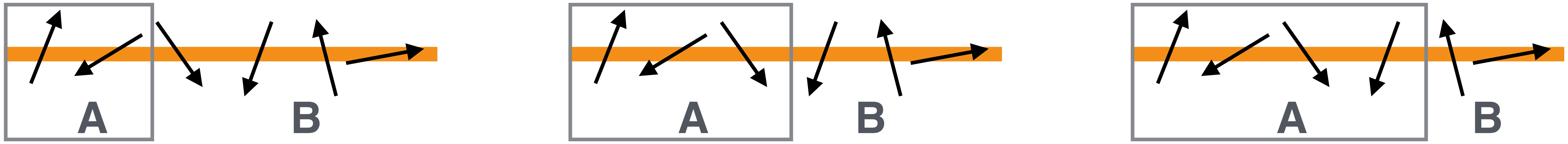
Arbitrariness of quantitative determination of phase boundary

$$\bar{h}_{\mathrm{c}} = 3.6 \pm 0.5$$

Correlation between average absolute field value and transition for 40 disorder realizations

Correlation coefficient: 0.76

Results: **Local structure**



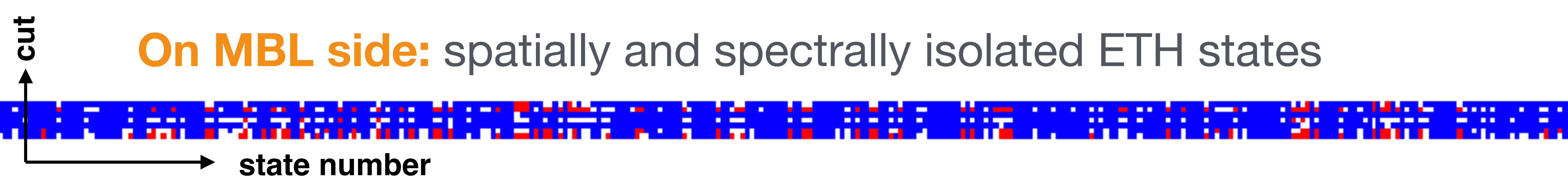
Compare classification results for different entanglement cuts in the same disorder realization

N = 18; cuts from 6 … 12

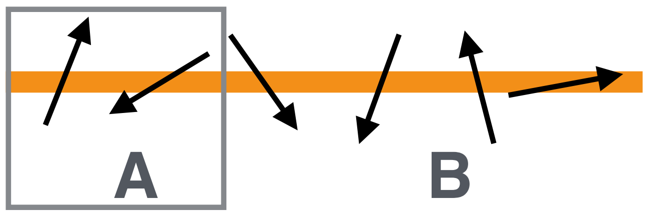
red: ETH blue: MBL white: not confident

On ETH side: spatially extended, spectrally isolated MBL states

On MBL side: spatially and spectrally isolated ETH states



Results: Local structure



Compare classificatio
cuts in the same diso

N = 18; cuts from 6 ..

red: ETH   blue: MBL

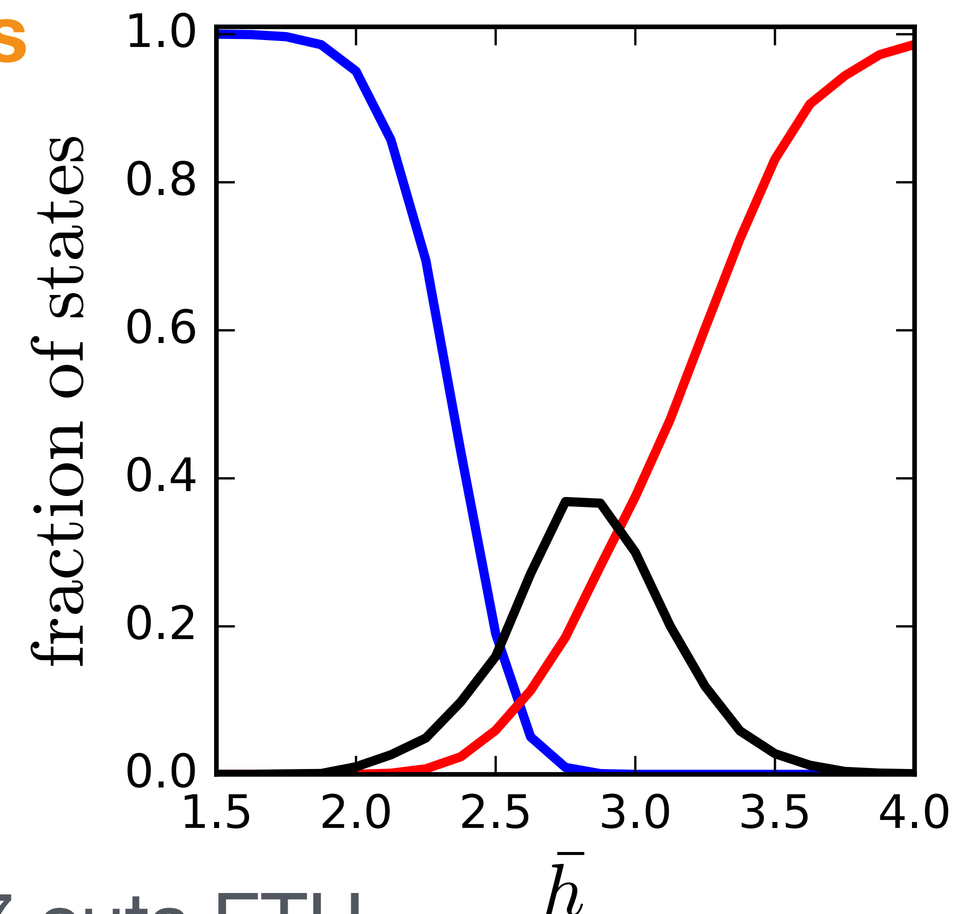
On ETH side: spat

On MBL side: spa

cut

state number

Statistics



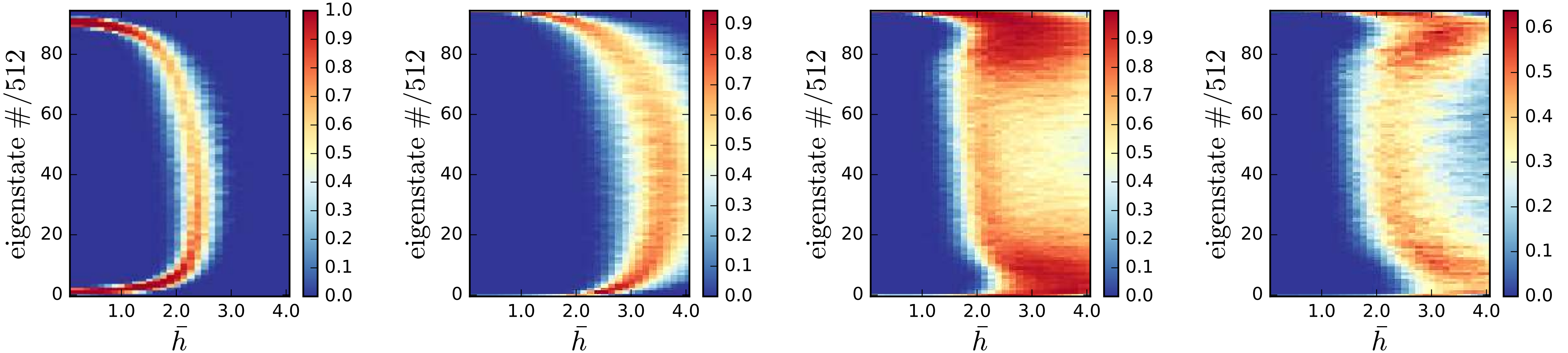
blue: all 7 cuts ETH
red: all 7 cuts MBL
black: at least one ETH and one MBL cut

ETH/MBL asymmetry in local structure near the transition: reaffirms bubble hypothesis

Results: **What can go wrong**

Fraction of uncertain spectra; same disorder realization, N = 18

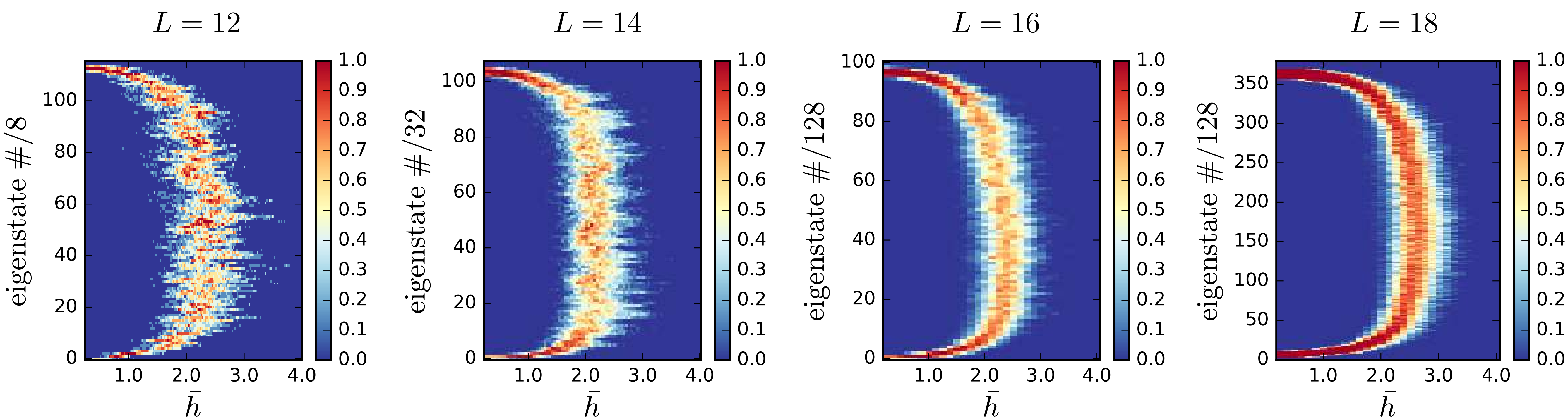
$$\mathrm{Cost}(\hat{f}, f) = -\sum_{x\in\mathrm{TD}}\sum_{i}^{2} f_i(x)\log \hat{f}_i(x) - \delta \sum_{x\in\mathrm{TR}}\sum_{i}^{2} \hat{f}_i(x)\log \hat{f}_i(x) + \mu |V|^2$$



confidence optimization	~~confidence optimization~~	confidence optimization	~~confidence optimization~~
weight decay	weight decay	~~weight decay~~	~~weight decay~~

Need both terms in cost function

Results: Finite size effects



- artifact structures near transition for smaller systems
- smooth and sharp phase boundary at largest system size
- confirms that confidence threshold 0.9 is appropriate for the system size

Dreaming: **What the network has learned**

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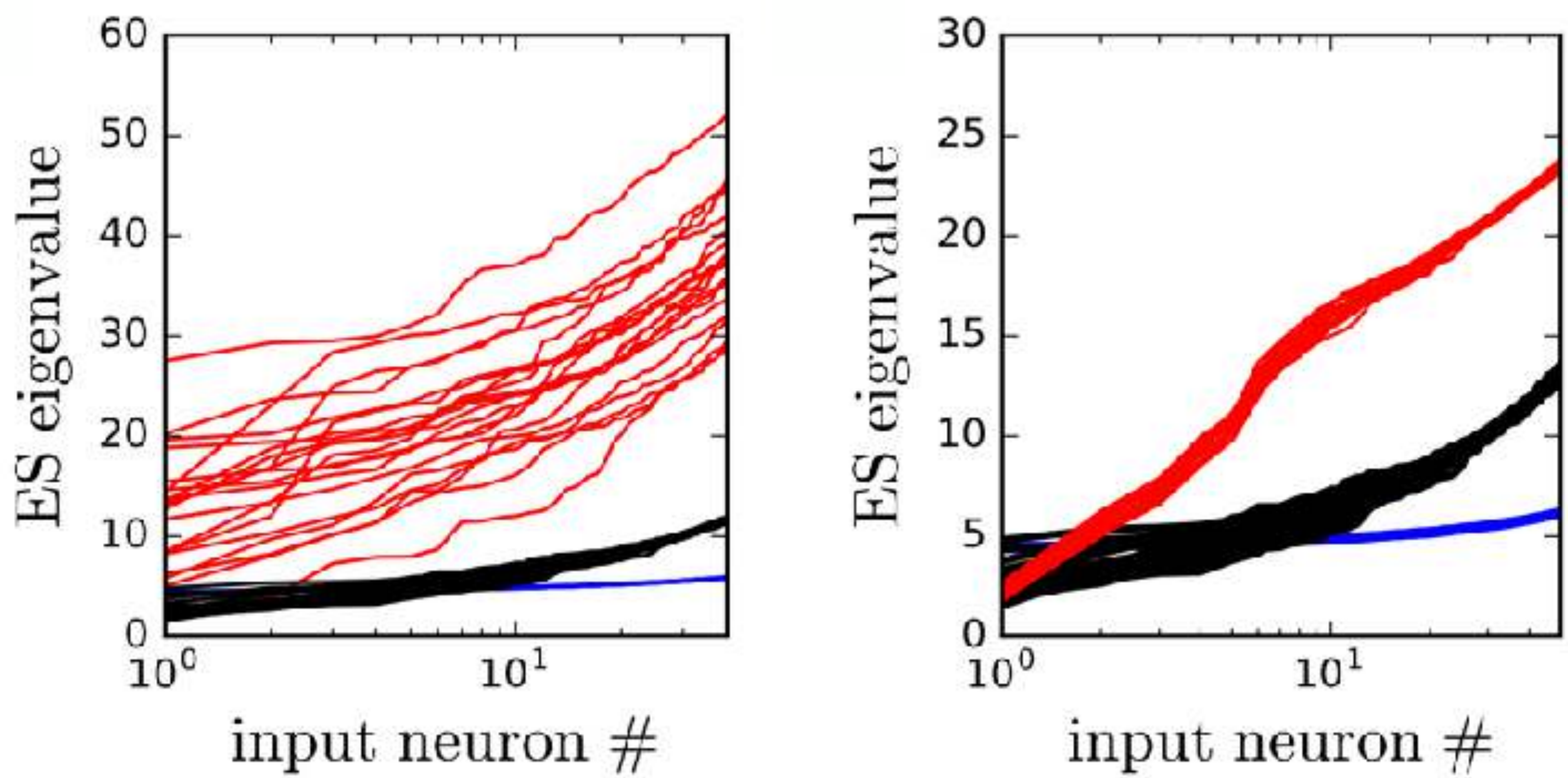


actual entanglement spectra

dreamed entanglement spectra

Shape reproduced, magnitude not

Reproduces power-law form of entanglement spectra

[Serbyn et al., PRL 2016]

What we have learned:
Recipe for phase classification

- train NN deep in the phases
- increase number of hidden layers until convergence on test set
- use dropout regularization
- use weight decay
- use **confidence optimization** near phase transition region

Problems

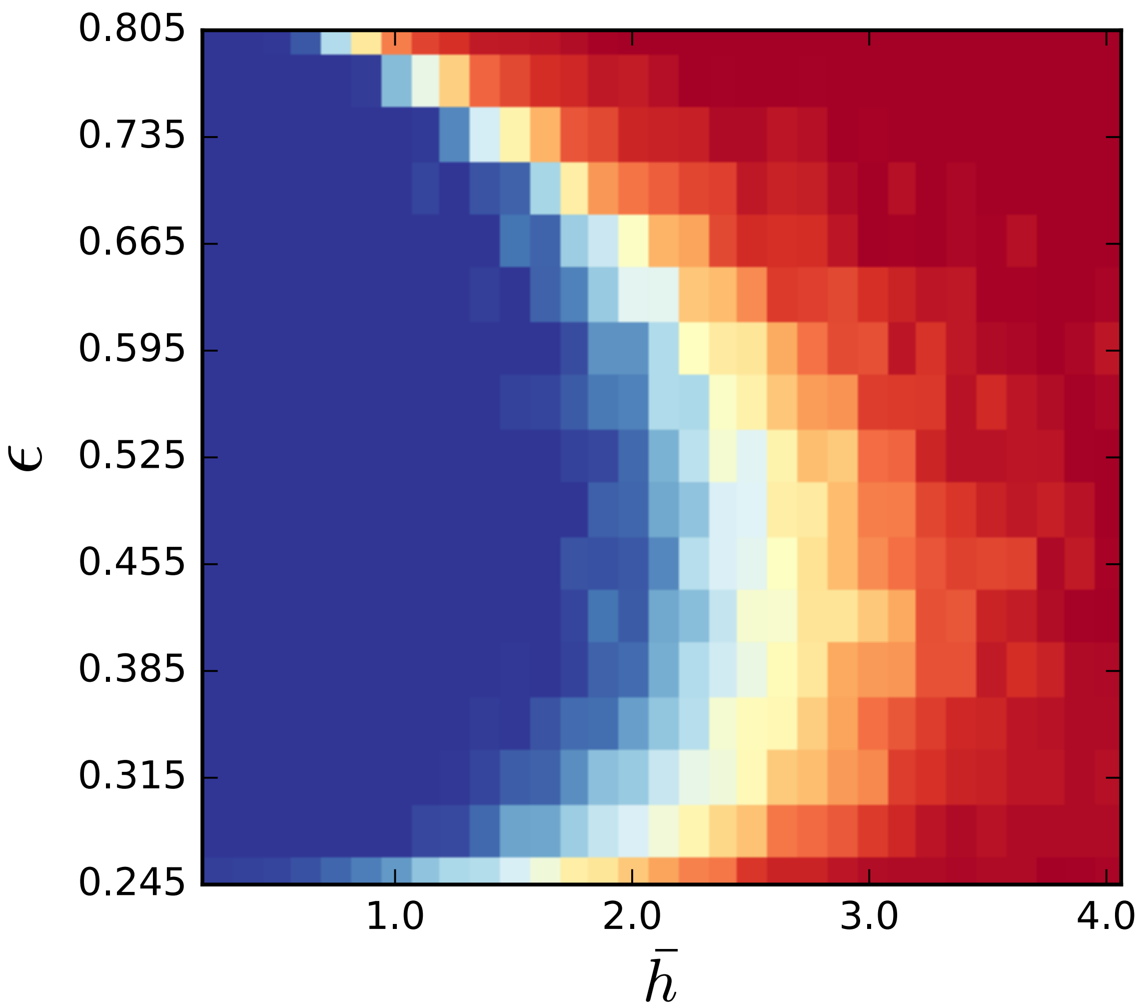
- quantitative correctness not guaranteed
- discovery of new phases
- interpretability

Advantages

- simple and performant
- no physical insight about phase characteristics assumed

Summary

- performance comparable to established (physical) methods
- works for single disorder realizations, **individual eigenstates**, small systems
- **simple and natural** choice of network and cost function; no tweaking
- blueprint for other phase classification applications using NNs



Open source code

Low entry barrier through packages like Google's TensorFlow