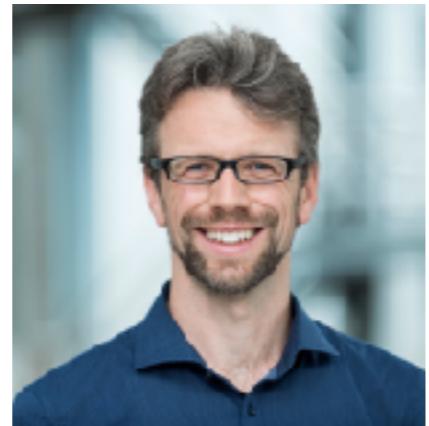




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RIKEN, 14 September 2017

# Probing many-body localization with neural networks



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**PRB 95, 245134 (2017)**

- 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

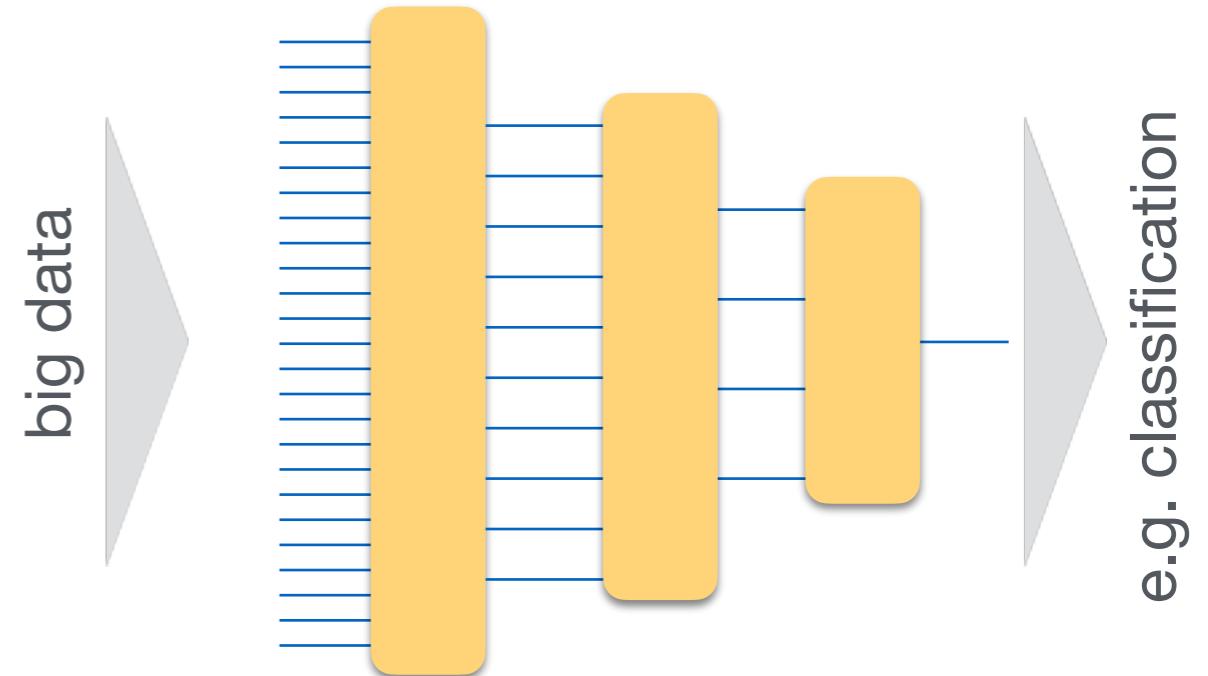
# labelled data (input-output pairs):

Reduce **cost function** (distance measure between network output and labels) via gradient descent.

**Verify** network performance on distinct test data set.

# Input

# Output



# Unsupervised learning

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

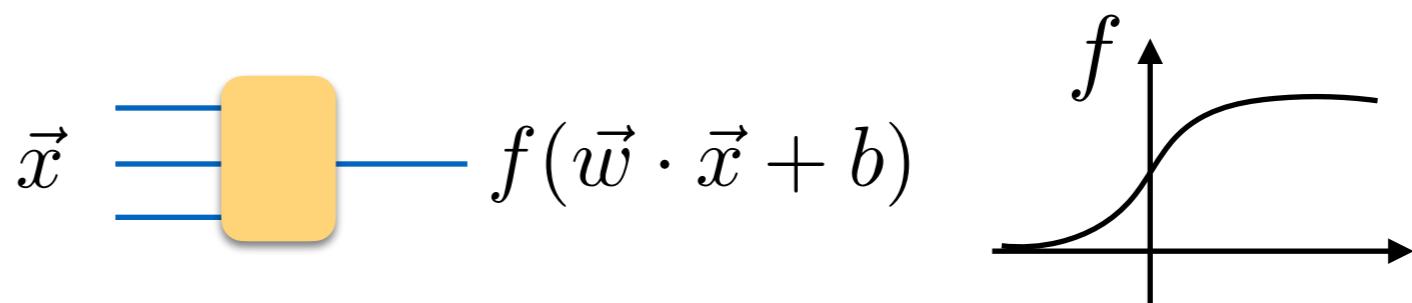
# Holy grail of the field

# Supervised learning with Artificial Neural Networks

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

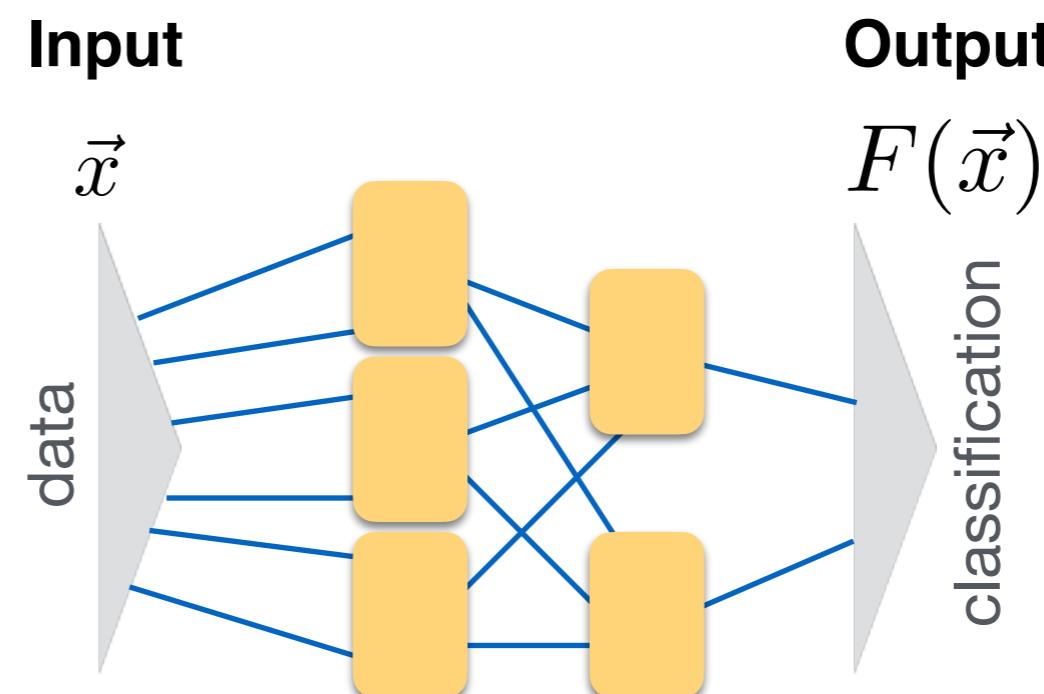
## Individual neuron:

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



## Deep network:

many layers of neurons



## **Objective:**

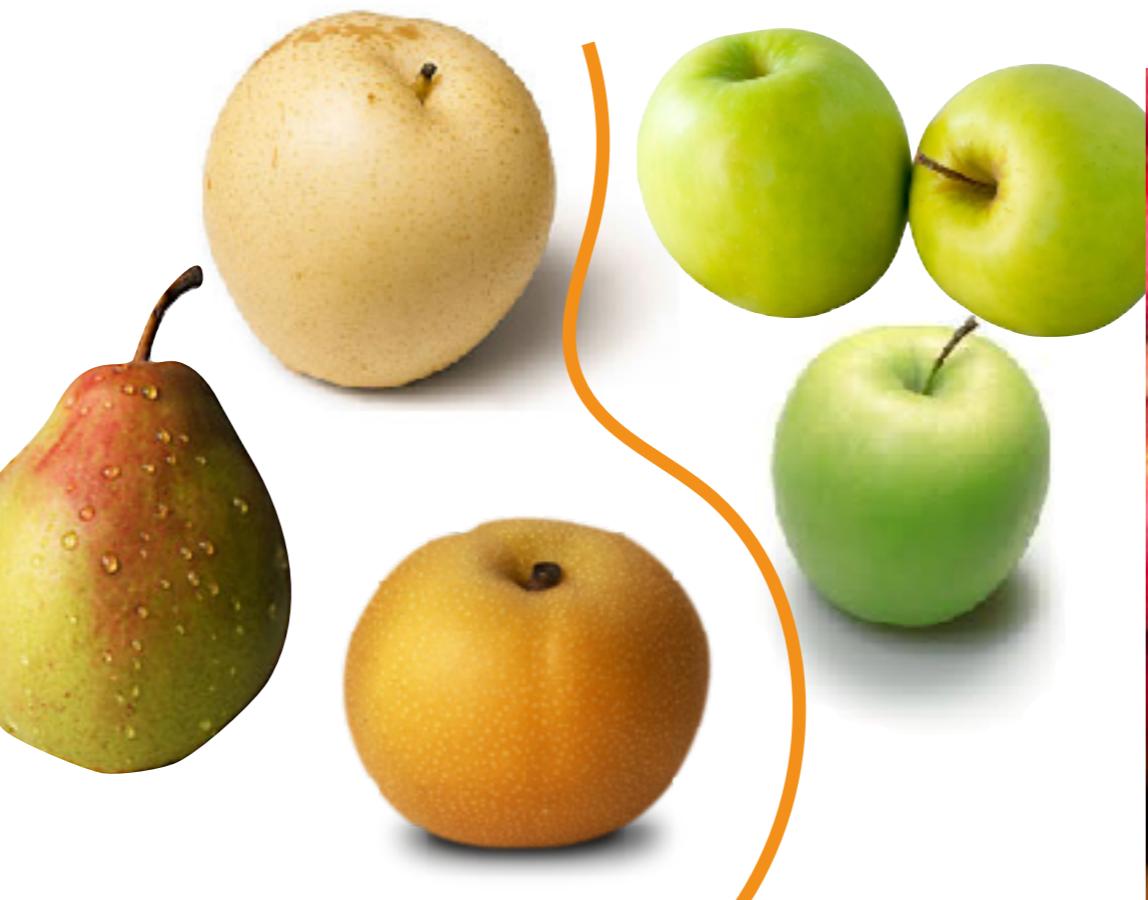
Classification of phases of matter using entanglement spectra

## **Supervised learning:**

Train network with data deep in the respective phase

## **Determine phase boundary:**

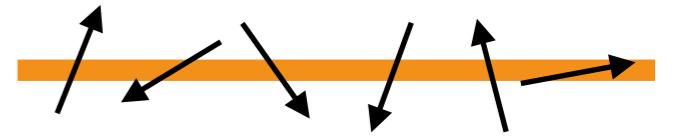
Apply network to states for which classification is less clear



# Toy problem: Many-body localization

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

$$H = J \sum_{r=1}^{N-1} \mathbf{S}_r \cdot \mathbf{S}_{r+1} + \sum_{r=1}^N h_r S_r^z$$



$$J = 1$$

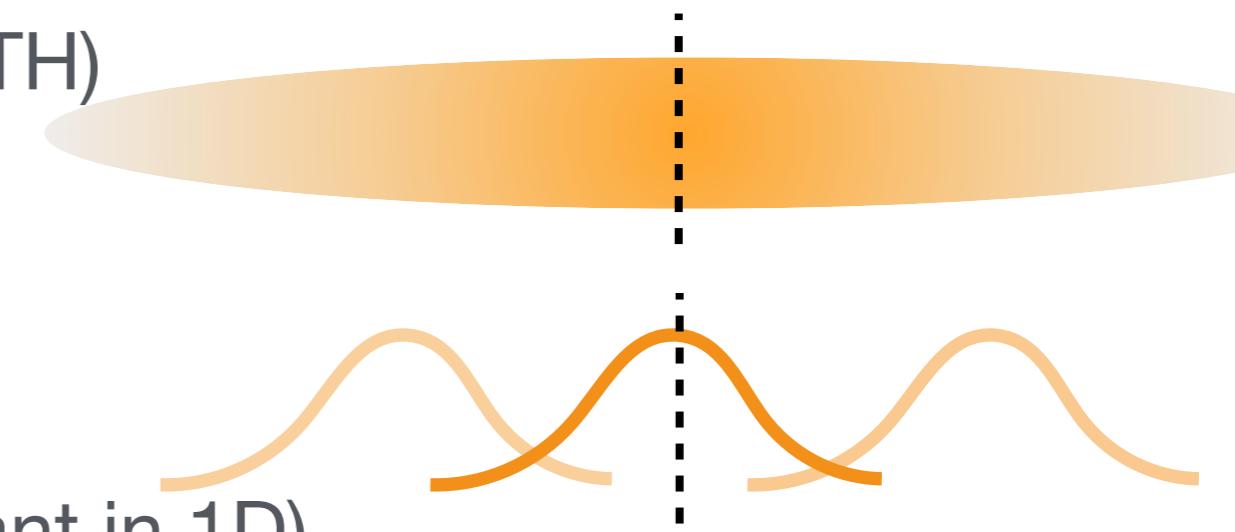
$$h_r \in [-\bar{h}, \bar{h}]$$

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

volume law entanglement

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

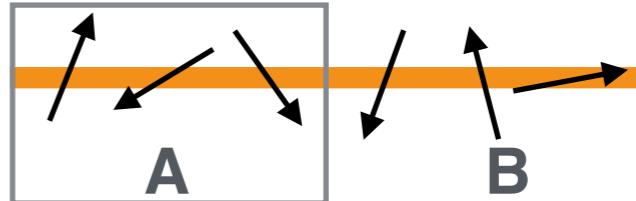
area law entanglement (constant in 1D)



# Conventional classification methods

based on energy level spectrum or entanglement entropy/spectrum

$$\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi| \equiv e^{-H_e}$$

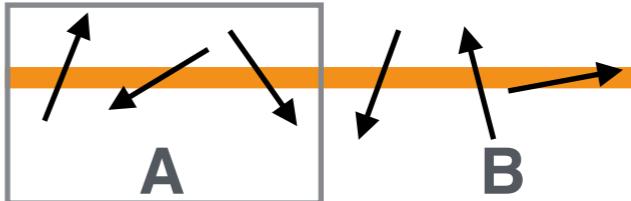


- i) **Schmidt gap:**  $\lambda_1(\rho_A) - \lambda_2(\rho_A)$ 
  - $\rightarrow 1$  for MBL (nearly pure)
  - $\ll 1$  for ETH
- ii) Volume vs. area law **scaling** of  $S(N_A)$  with  $N_A$
- iii) **Standard deviation** of  $S(N_A)$  over many consecutive eigenstates
  - large near the transition where 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

based on energy level spectrum or entanglement entropy/spectrum

$$\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi| \equiv e^{-H_e}$$



crude

i) **Schmidt gap:**  $\lambda_1(\rho_A) - \lambda_2(\rho_A) \rightarrow 1$  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  $S(N_A)$

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

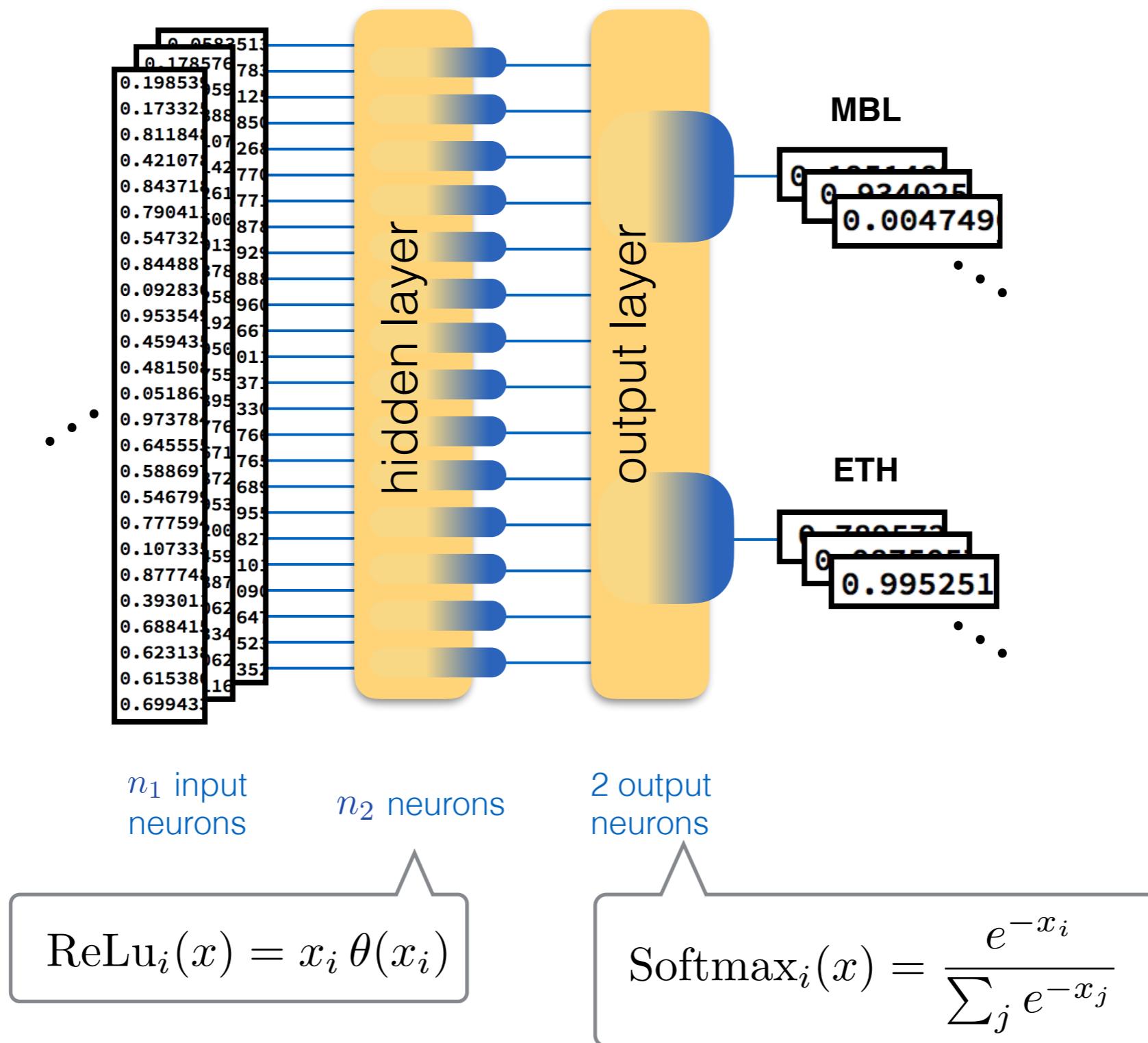
iii) **Level statistics** of either the entanglement spectrum or the energy spectrum follow distinct statistical distributions in each regime

needs large systems

# Structure of neural network

**Input:**  
entanglement spectra

**Output:**  
confidence for



# Cost function and regularization

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

## Cross entropy

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

labelled  
training  
data

classifying  
output  
neurons:  
2 options,  
ETH or MBL

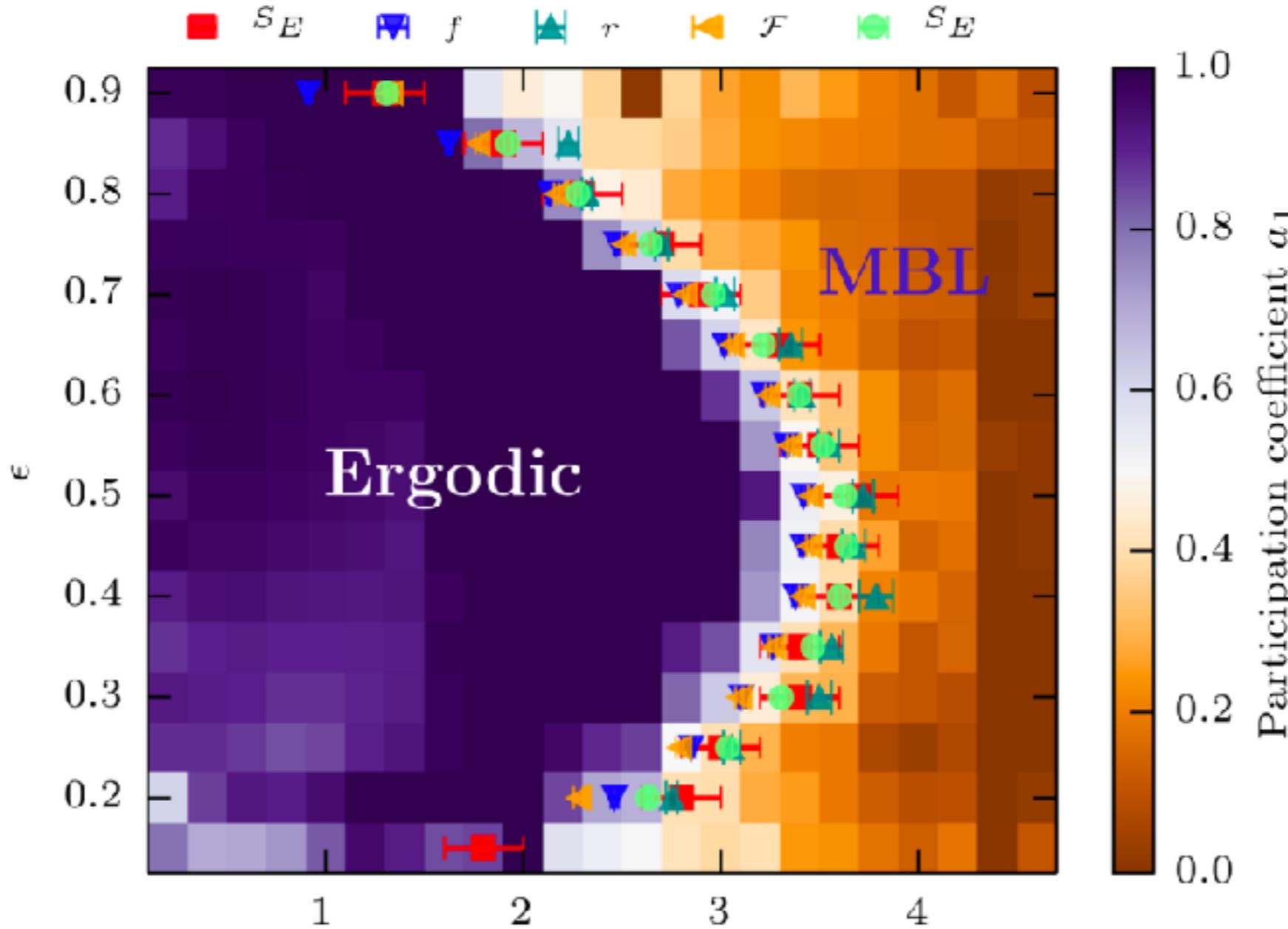
Weight decay  
  
favors having only  
few nonzero  
weights/using as  
few neurons as  
possible

Confidence  
optimization

favors unlabelled data  
near phase transition to  
be classified  
confidently

random subset of  
spectra near transition

# For comparison: Conventional methods



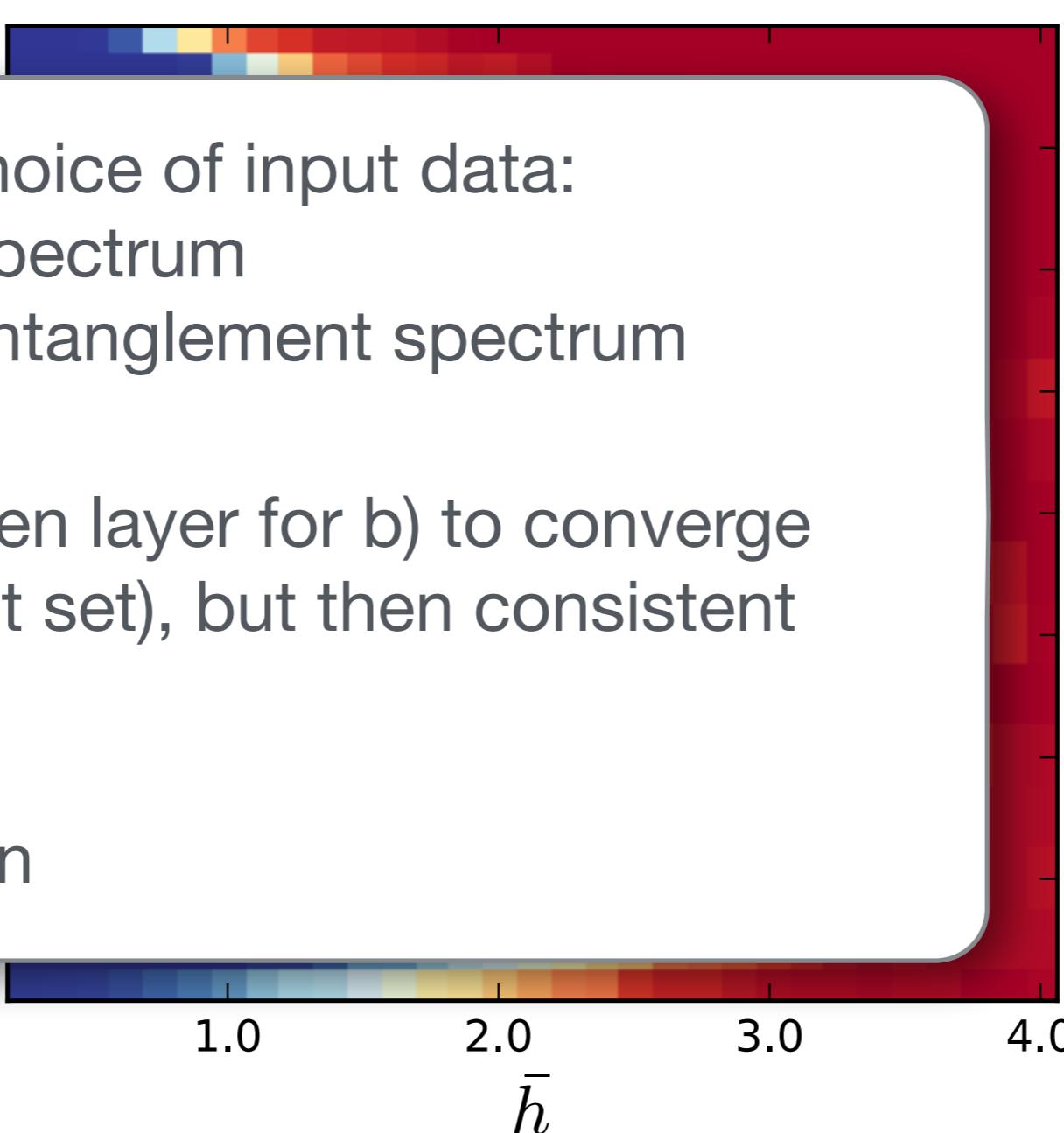
Volume law coefficient of the entanglement entropy

[Luitz et al., PRB 2015]

# Results: Disorder-averaged phase diagram

0.805

0.245



**Robust** against choice of input data:

- a) entanglement spectrum
- b) differences in entanglement spectrum

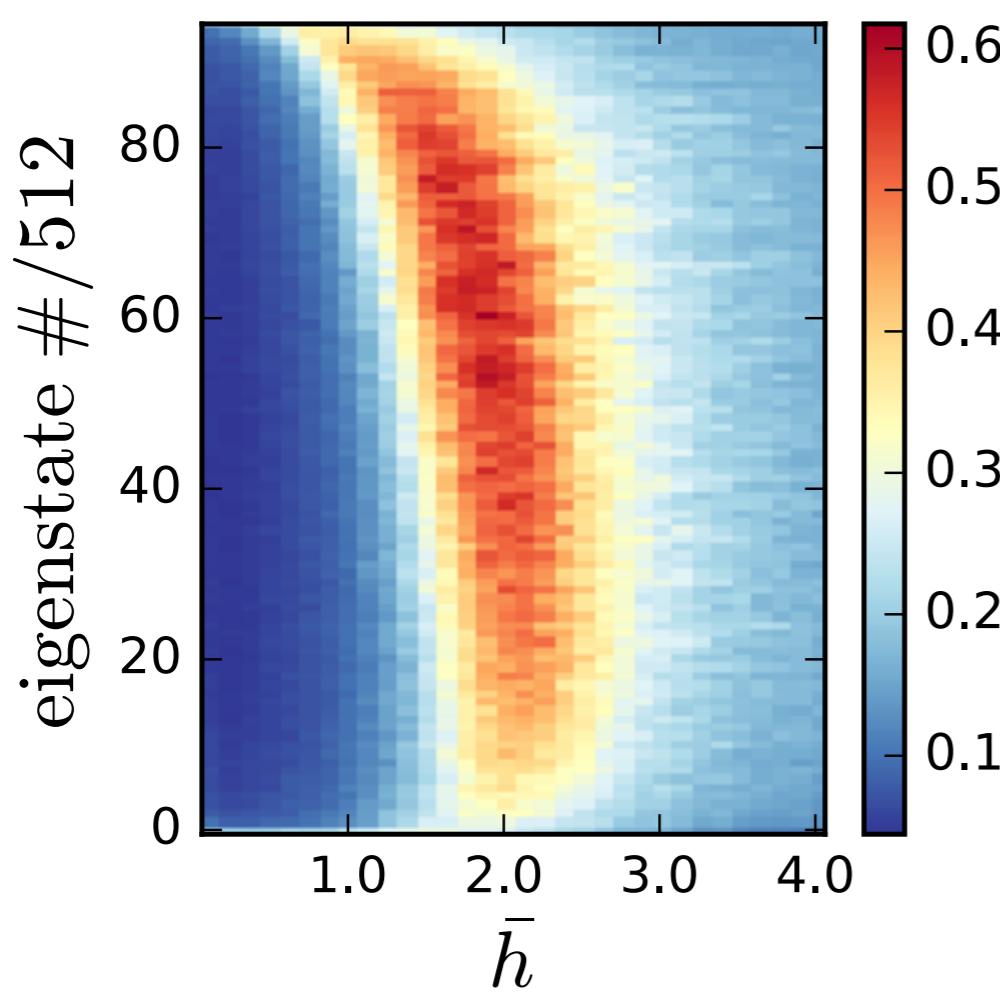
Need second hidden layer for b) to converge  
(yield 100% on test set), but then consistent  
results

Use a) from here on

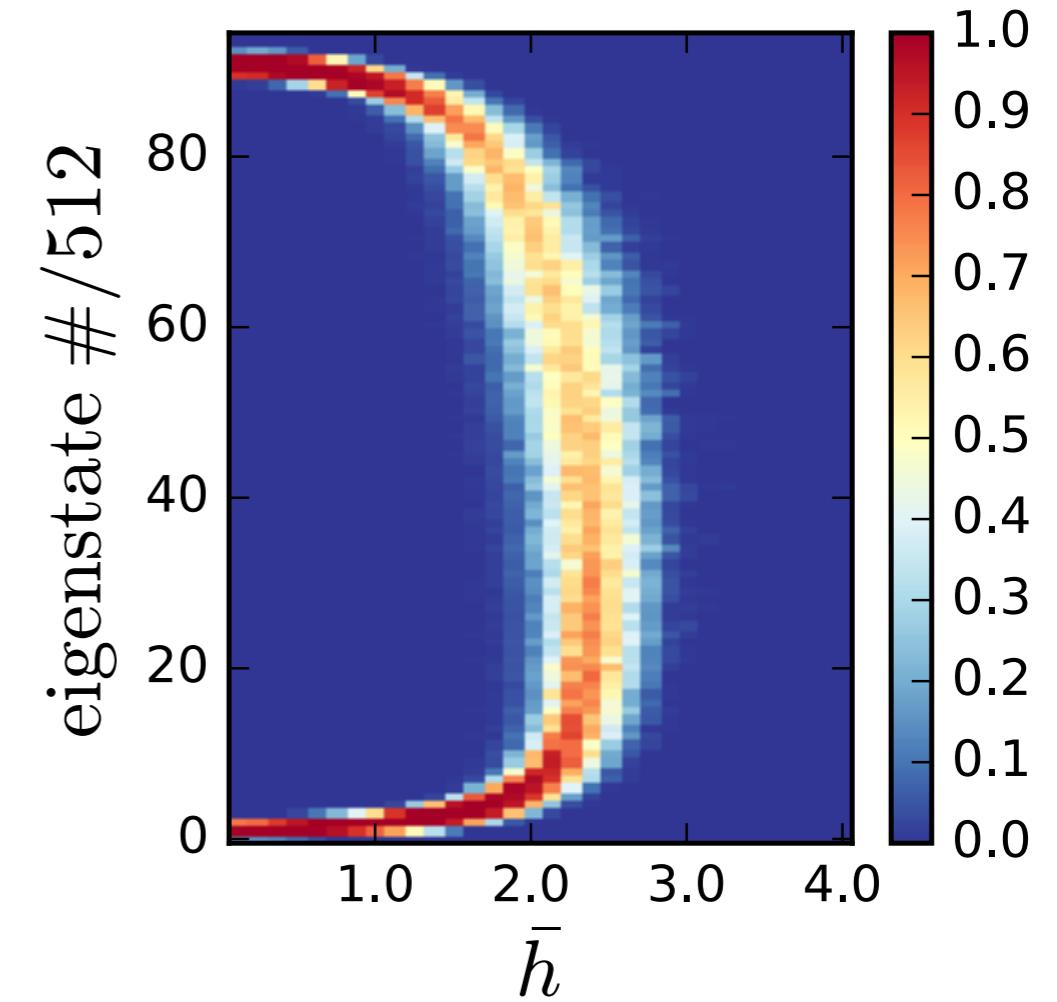
Confidence for MBL averaged over  
disorder realization and eigenstates in  
energy window

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

# Results: Transition in single disorder realization



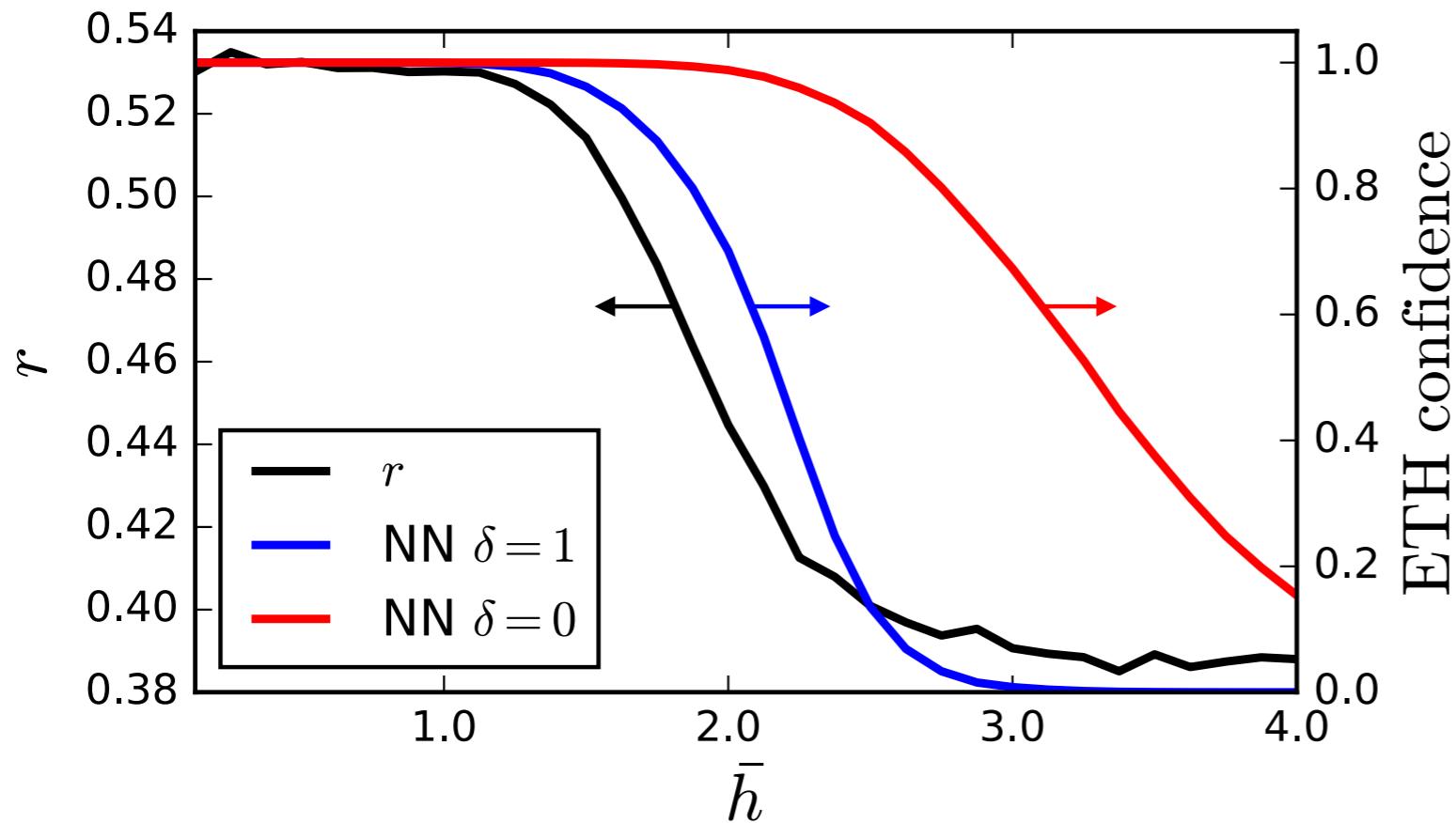
standard deviation of  
entanglement entropy over 512  
consecutive eigenstates



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:

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

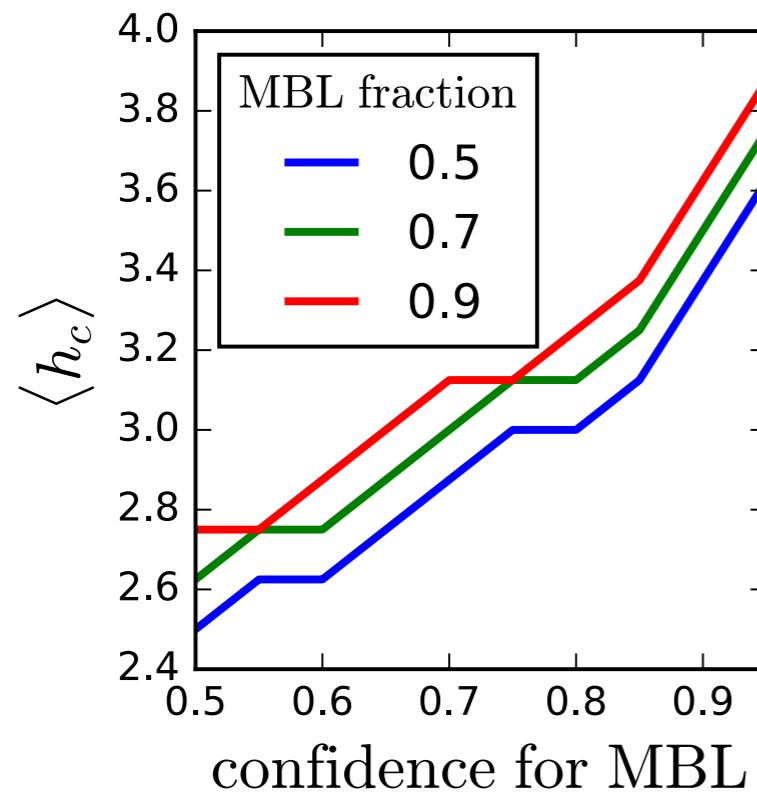
**ETH:** GOE statistics

$r \sim 0.530$

**MBL:** Poisson statistics

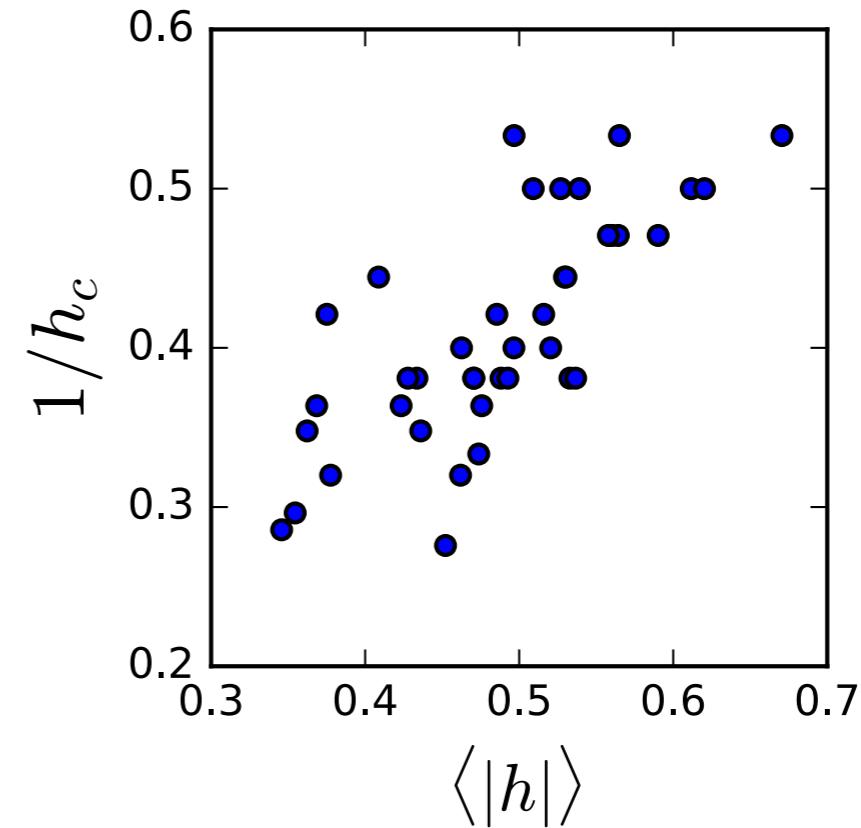
$r \sim 0.386$

# Results: Determination of critical field



Arbitrariness of quantitative determination of phase boundary

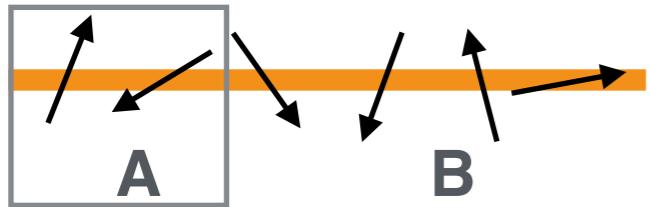
$$\bar{h}_c = 3.6 \pm 0.5$$



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

Correlation coefficient: 0.76

# Results: Local structure



Compare classification cuts in the same disorder

$N = 18$ ; cuts from 6 ..

red: ETH    blue: MBL

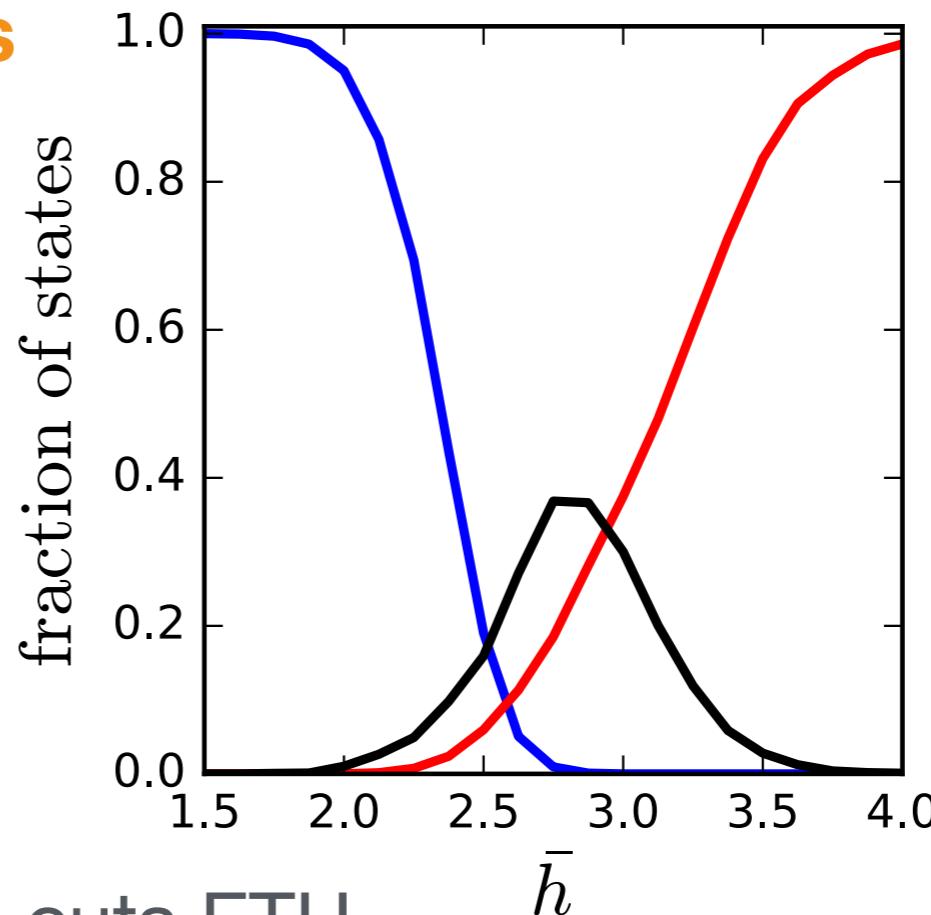
On ETH side: spatial



On MBL side: spatial



## Statistics



blue: all 7 cuts ETH

red: all 7 cuts MBL

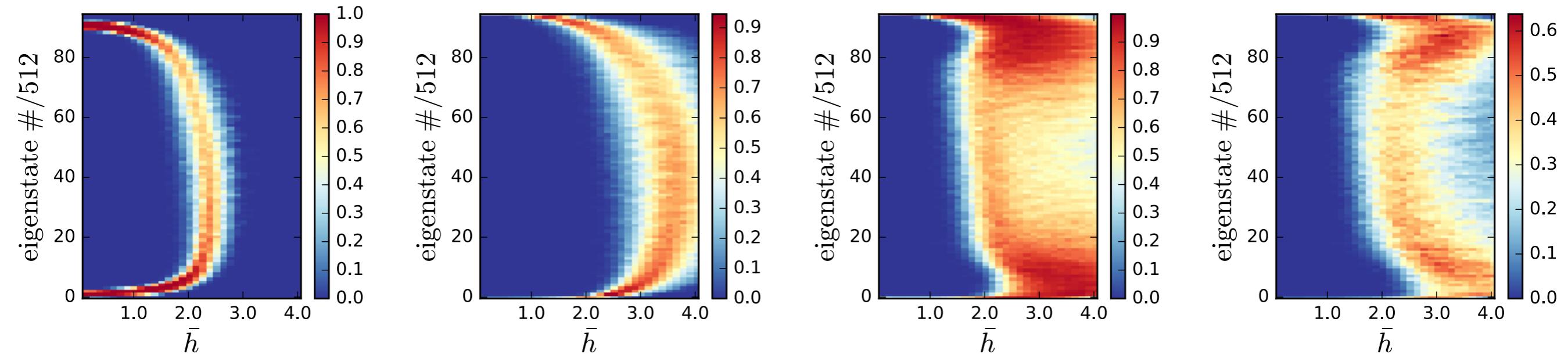
black: at least one ETH and one MBL cut

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

# Results: What can go wrong

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

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



confidence  
optimization

confidence  
optimization

confidence  
optimization

confidence  
optimization

weight  
decay

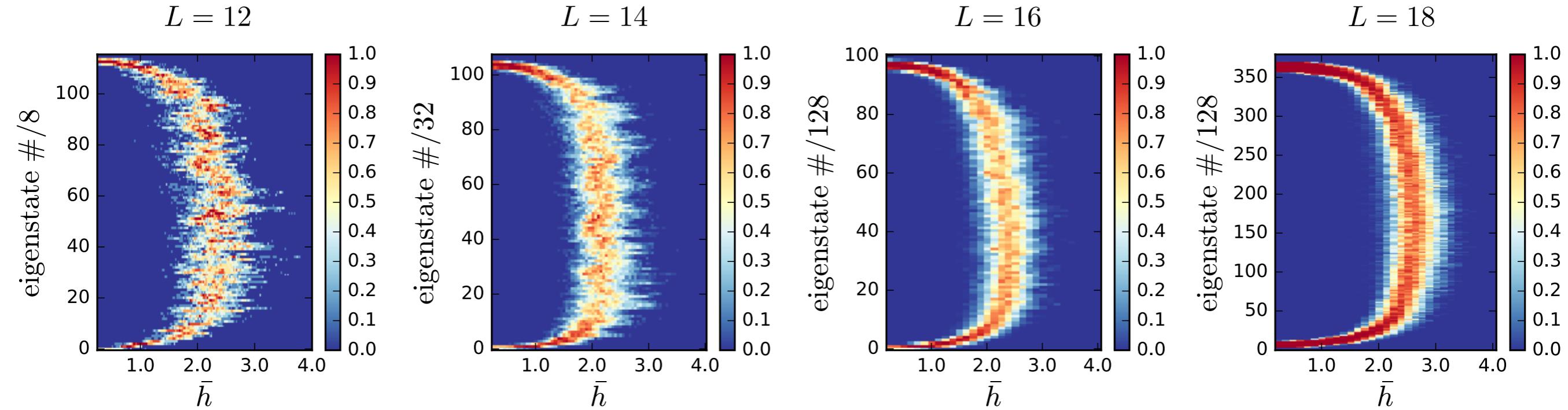
weight  
decay

weight  
decay

weight  
decay

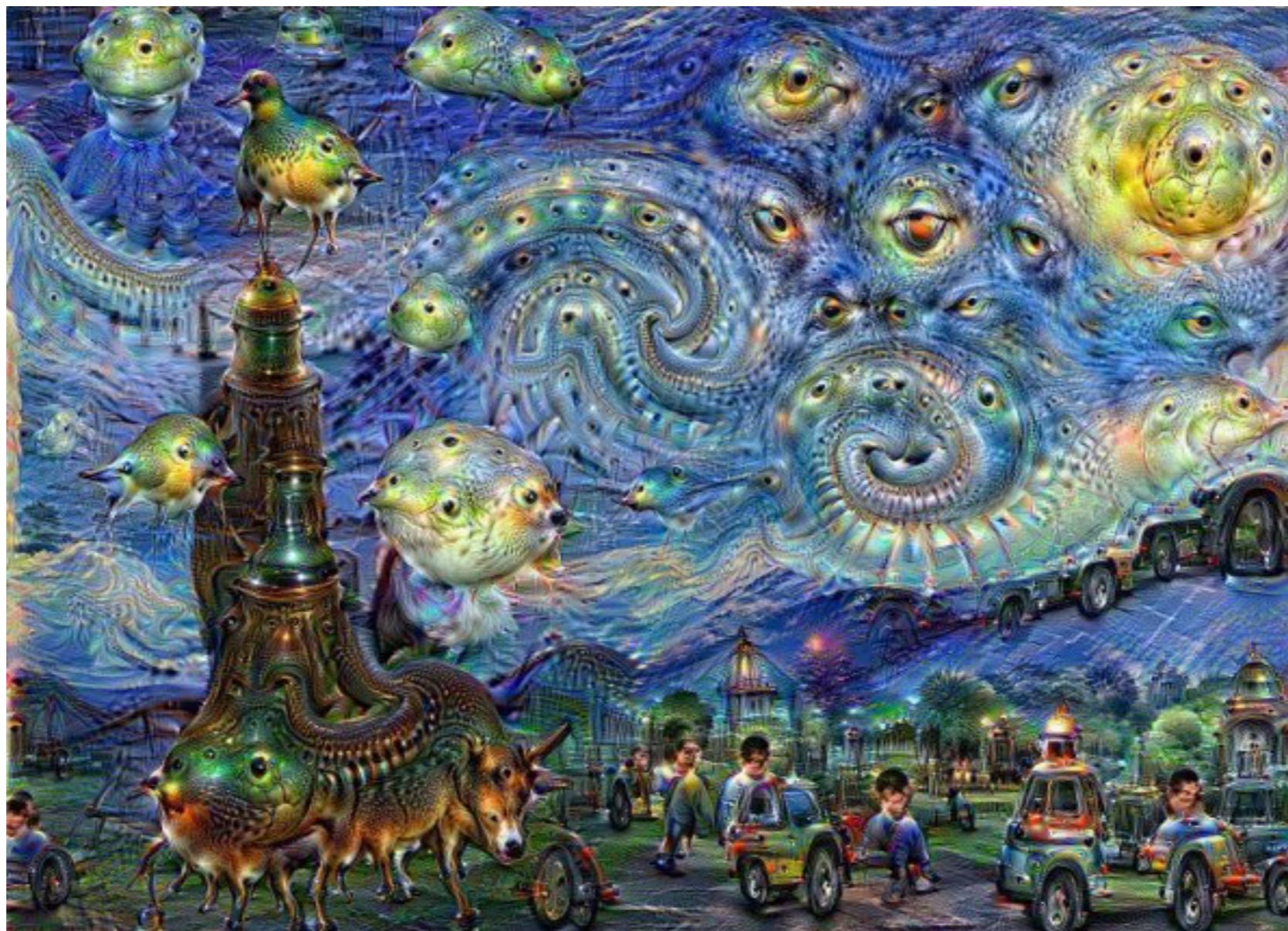
Need both terms in cost function

# Results: Finite size effects

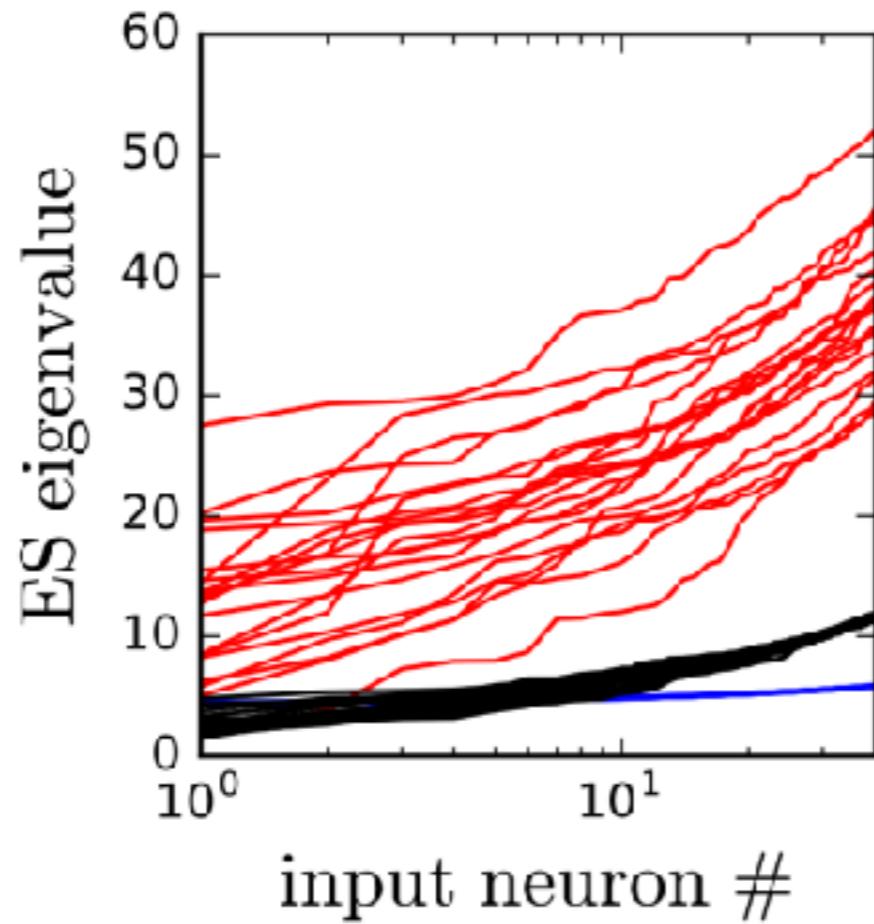


- artifact structures near transition for smaller systems
- smooth and sharp phase boundary at largest system size
- confirms that confidence threshold 0.9 is appropriate for the system size

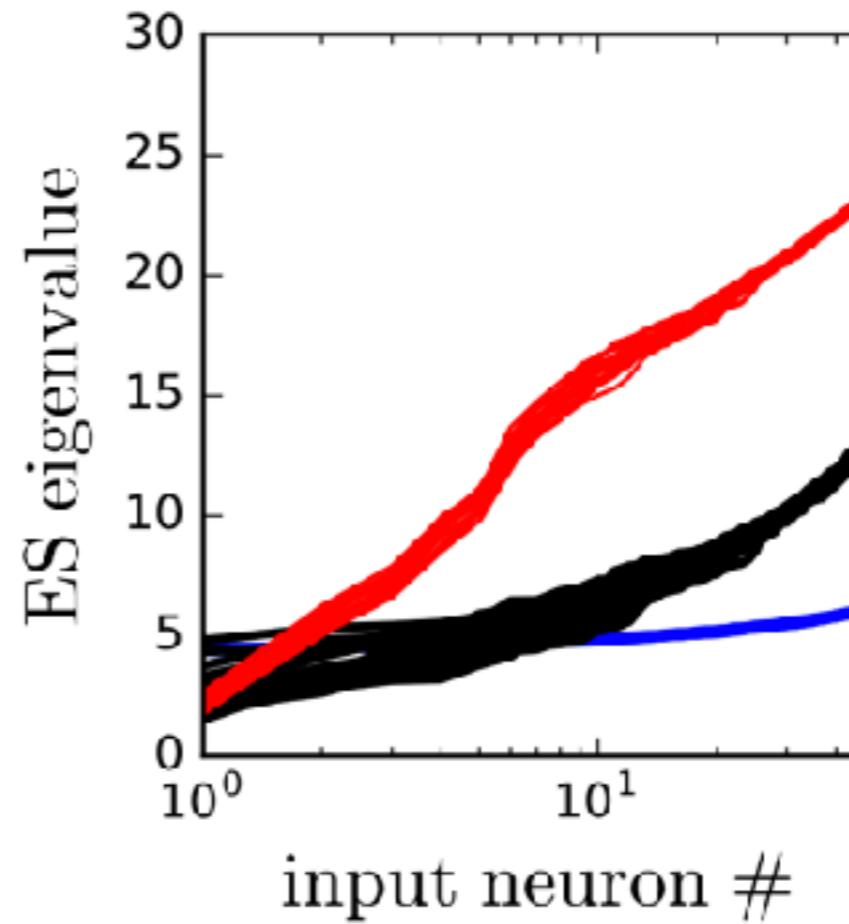
# Dreaming: What the network has learned



# Dreaming: What the network has learned



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

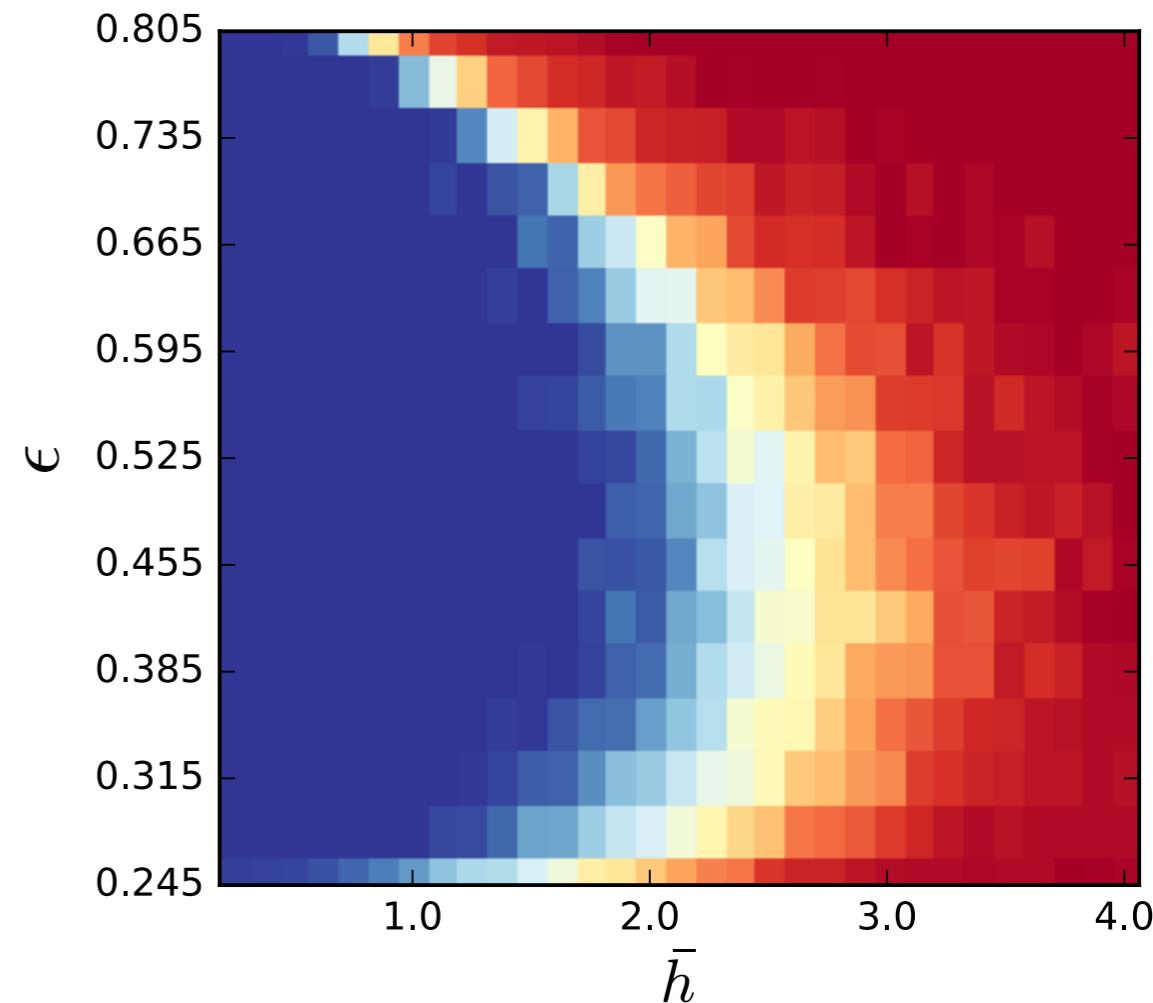
- quantitative correctness not guaranteed
- discovery of new phases
- interpretability

## Advantages

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

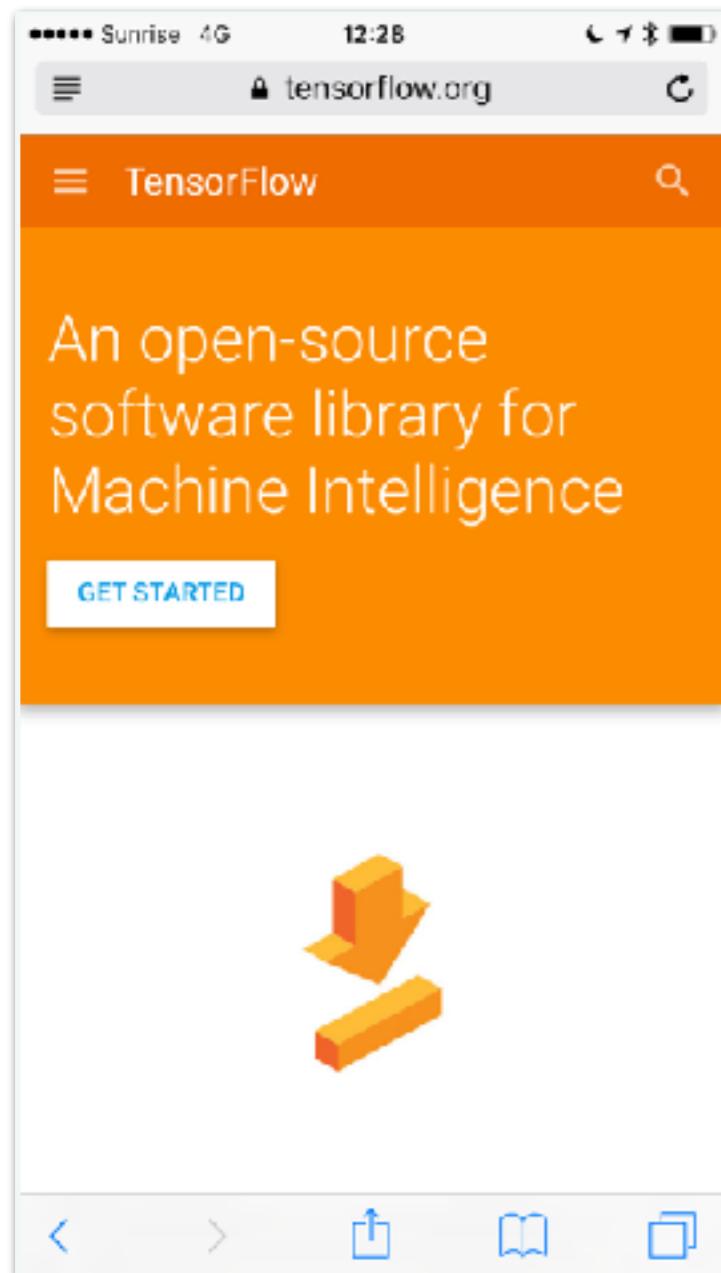
# Summary

- 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



Companies using  
TensorFlow

Google

IBM Power Systems

airbnb

AIRBUS  
DEFENCE & SPACE

intel

J.D.COM 京东

ARM

CEVA

QUALCOMM

quansight

CISI

DeepMind

SAP



Dropbox

eBay

