Learning Quantum Emergence with AI

Eun-Ah Kim (Cornell)

CIFAR summer school 2018

Challenges of Complexity

Regression,
Classification

Simple
Principles

Complex Reality
of Data

Generation,
Prediction

Entropy
Phonons
Topological Invariant
Fermi statistics

Phase Diagrams
Many-body Wave Functions

Data Revolution in R-space

Tunneling Density of States, in 1962

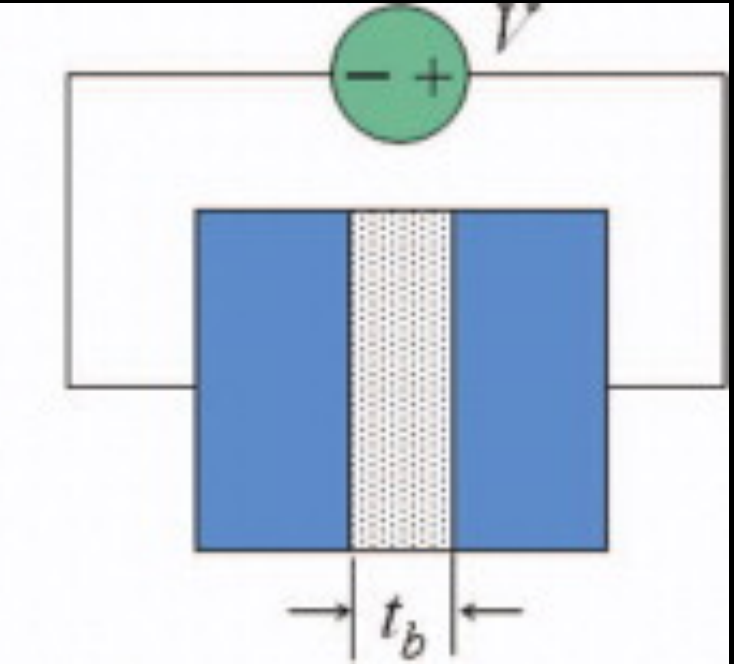
PHYSICAL REVIEW VOLUME 126, NUMBER 3 MAY 1, 1962

Tunneling into Superconductors at Temperatures below 1°K

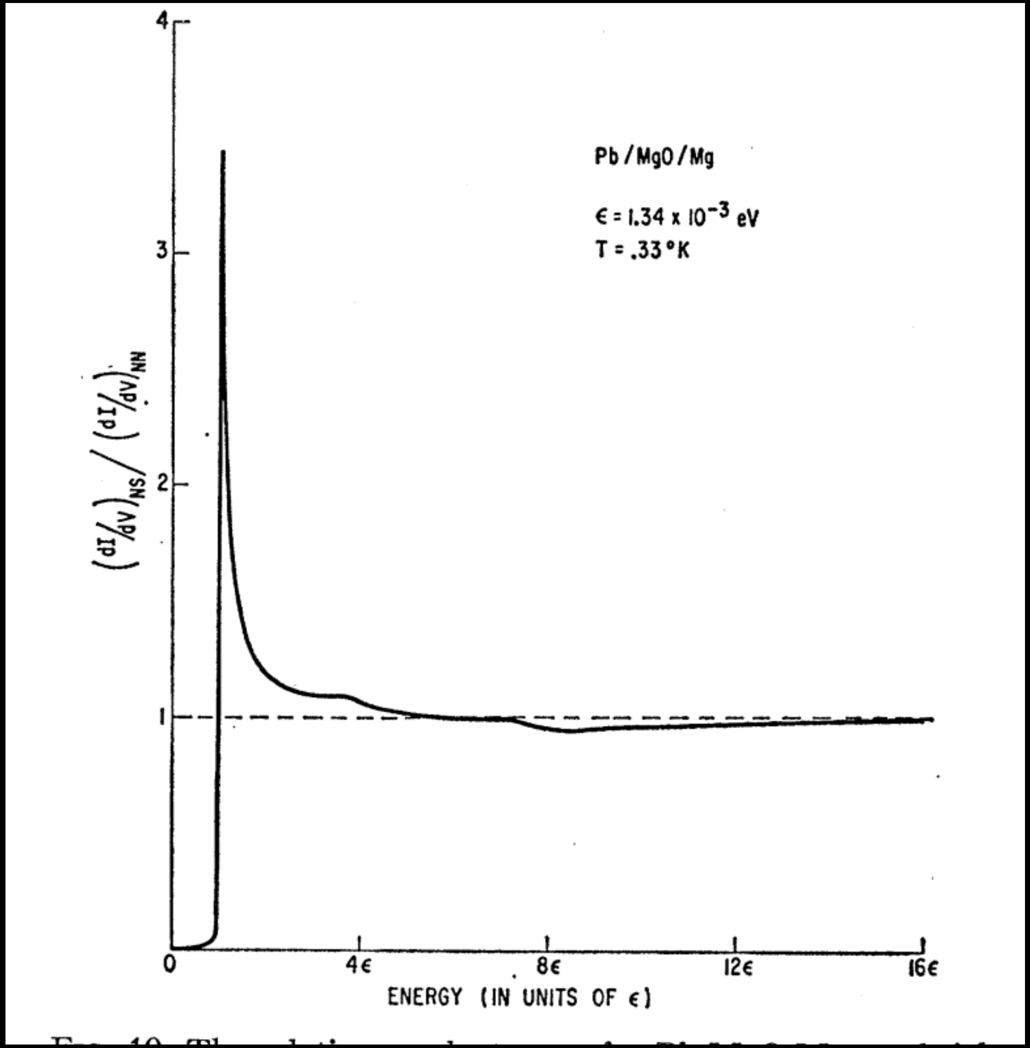
I. Giaever, H. R. Hart, Jr., and K. Megerle
General Electric Research Laboratory, Schenectady, New York
(Received November 16, 1961)

The density of states in four superconductors, lead, tin, indium, and aluminum, has been studied using the tunneling technique. The experimental results agree remarkably well with the Bardeen-Cooper-Schrieffer theory; however, two exceptions were found. The energy gap is not as sharp in the experiment as in the theory, but this may merely be due to imperfect samples. The density of states in lead has definite but small divergences from the theory.

Tunneling Density of States, in 1962

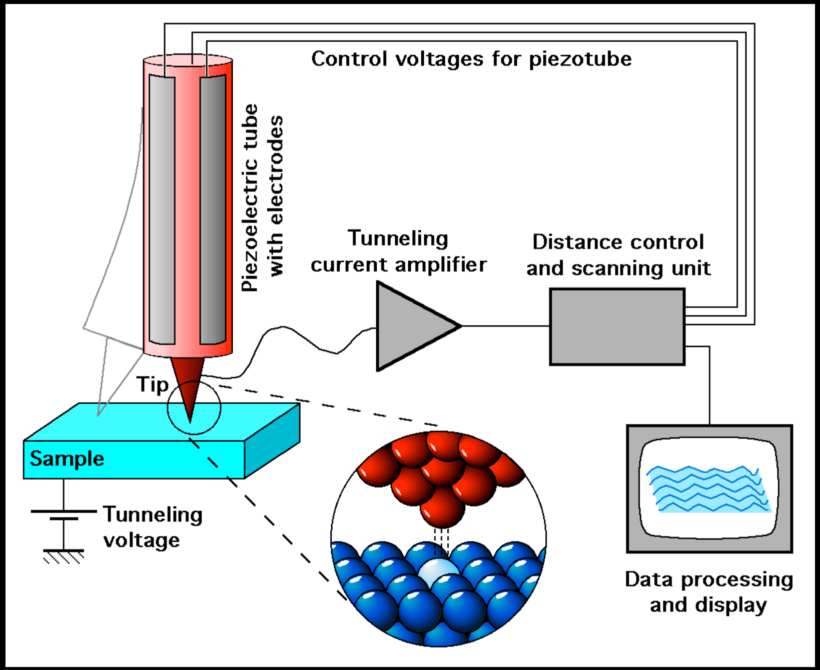


Differential conductance dI/dV @ V proportional to N(E=eV)

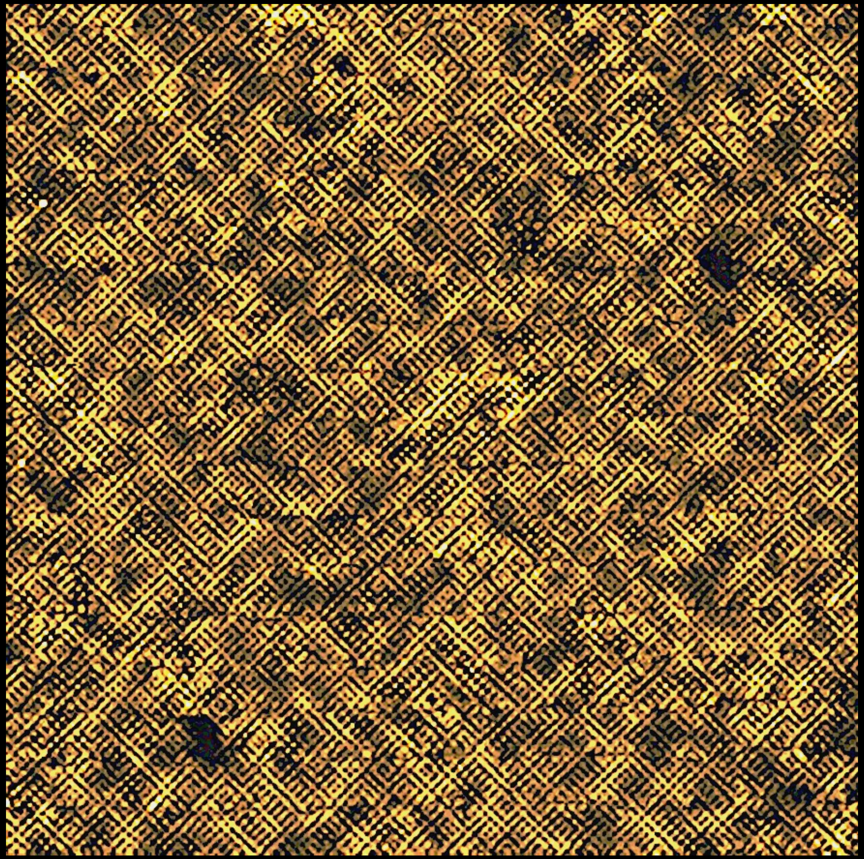


Giaever et al, Phys. Rev. 126, 941 (1962)

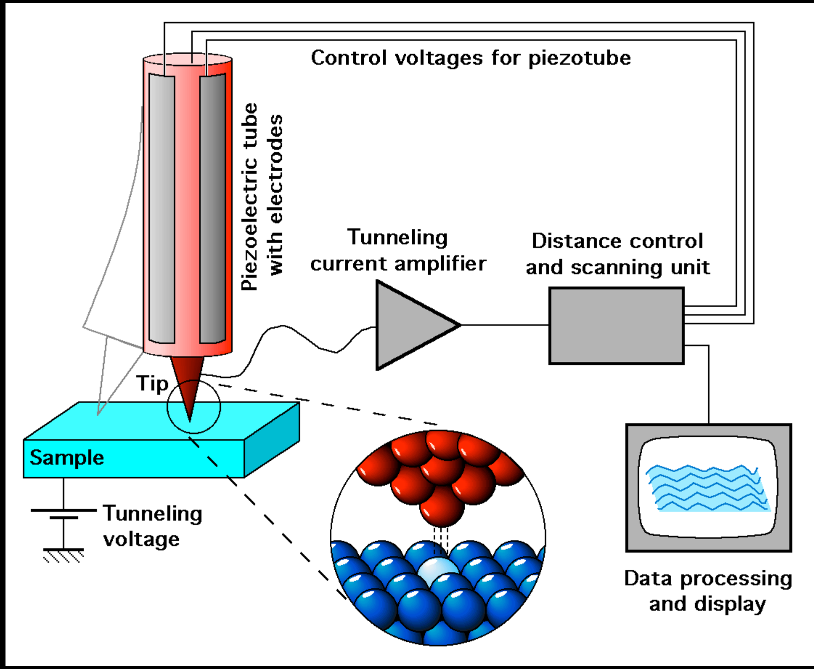
Tunneling Density of States, in 2000's



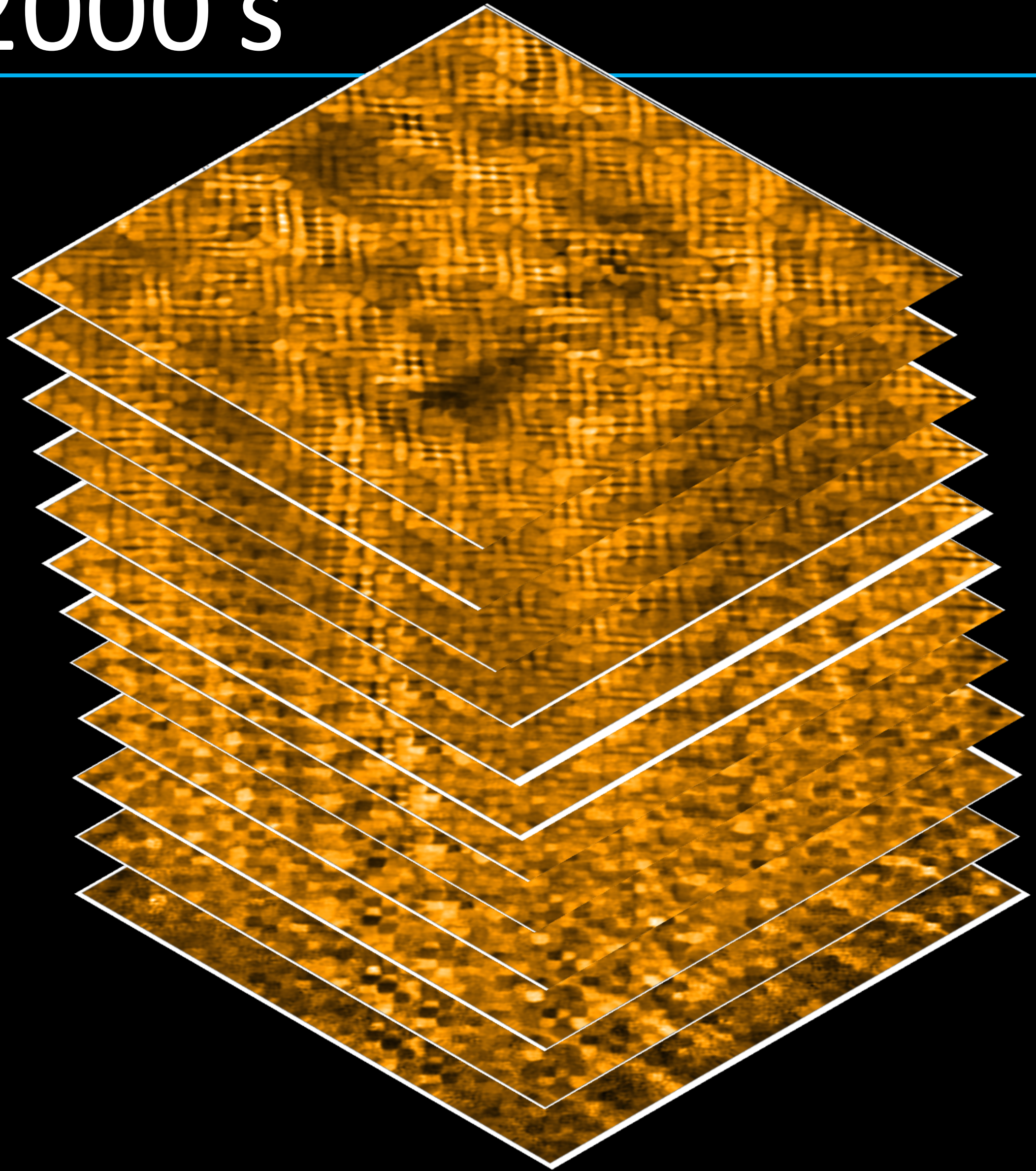
Imaging N(r,E):
Scanning Tunneling Spectroscopy



Tunneling Density of States, in 2000's

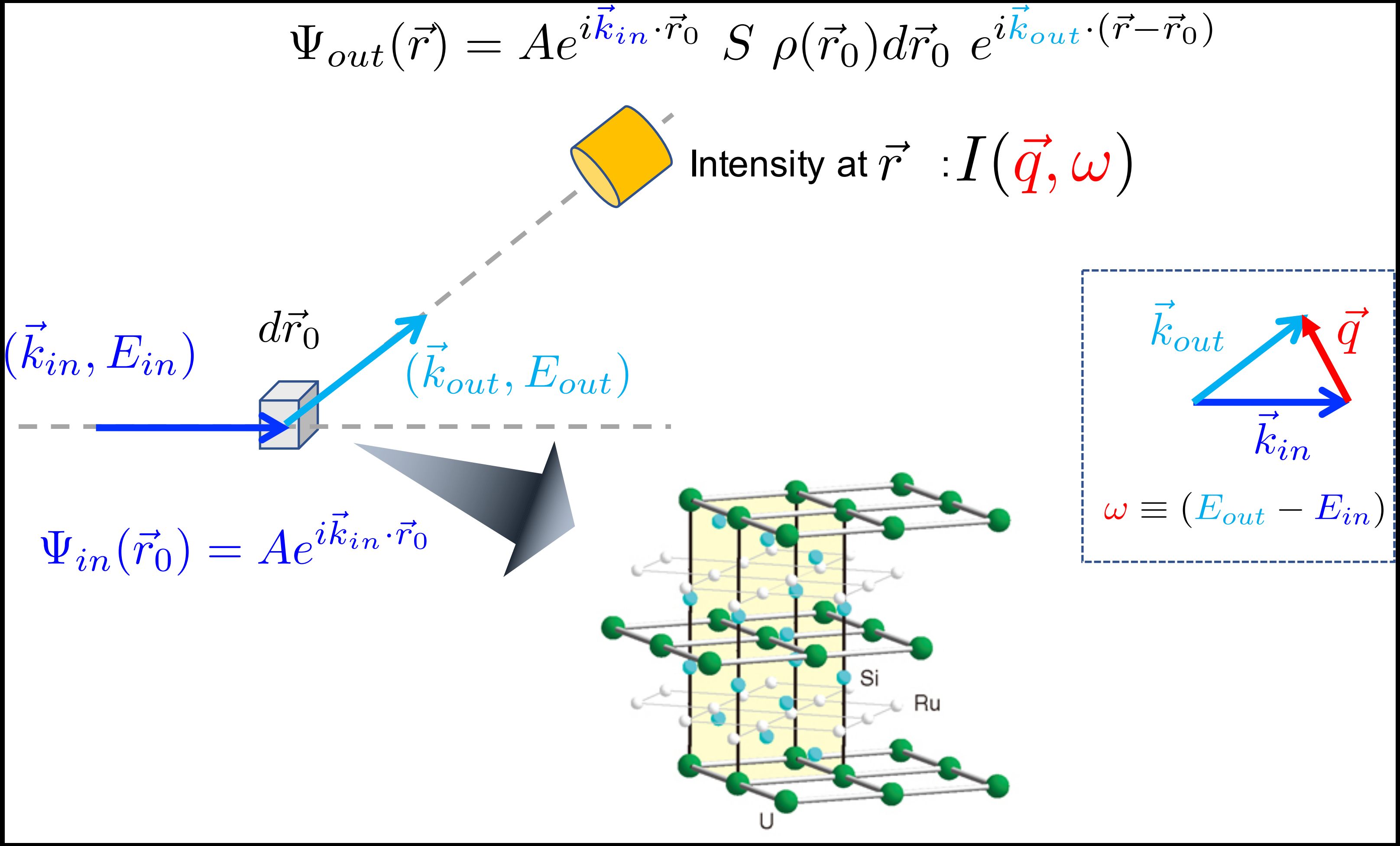


Imaging N(r,E):
Scanning Tunneling Spectroscopy

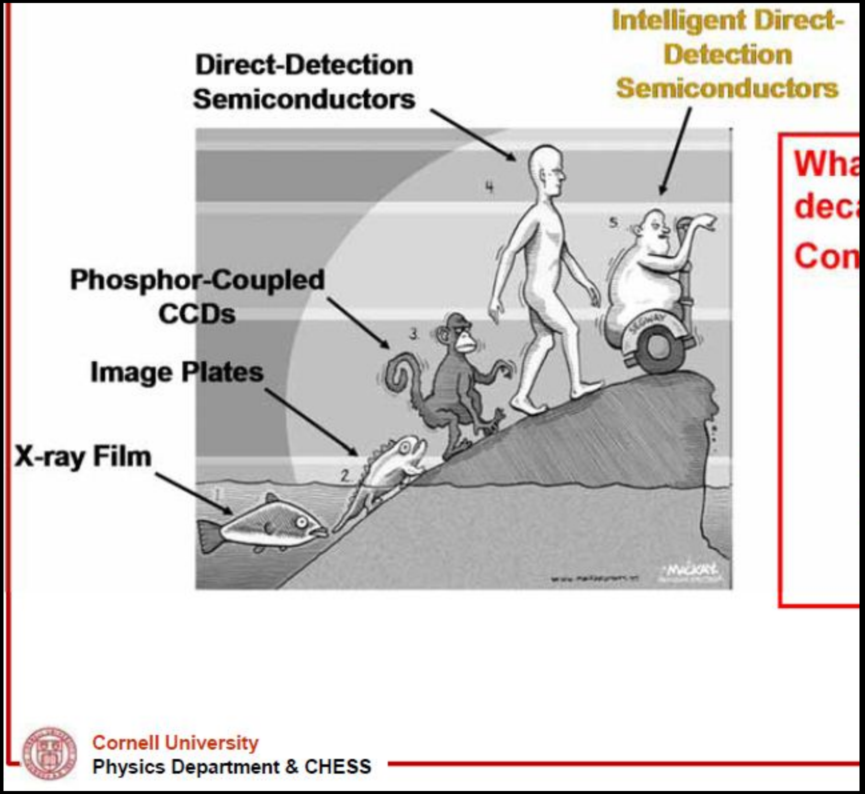


Data Revolution in Q-space

Sparse Data with Point Detectors



Comprehensive Data with Modern Detectors

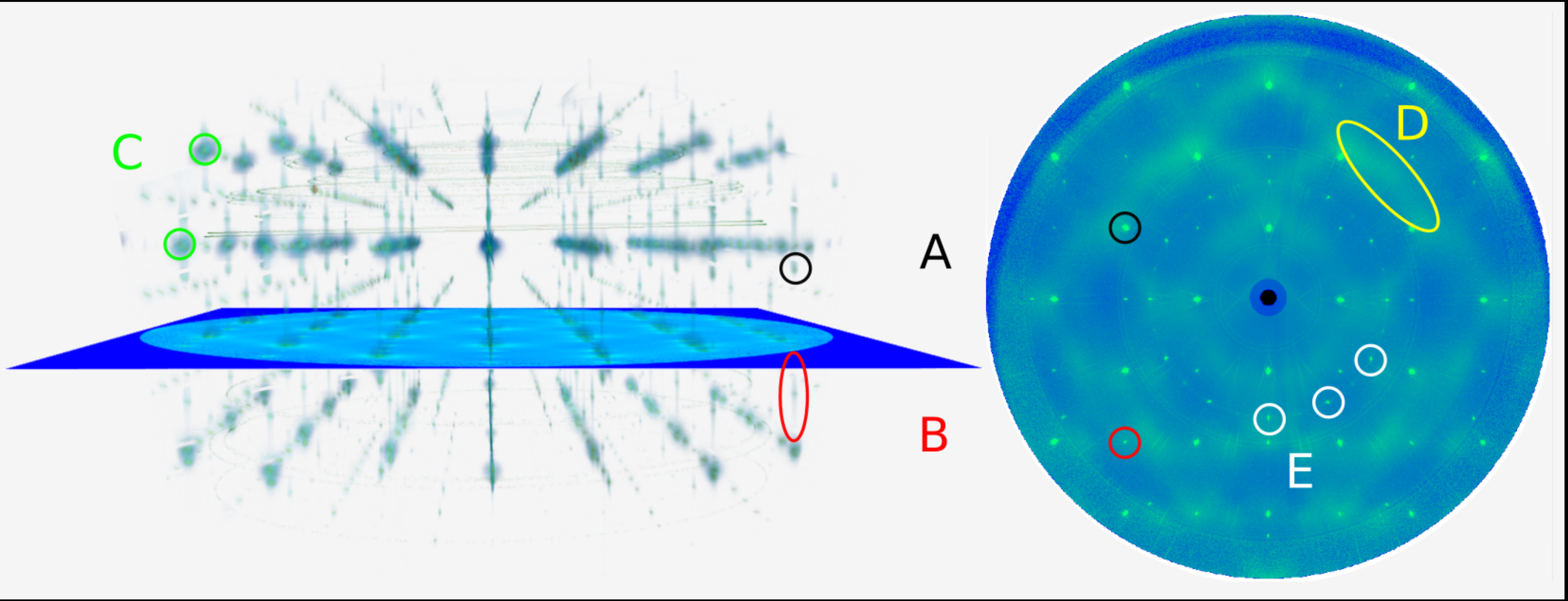


High energy X-ray Data at CHESS
> Possibly 5 TB per day

https://neutrons.ornl.gov/sequoia

Neutron data from Spallation Neutron Source
> Possibly 200 GB per hour

Comprehensive, too comprehensive!



Data-driven Challenges?

NSF'S 10 BIG IDEAS

to new data-driven research challenges. The challenges posed by complex data elements such …unstructured and heterogeneous data formats; streaming and dynamic data; complex dependence structures; missing, uncertain, and noisy information; sparsity; and information hidden at the noise level will require research that (a) addresses the core algorithmic, mathematical, and statistical principles; and (b) leads to new approaches, computational tools, and software for data-driven discovery…

https://www.nsf.gov/pubs/2018/nsf18542/nsf18542.htm

Chemical shifts from tiny NMR samples *pp. 38 & 67*

Regulating products that target gut microbiomes *p. 39*

Preschool games promote math skills in India *p. 47*

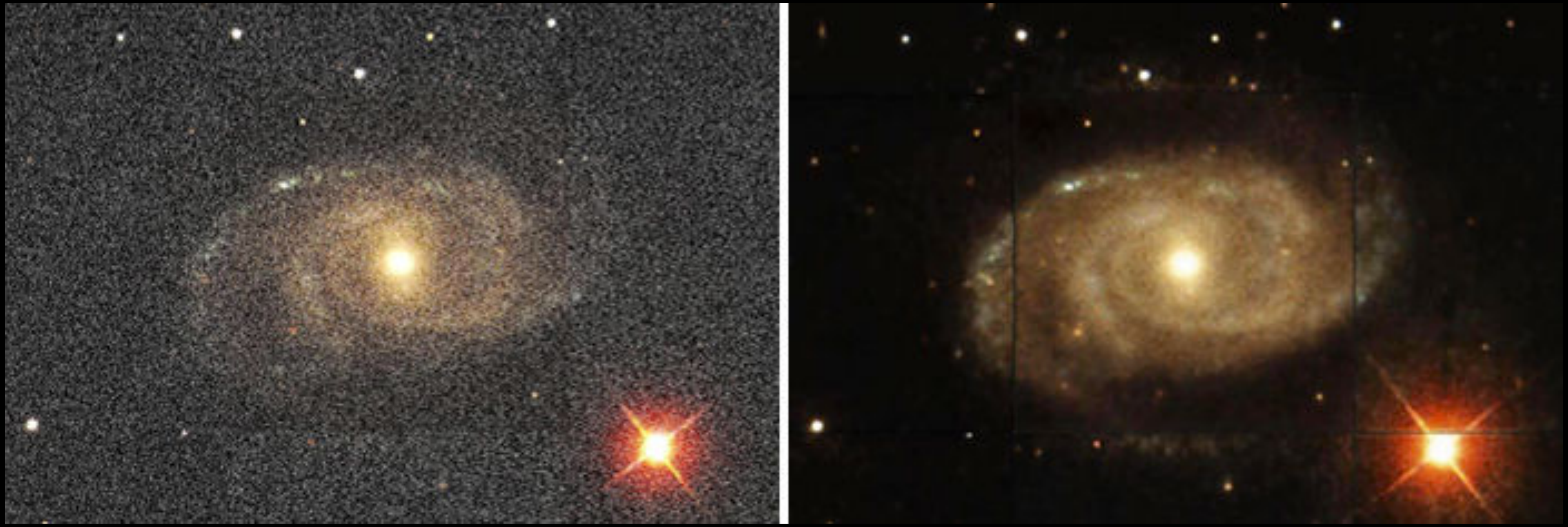
Science

$15
7 JULY 2017
sciencemag.org
AAAS

AI TRANSFORMS SCIENCE

p. 16

Astronmy, Particle Physics, Genomics, demographics, Medicine, …



AI that "knows" what a galaxy should look like transforms a fuzzy image (left) into a crisp one (right).

Why ML for Quantum Matter?

1. Experimental and Computational Data-driven Challenges
2. Understanding = Knowledge Compression: Regression/Generation

Challenges of Complexity

Simple Principles

Entropy
Phonons
Topological Invariant
Fermi statistics

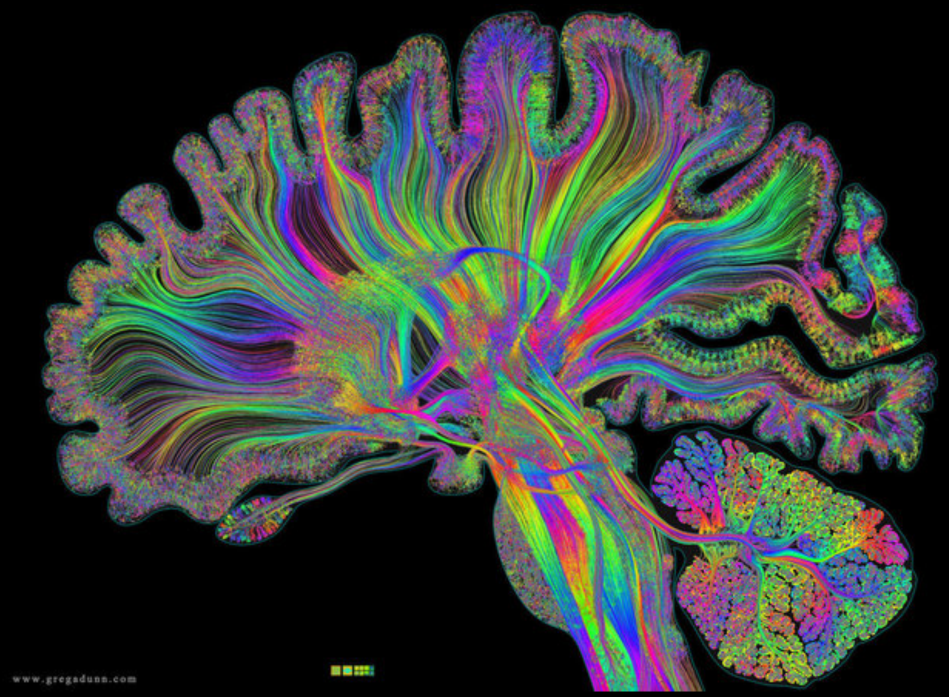
Regression, Classification

Generation, Prediction

Complex Reality of Data

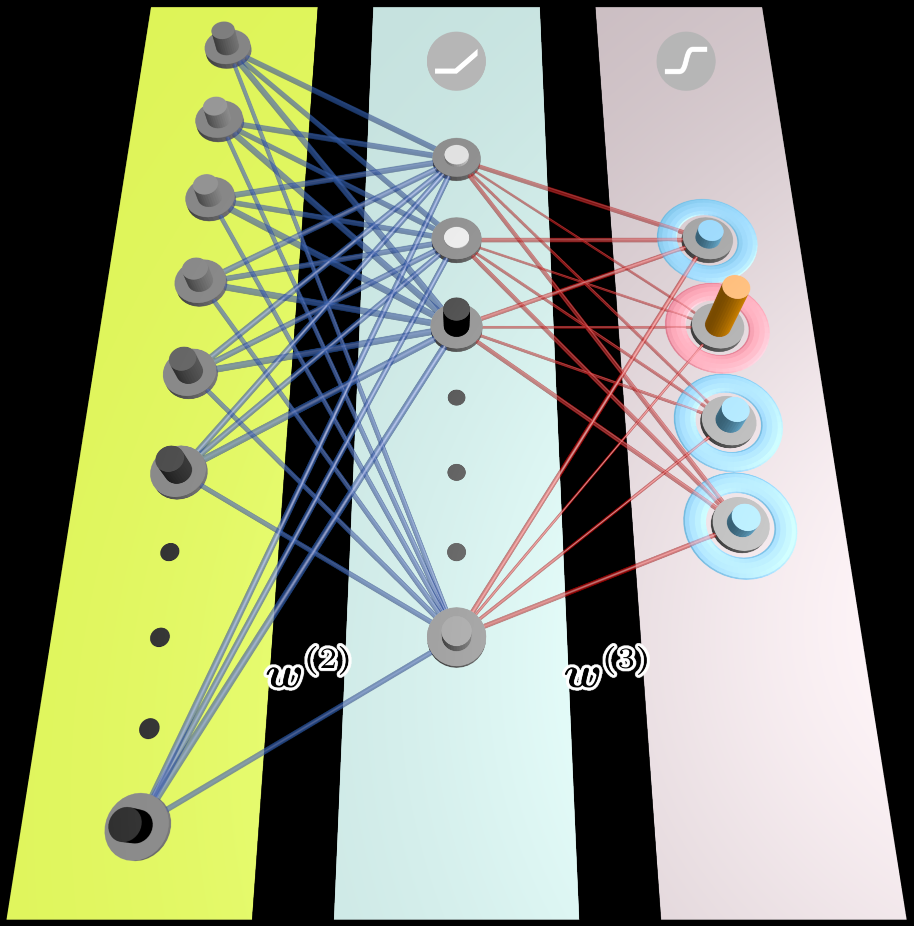
Phase Diagrams
Many-body Wave Functions

New Insight through Synergy



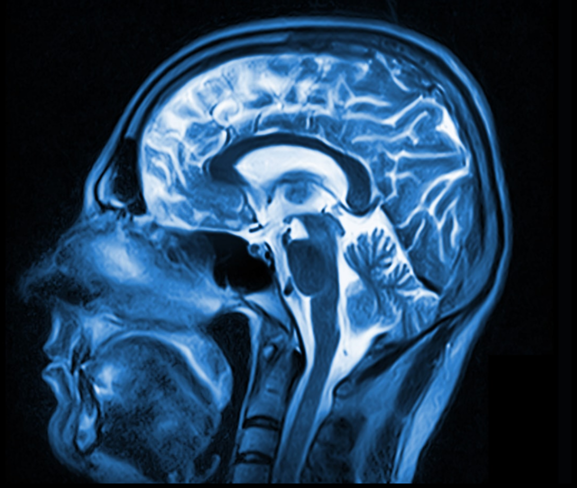
GREG DUNN AND BRIAN EDWARDS

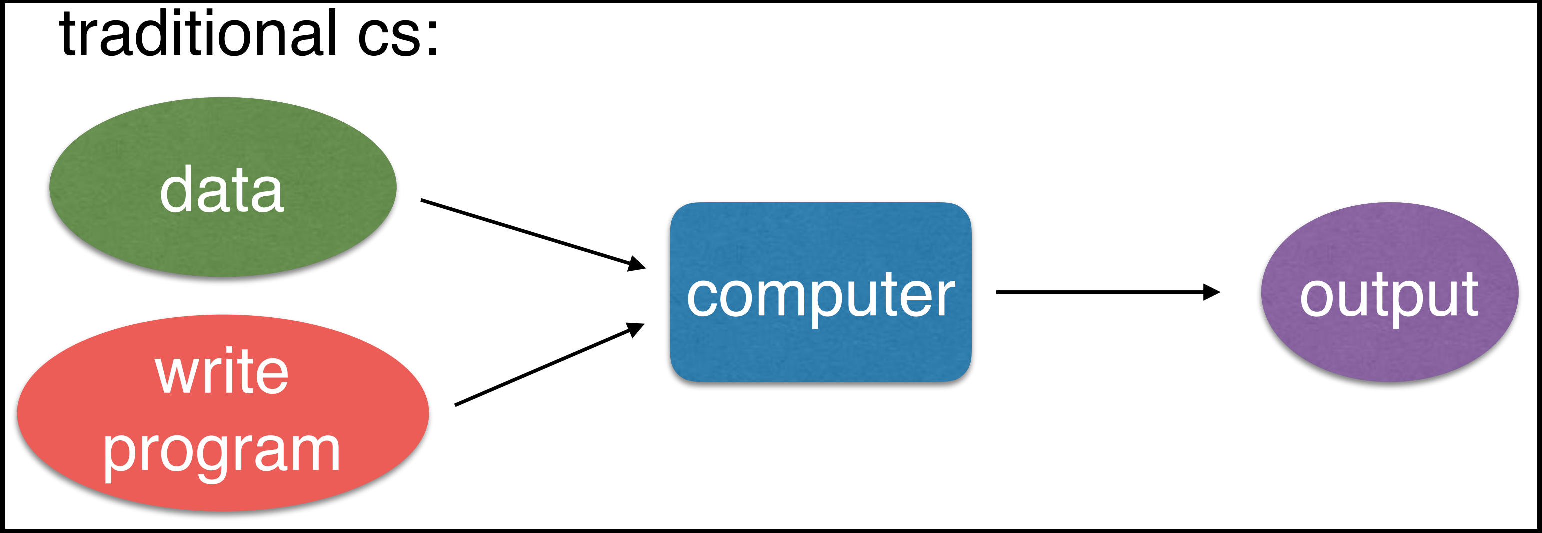
$\otimes$

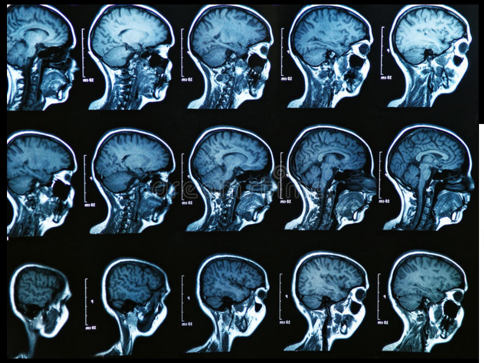


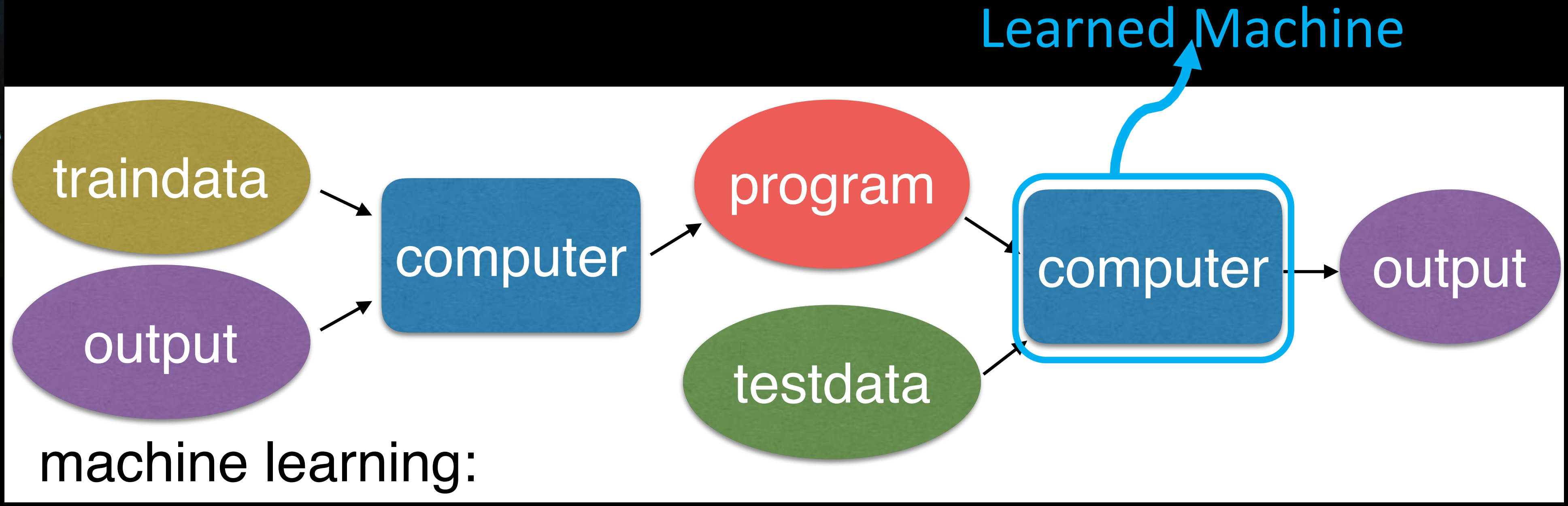
Machine Learning

Challenges of Complexity: Altzheimer







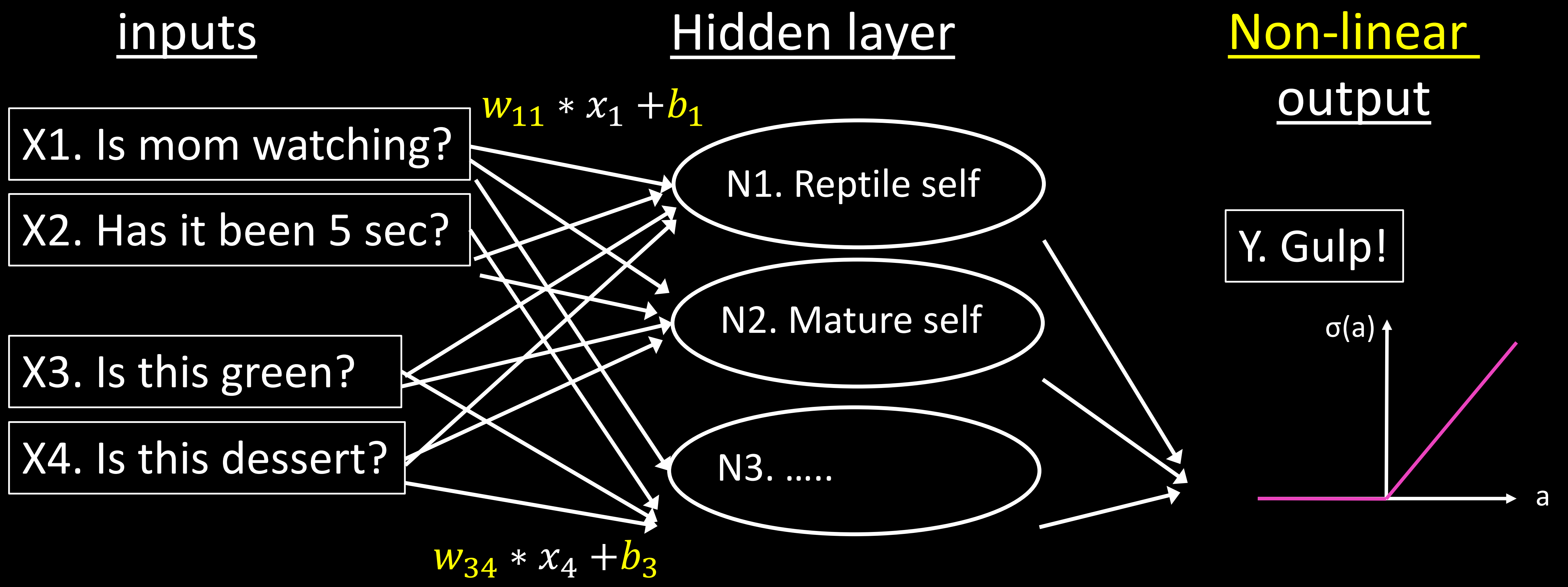


How Neural Network Learns

to make the correct decision

Decision (regression) based on w(t) and b(t)

- Kid's decision upon dropping food…



Gradient Descent with a Cost Function C(w,b)

<u>inputs</u>

X1. Is mom watching?

X2. Has it been 5 sec?

X3. Is this green?

X4. Is this dessert?

- ❑ Non-linear output, e.g., (rectifier)

$$\boxed{a(x; w, b) = \max(0, wx + b)}$$

- ❑ Desired output for a particular input x

$$\boxed{y(x) = 0}$$

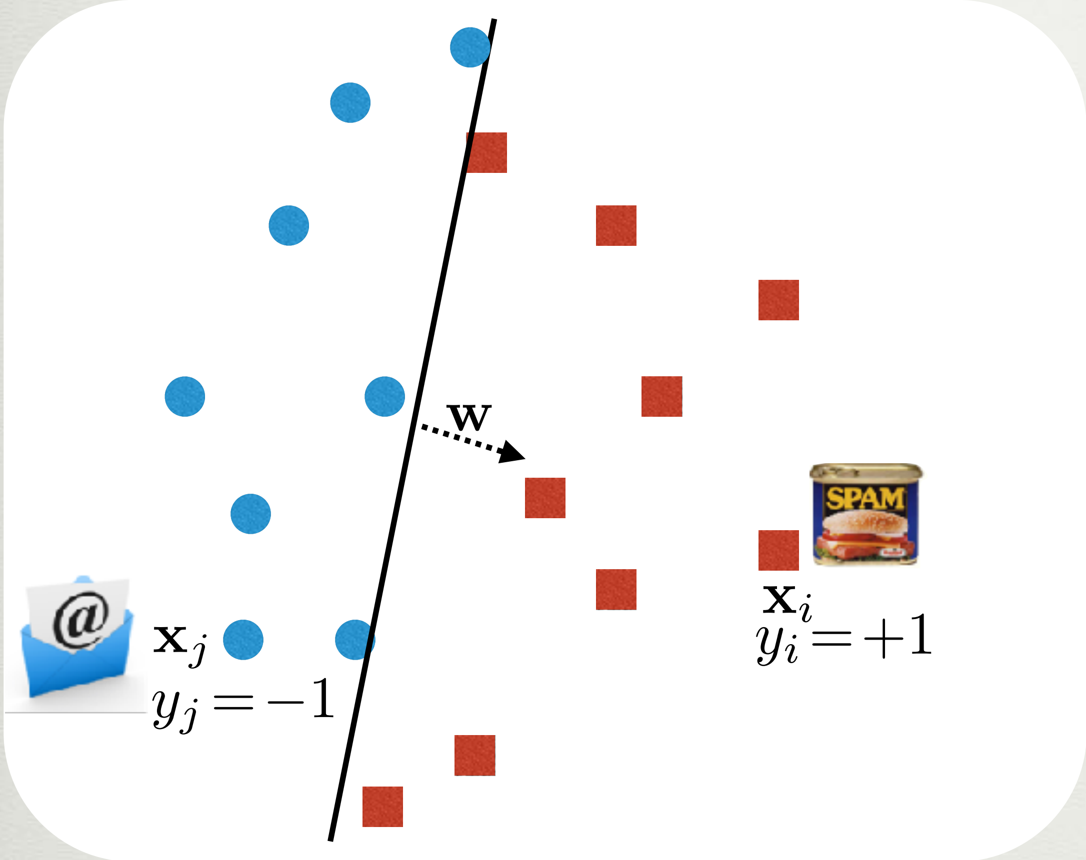
- ❑ Cost Function, e.g. cross entropy

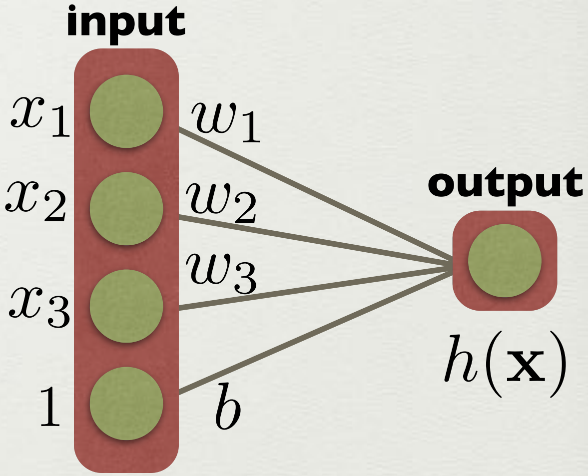
$$\boxed{C(w, b) = -\frac{1}{n}\sum_x [y\ln a + (1-y)\ln(1-a)]}$$

What can we do with ANN?

Perceptron

[Rosenblatt 1957]





Slide from Kilian Weinberger, Cornell

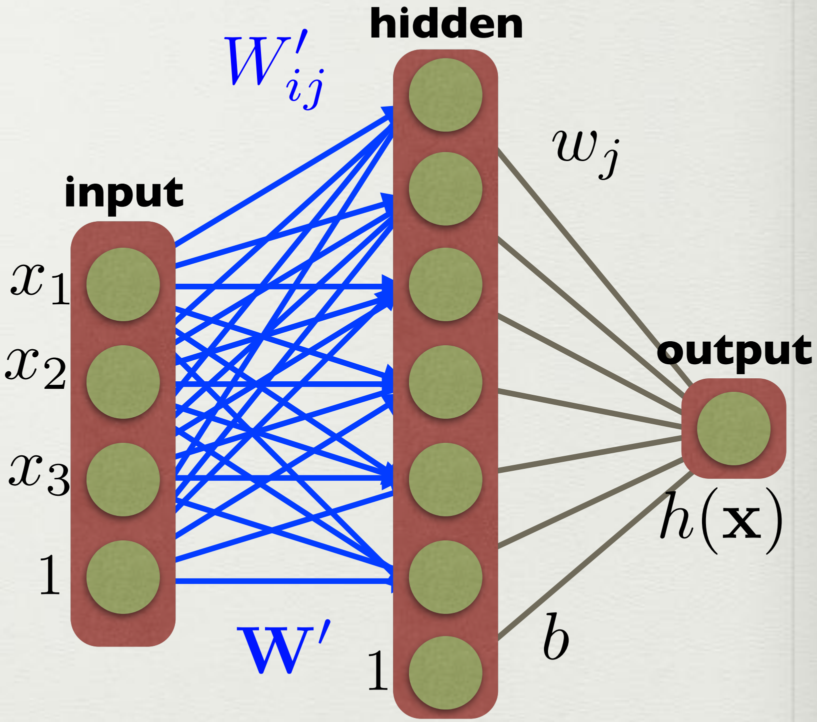
$$h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

http://cornell.videonote.com/videos/1000481/play?t=1654.958939

Multi-Layer Perceptron

(a.k.a. Neural Networks)

[Rosenblatt 1961]



$$\sigma(a) = \max(a, 0)$$

Rectified Linear Units

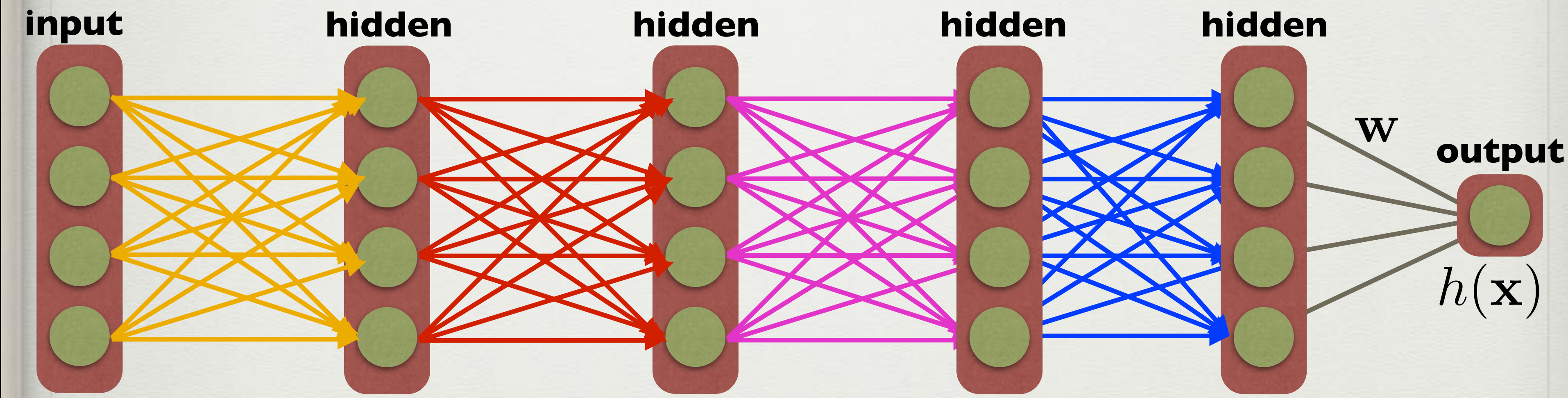
$$h(\mathbf{x}) = \mathbf{w}^\top \sigma\left(\mathbf{W}'\mathbf{x} + \mathbf{c}\right) + b$$

Slide from Kilian Weinberger, Cornell

Multi-Layer Perceptron

(a.k.a. Neural Networks, Deep Learning)

[Rosenblatt 1961]



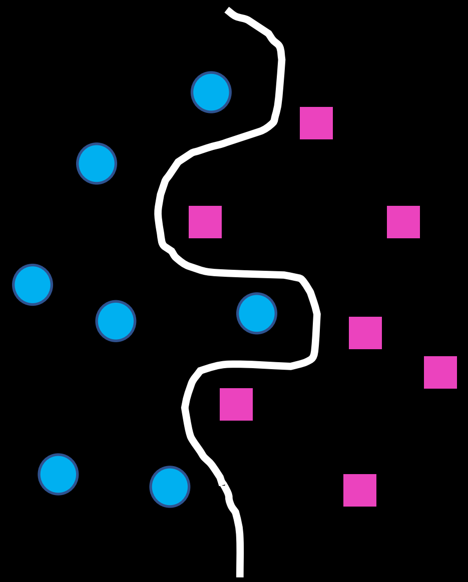
$$h(\mathbf{x}) = \mathbf{w}^\top \sigma(\mathbf{W}'\sigma(\mathbf{W}^2\sigma(\mathbf{W}^3\sigma(\mathbf{W}^4\mathbf{x}))))$$

Slide from Kilian Weinberger, Cornell

Use Neural Networks to

Represent

Many-Body Wave Functions



Classify

Numerical & Experimental Data

ML in Quantum Matter Physics

- Representing Wave function
  - Variational Wave Function represented through neural networks
    https://arxiv.org/abs/1606.02318, Carleo & Troyer, Science (2017)
  - Mapping Tensor Network to Neural network
    https://arxiv.org/pdf/1701.04831.pdf Tao Xiang
  - Neural Network Representation of Ground State WF of solvable models
    Dong-Ling Deng, Xiaopeng Li, Das Sarma
    https://arxiv.org/abs/1609.09060
    https://arxiv.org/abs/1701.04844, PRX (2017)
- Detecting Phases
  - Supervised
    - 2D Ising model & 2D Ising lattice gauge theory **arXiv:1605.01735** Carrasquilla and Melko, Nature Physics (2017)
    - Finite-T repulsive U 3D Hubbard **arXiv:1609.02552** Melko, Khatami et al
    - Zero-T repulsive U honeycomb Hubbard **arXiv:1608.07848** Melko, Trebst et al
    - Fractional Chern Insulator, **arXiv:1611.01518**, Yi Zhang & E-AK, PRL, Physics Viewpoint (2017)
    - Z2 QSL with mutual statistics, **arXiv:1705.01947**, Yi Zhang, Melko, E-AK
    - MBL, **arXiv:1704.01578** Neupert et al
    - Hard-core bosons: superfluids, KT, Semi-unsupervised, **arXiv:1707.00663**, Broecker, Assaad, Trebst

  - Unsupervised (PCA and Autoencoders): so far, all classical.
    arXiv:1606.00318 Lei Wang: 2D Ising
    https://arxiv.org/abs/1703.02435 S. Wetzel: 2D Ising, 3D XY
    https://arxiv.org/pdf/1704.00080.pdf Hu, Singh, Scalatter, Various spin models including highly frustrated three component (S in {-1,0,1}) spin model).
    https://arxiv.org/pdf/1706.07977.pdf Ce Wang &Hui Zhai, Classical frustrated spin model
- Theoretical Physics of Deep Neural Networks:
  - Connection between RG and fully connected deep network, **arXiv:1410.3831**, Mehta and Schwab

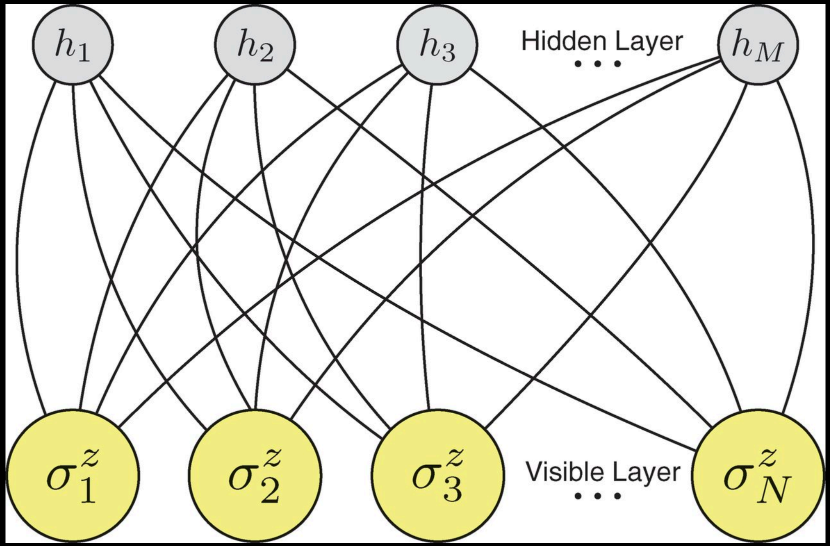
Used Neural Networks to

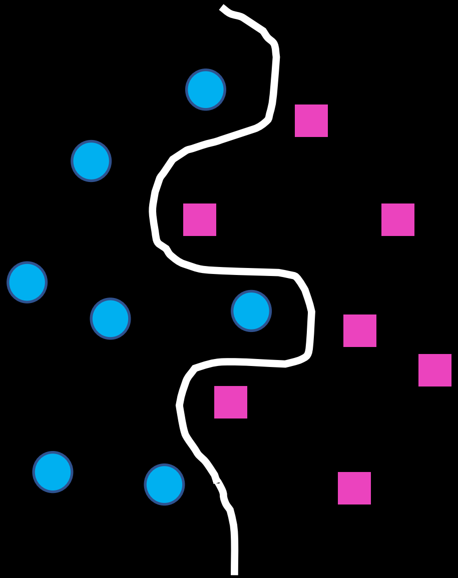
Represent

Many-Body Wave Functions

Carleo and Troyer, Science 355, 602 (Feb, 2017)

$$\Psi_{\mathcal{M}}(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} \exp\left[\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z\right]$$

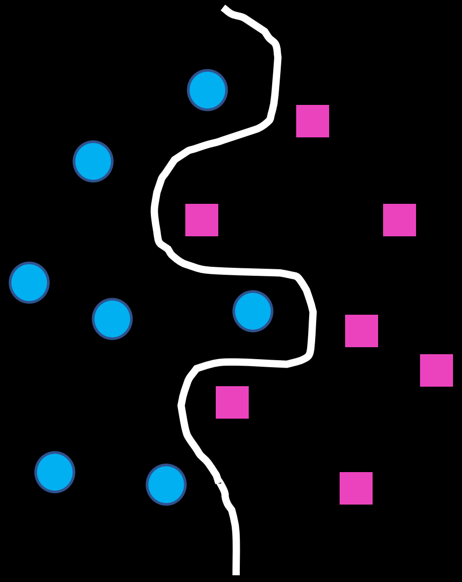




The network parameters $\mathcal{W} = \{a, b, W\}$

: A compact representation of the many-body state

Used Neural Networks to

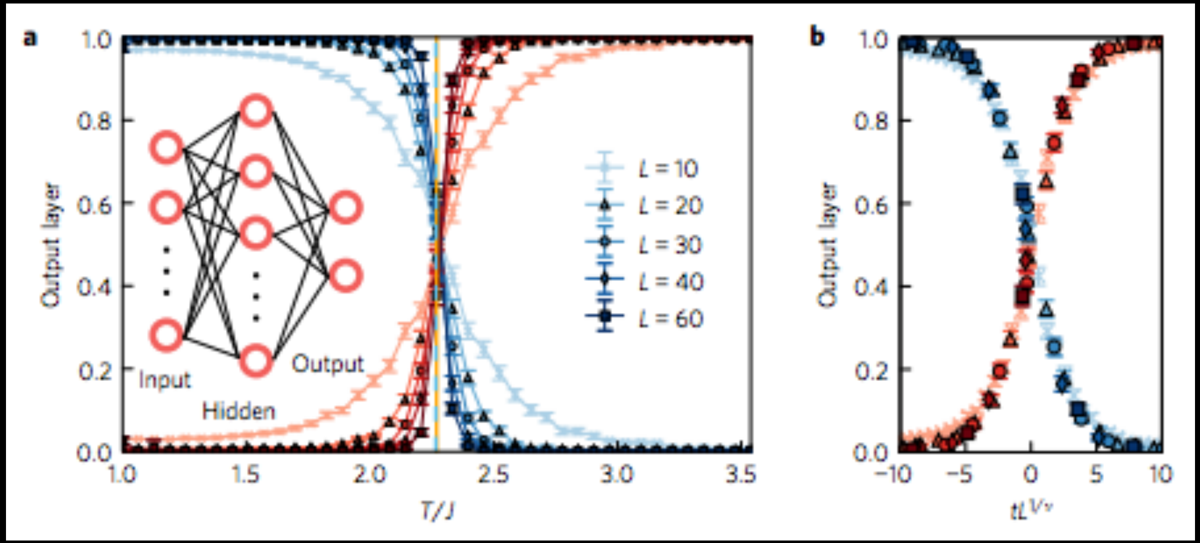


Classify

Numerical Data

Carrasquilla and Melko, Nat. Phys. ,13, 431 (May, 2017)

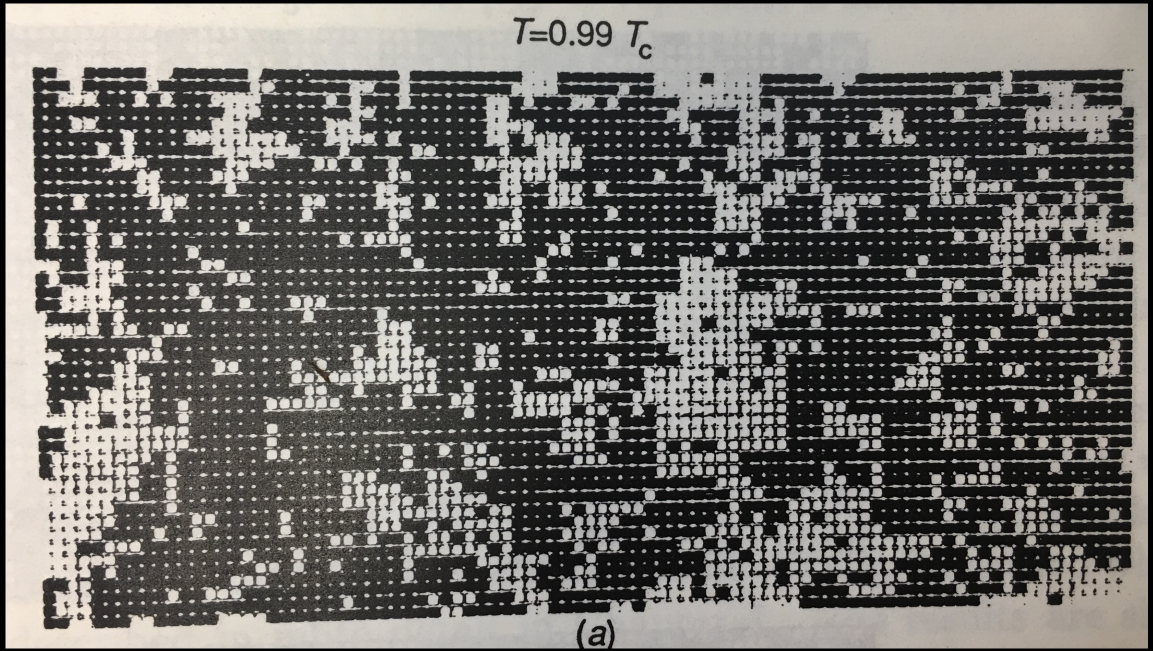
- Supervised Learning on the (thermalized) raw configurations
- Speed-up from "seeing through" noisy data.

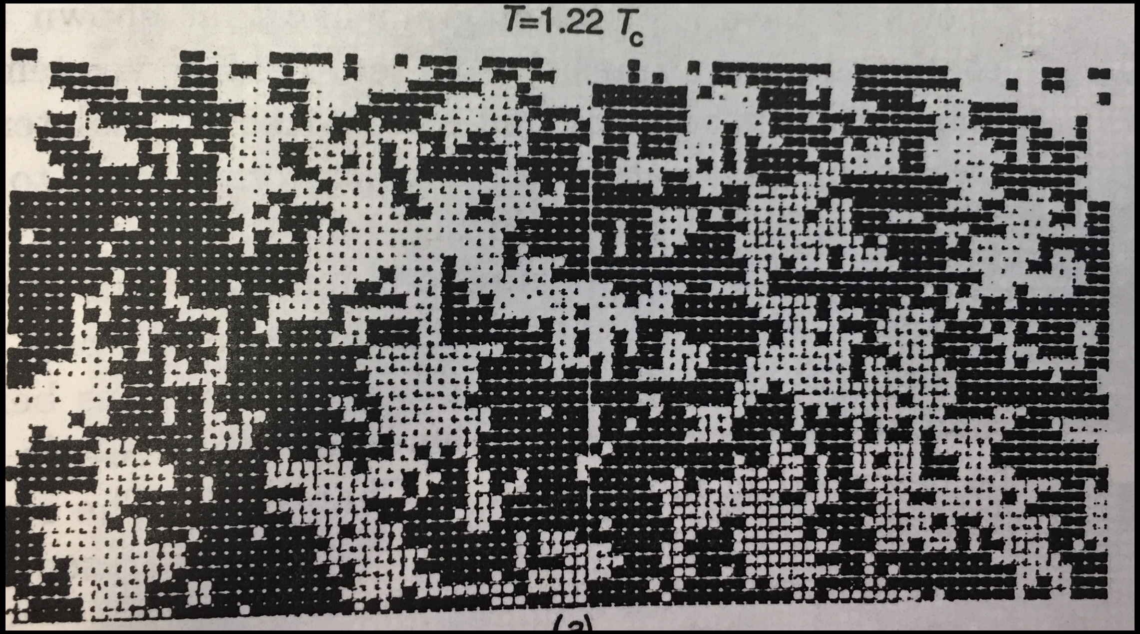


Bench-Marked against known results for

- The 1D Transverse Field Ising Model
- The Antiferromagnetic Heisenberg Model in 1D and 2D (square lattice)
- The Ferromagnetic Ising Model

But all Long-Range Ordered States are Classical!!





Beyond Long Range Order…

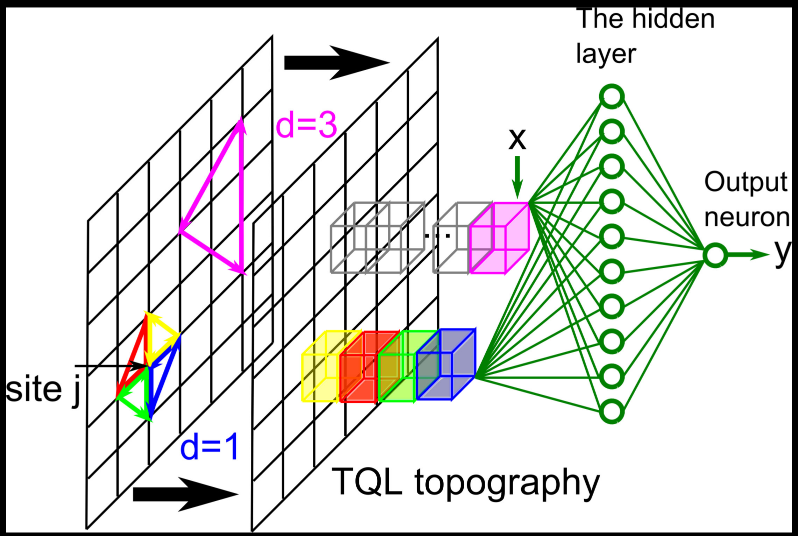
1. Discerning Topological Phases in Computational Data.

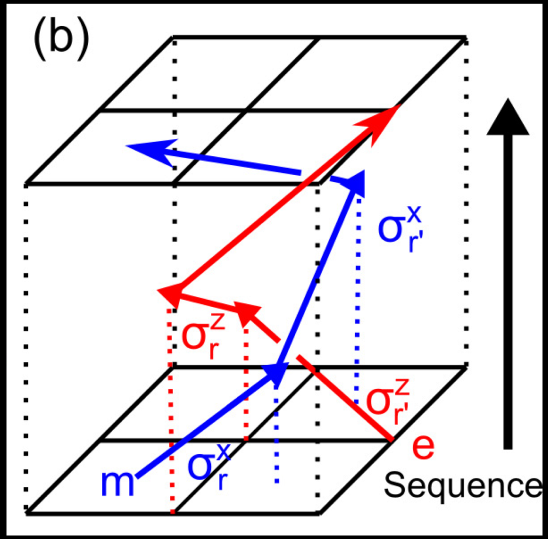
2. Seeking Theoretical Insights in Experimental Data from STM.

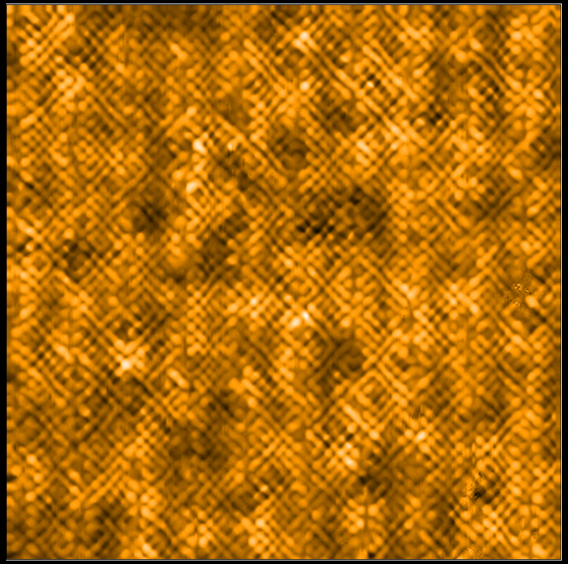
QPT

Mutual Statistics

CDW







Yi Zhang &E-AK, PRL **118**, 216401 (2017), Physics Viewpoint

Yi Zhang , R. Melko &E-AK, PRB, 96, 245119 (2017)

Mesaros et al, &E-AK, 2018

Discerning Numerical Data

Yi Zhang

- Chern Insulators

Featured in Physics | Editors' Suggestion

Quantum Loop Topography for Machine Learning

Yi Zhang and Eun-Ah Kim
Phys. Rev. Lett. **118**, 216401 – Published 22 May 2017

Physics See Viewpoint: Neural Networks Identify Topological Phases

- Z2 Quantum Spin Liquid

PHYSICAL REVIEW B **96**, 245119 (2017)

Machine learning $\mathbb{Z}_2$ quantum spin liquids with quasiparticle statistics

Yi Zhang,[1,*] Roger G. Melko,[2,3] and Eun-Ah Kim[1,†]

Interpretability:
What did Neural Network Learn?

Yi Zhang

Discerning Numerical Data

- Chern Insulators

Featured in Physics | Editors' Suggestion

Quantum Loop Topography for Machine Learning

Yi Zhang and Eun-Ah Kim
Phys. Rev. Lett. **118**, 216401 – Published 22 May 2017

Physics See Viewpoint: Neural Networks Identify Topological Phases

- Z2 Quantum Spin Liquid

PHYSICAL REVIEW B **96**, 245119 (2017)

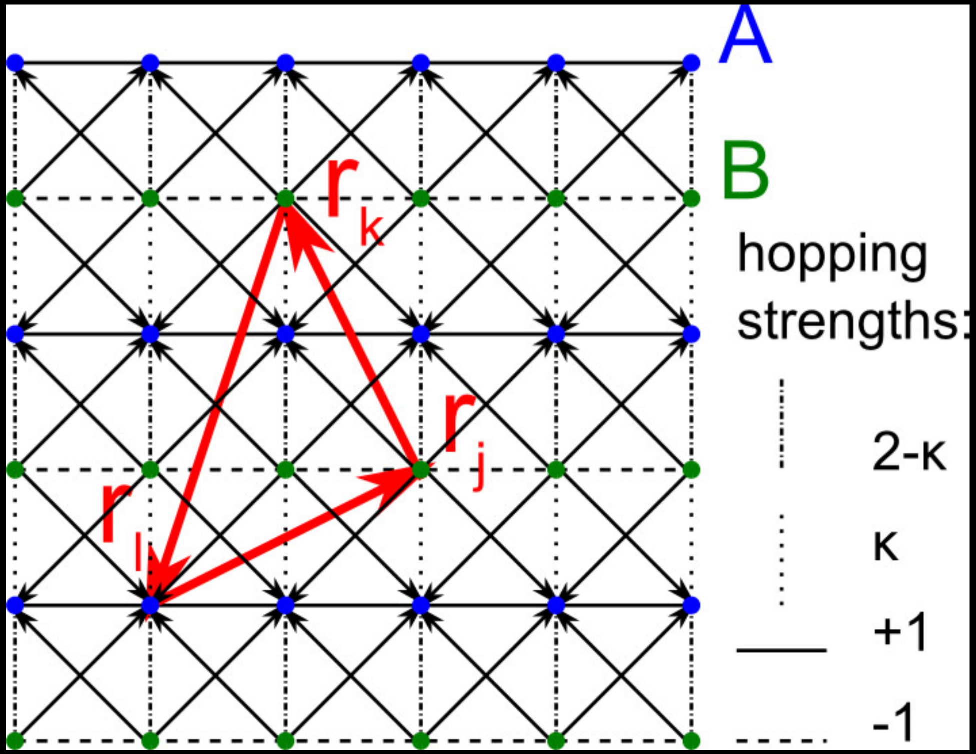
Machine learning $\mathbb{Z}_2$ quantum spin liquids with quasiparticle statistics

Yi Zhang,[1,*] Roger G. Melko,[2,3] and Eun-Ah Kim[1,†]

Interpretability:
What did Neural Network Learn?

Chiral Topological Phase: Chern insulator TQPT

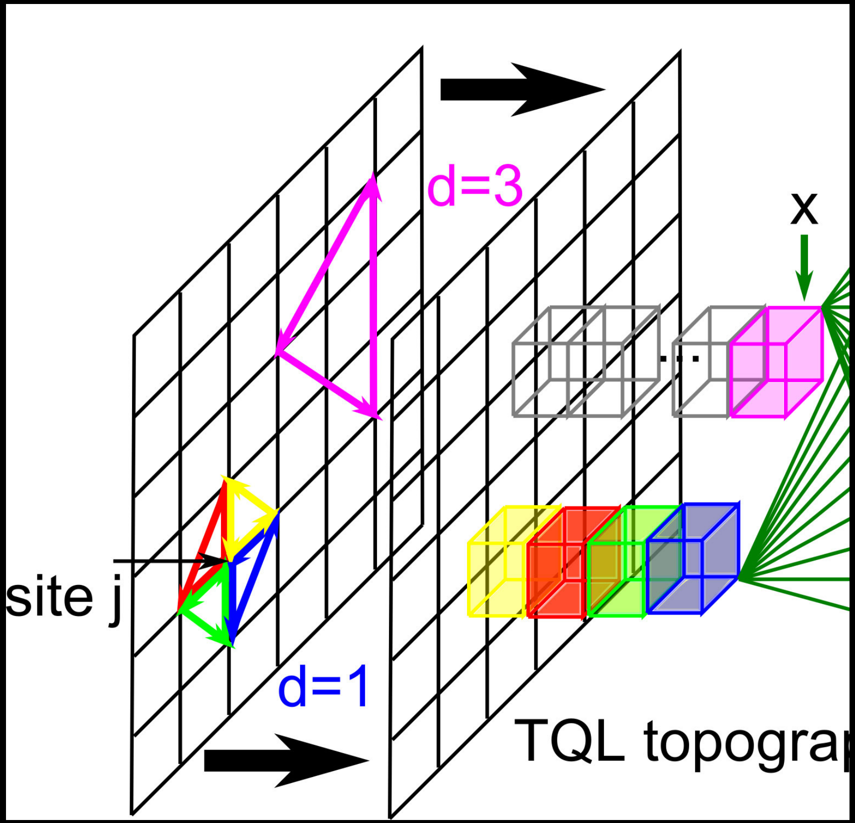
Model part I: Free Fermion



$$H(\kappa) = \sum_{\vec{r}} (-1)^y c^\dagger_{\vec{r}+\hat{x}} c_{\vec{r}} + [1 + (-1)^y(1-\kappa)] c^\dagger_{\vec{r}+\hat{y}} c_{\vec{r}} + (-1)^y \frac{i\kappa}{2} \left[c^\dagger_{\vec{r}+\hat{x}+\hat{y}} c_{\vec{r}} + c^\dagger_{\vec{r}+\hat{x}-\hat{y}} c_{\vec{r}} \right] + \mathrm{h.c.} \qquad (2)$$

- Topological Quantum Phase Transition at κ=0.5
- κ<0.5 trivial insulator
- κ>0.5 Chern insulator

Quantum Loop Topography



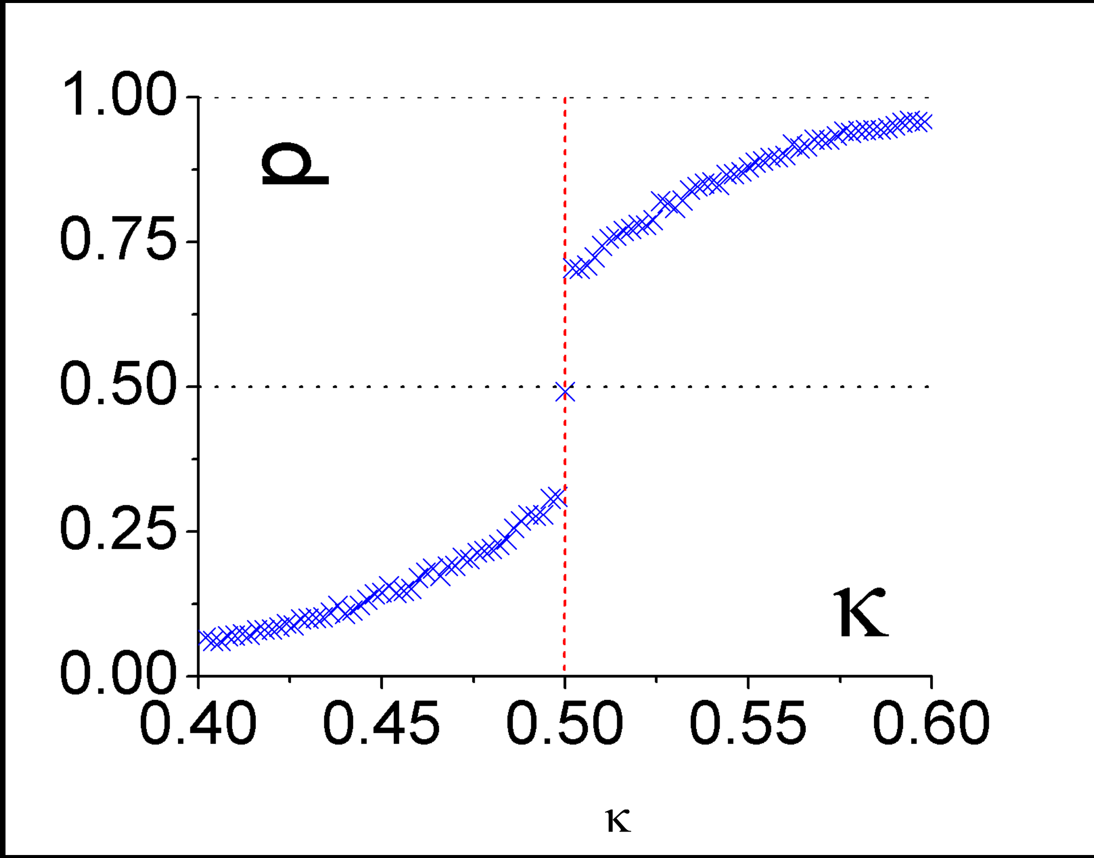
- QLT data entry for input x

$$\tilde{P}_{jk}\tilde{P}_{kl}\tilde{P}_{lj} \qquad \text{where } \tilde{P}_{jk} \equiv \left\langle c_j^\dagger c_k \right\rangle_\alpha$$

for a particular MC config.

- Each entry of x is complex valued
- Length(x)=2xLxLxD(d_c)

QLT as the input vector

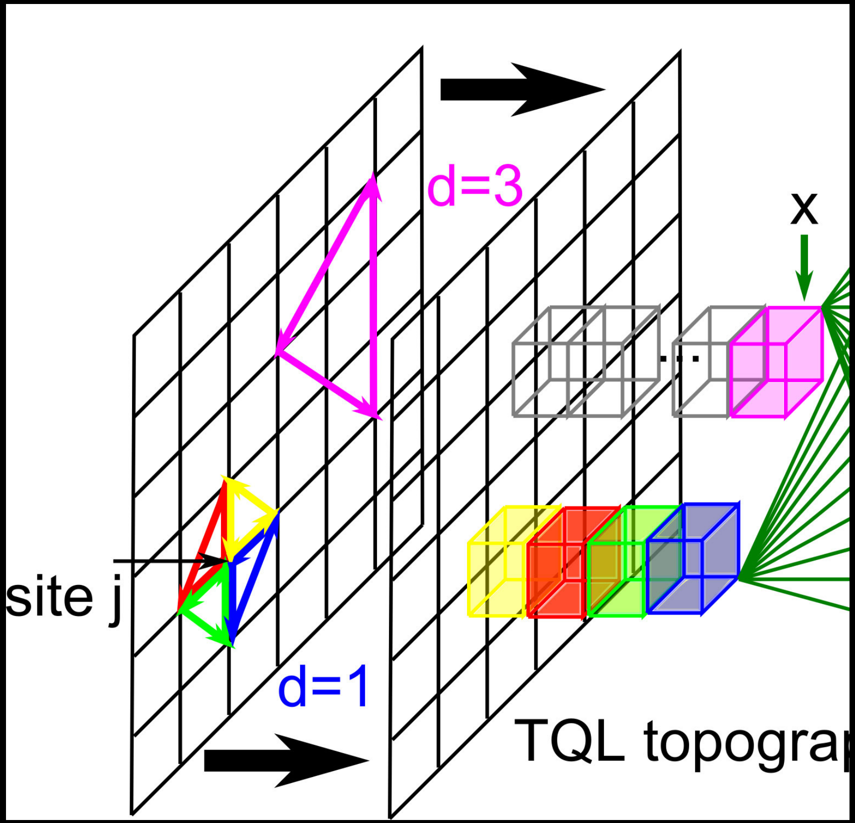


- Train with two known points:

  κ=0.1 (trivial), κ=1 (topo)

- Smallest triangles (d_c=1) are sufficient in the gapped phases
- Once trained, get PD in 10min on a laptop.
- 99.9% accuracy in the phase verified with 2k test samples.

How to ”image” Quantum Loops



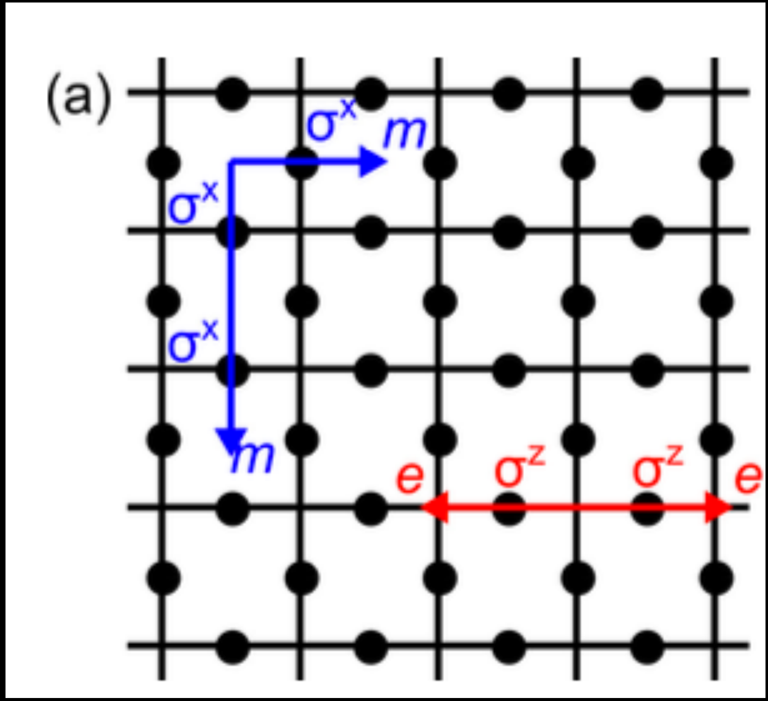
- Organize loops by lateral dimension d=1,2,3…
- Associate each site with all the triangles that involves the site as a vertex.
- Gap & quantization allow d_c<<L
- Quasi-2D ”image” input vector x

non-Chiral Topological Phase: Z2 quantum spin liquid

Yi Zhang , R. Melko &E-AK, PRB, 96, 245119 (2017)

Kitaev Model under field

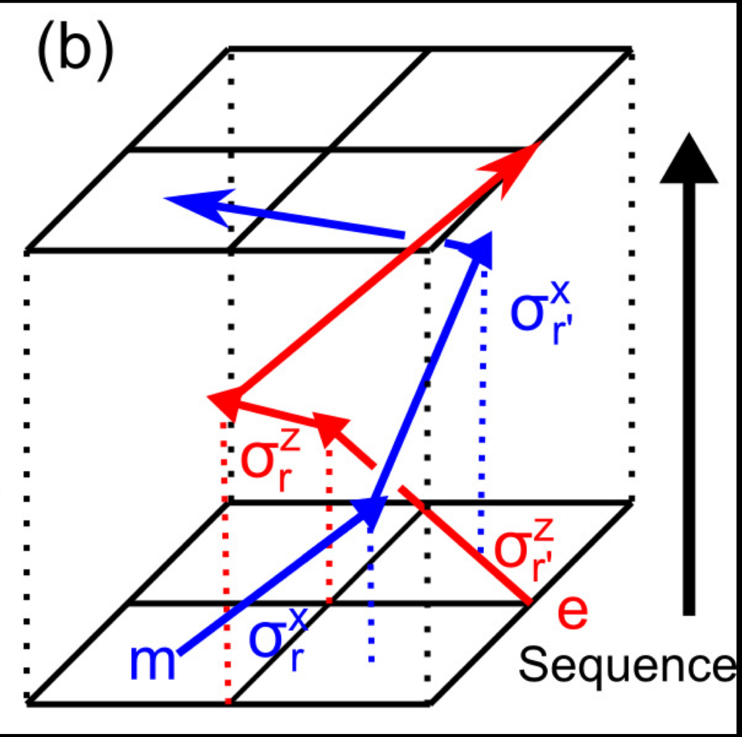
$$H_{2D} = -J_x \sum_s A_s - J_z \sum_p B_p - h_x \sum_b \sigma_b^x - h_z \sum_b \sigma_b^z$$



- Finite region of Z2 spin liquid with finite correlation length
- Spinons and Visons
- Mutual statistics

Quantum Loop Topography for Z2 QSL

$$H_{2D} = -J_x \sum_s A_s - J_z \sum_p B_p - h_x \sum_b \sigma_b^x - h_z \sum_b \sigma_b^z$$



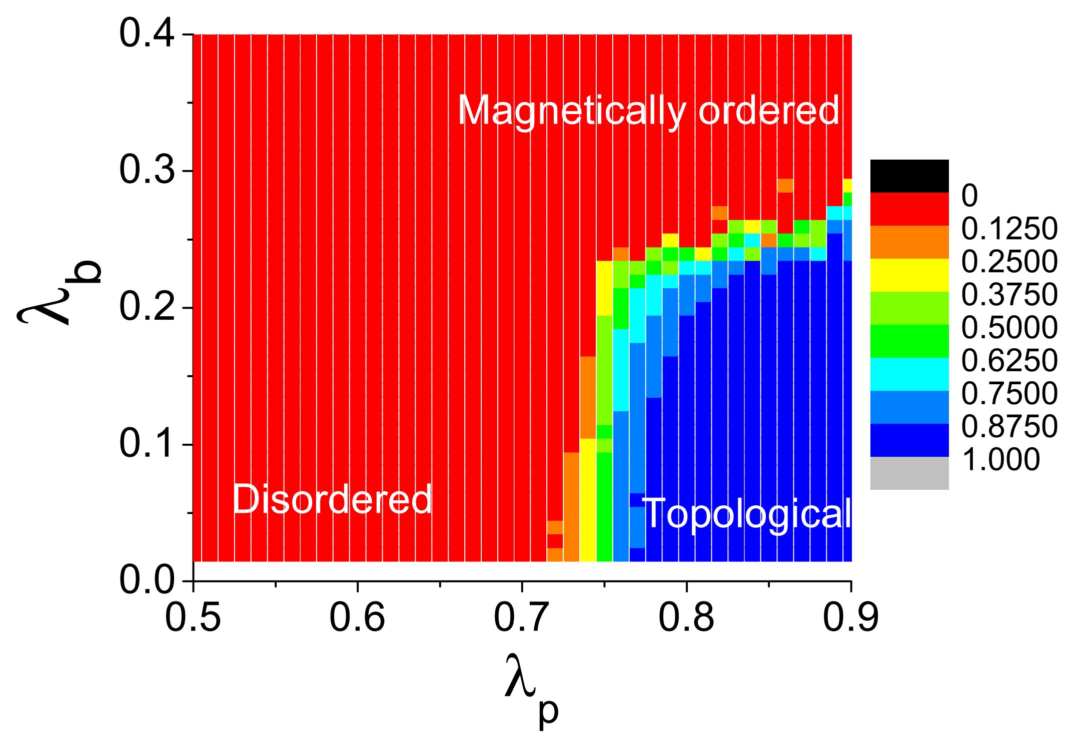
- QLT designed to probe mutual statistics

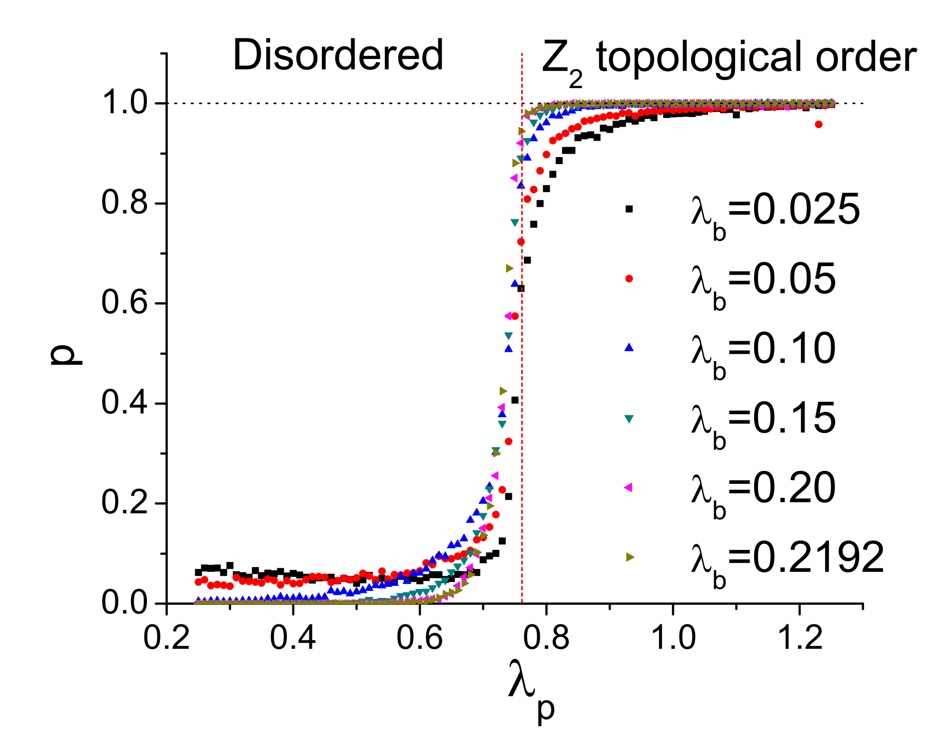
$$\left\langle \sigma_r^x \sigma_{r'}^z \sigma_{r'}^x \sigma_r^z \right\rangle = \mathrm{tr}\left[\rho \sigma_r^x \sigma_r^z \sigma_{r'}^z \sigma_{r'}^x\right]$$

Kitaev Model under field

$$H_{3D} = -\lambda_b \sum_b S_b - \lambda_p \sum_p \prod_{j \in p} S_j$$

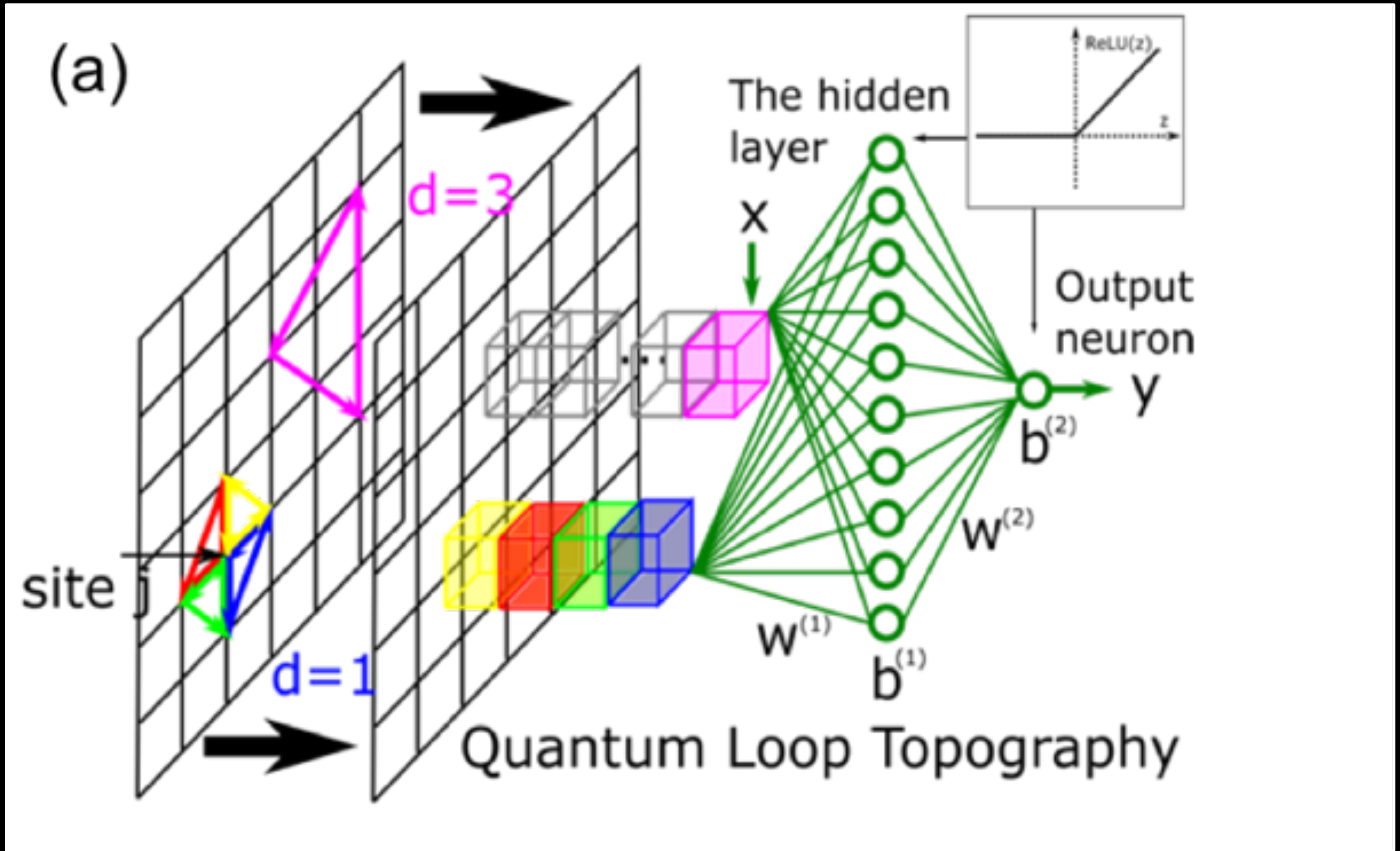
- 2+1D Kitaev Model under field ~Classical Z2 gauge Higgs model in 3D





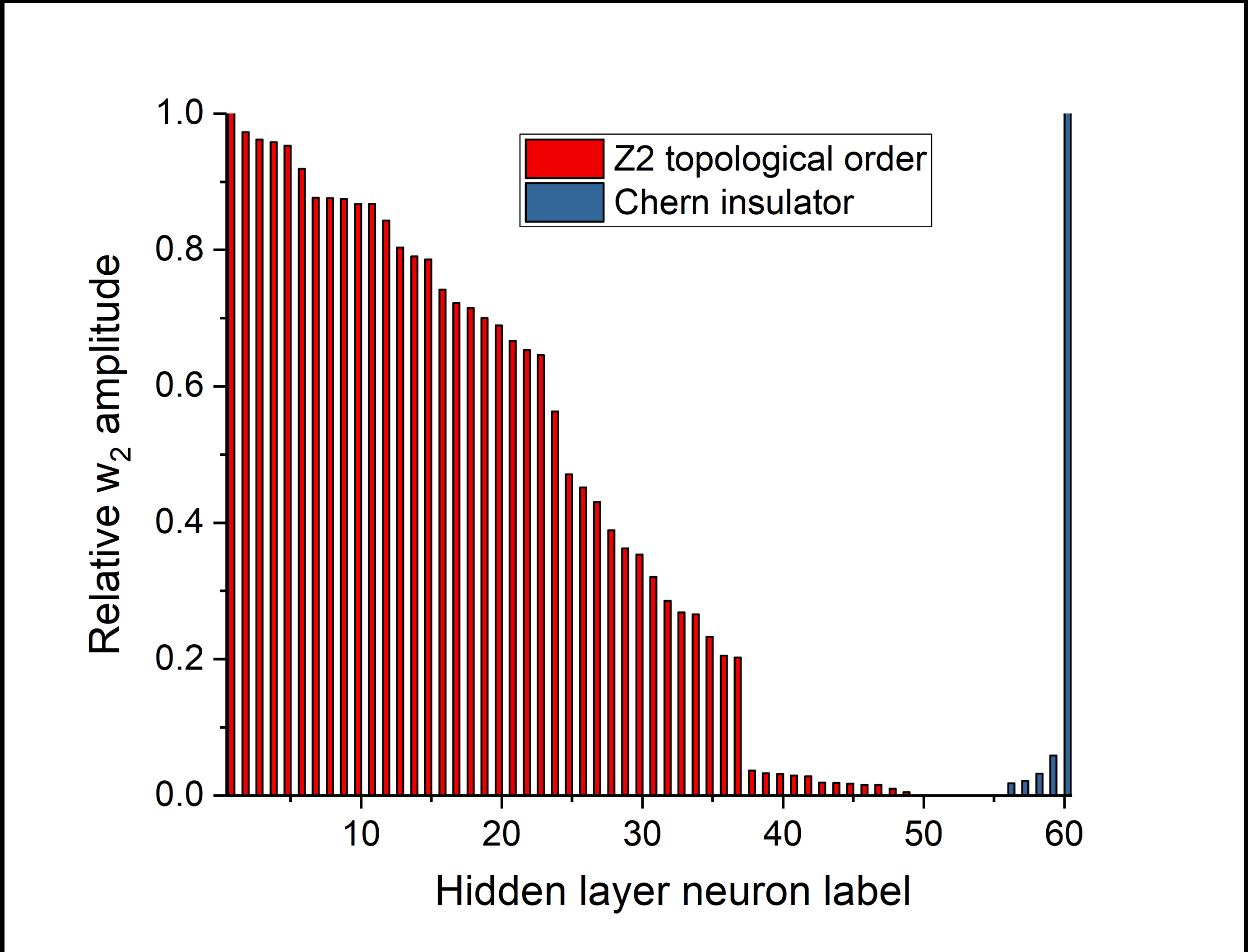
Yi Zhang , R. Melko &E-AK, PRB, 96, 245119 (2017)

Shallow Network, Deep Insight?



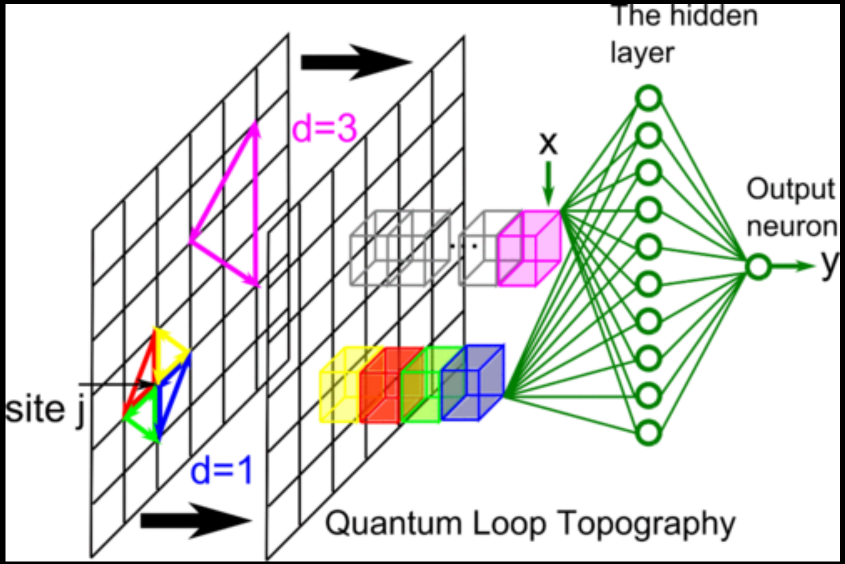
$$y(\vec{x}) = \sigma\left(\mathrm{w}_2^{\mathrm{T}} \cdot \sigma\left(\mathrm{w}_1 \vec{x} + \vec{b}_1\right) + b_2\right)$$

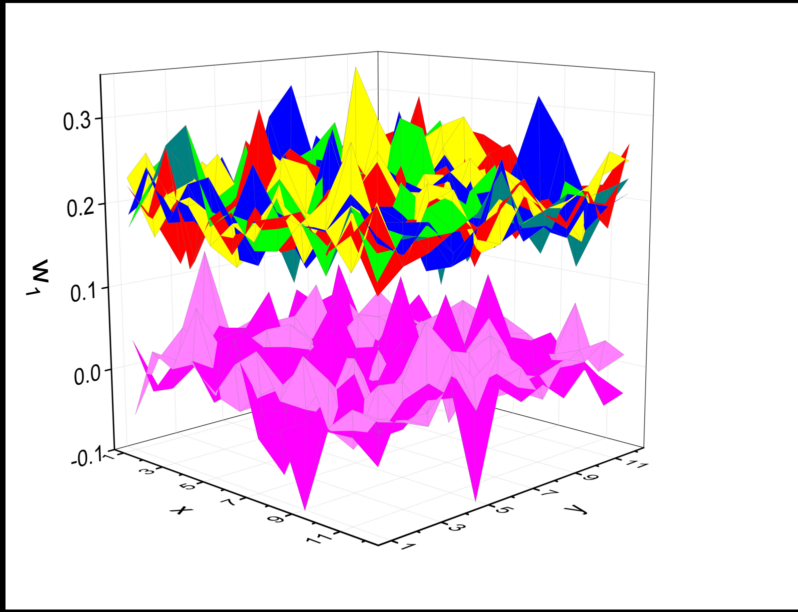
Hidden layer neurons actively involved in decision making for topological phases



What did the AI learn for CI?

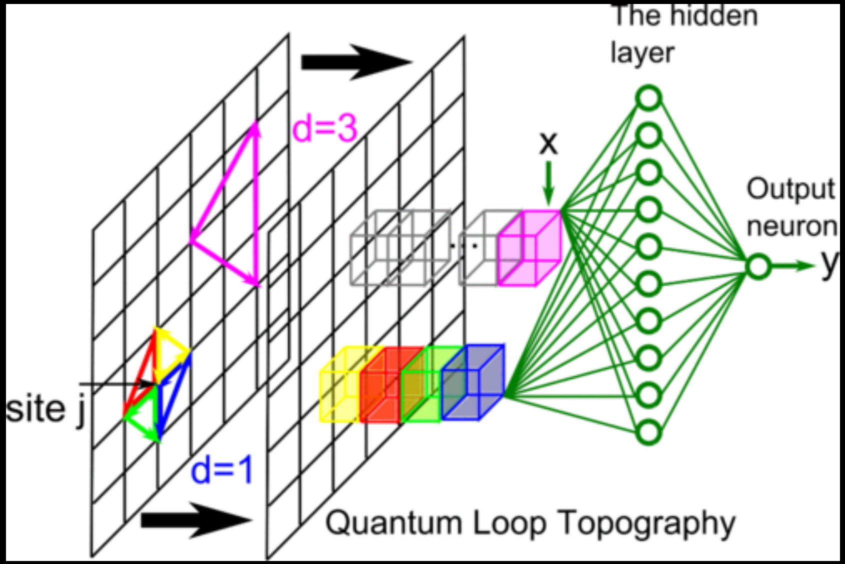
- Largest w_1 weights associated with the *imaginary* parts of the d_c=1 loops
- All sites contribute evenly.

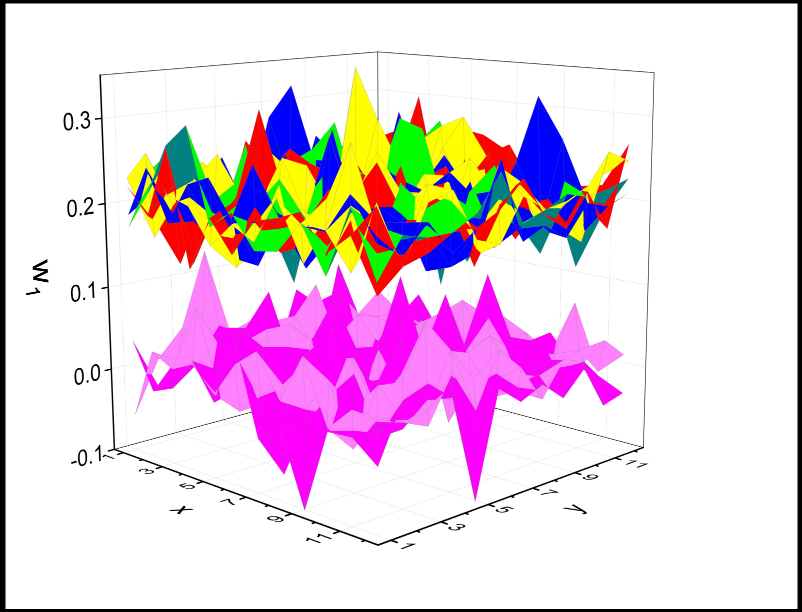




$$-4.84 \times max\left[0.208 \sum_{dc=1} \mathrm{i}P_{jk}P_{kl}P_{lj} + 3.73, 0\right] + 9.03 > 0 \quad \Leftrightarrow \quad \frac{1}{N}\sum_{dc=1} 2\pi \mathrm{i}P_{jk}P_{kl}P_{lj} > 0.392$$

What did the AI learn for CI?

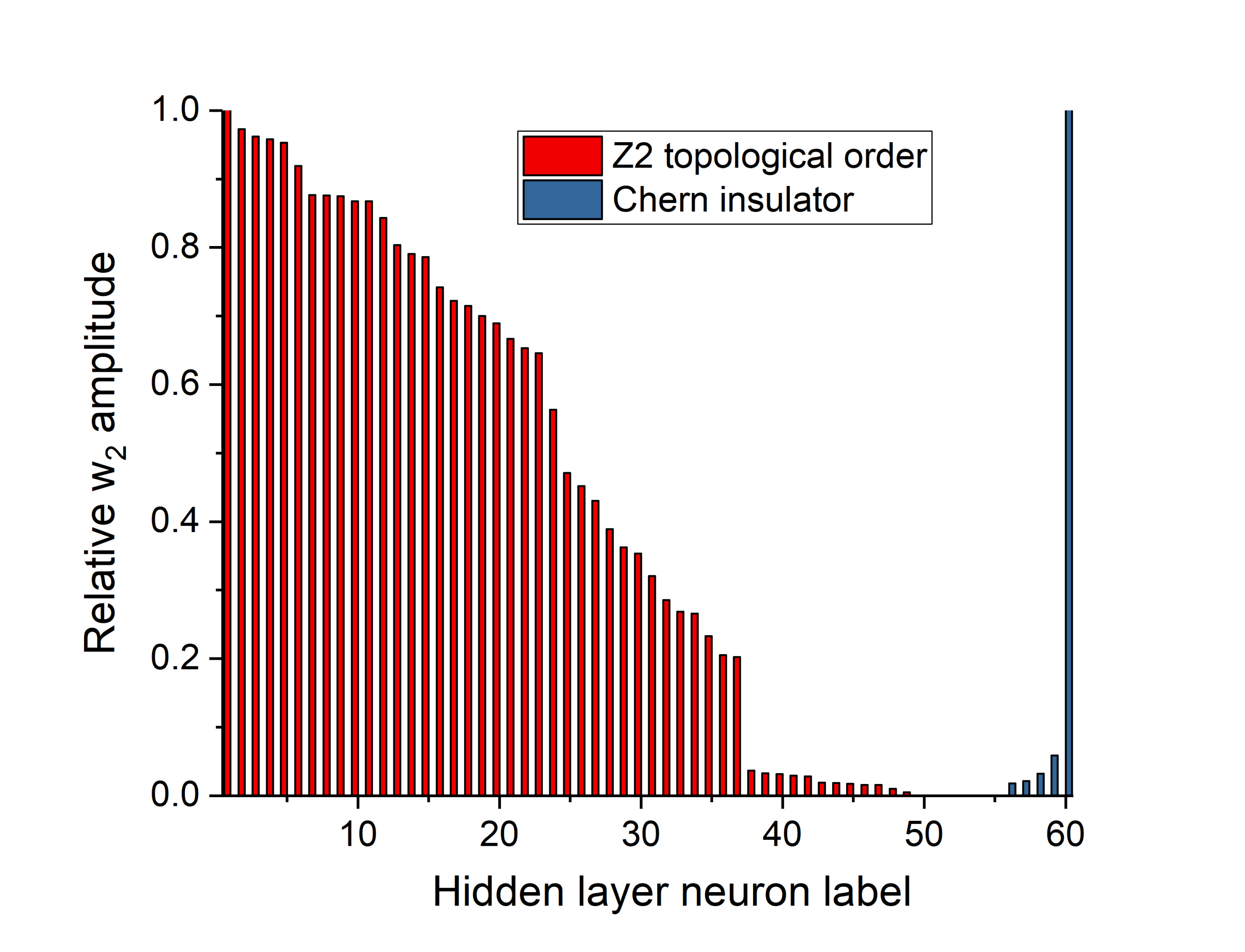




A topological invariant, the Chern Number:

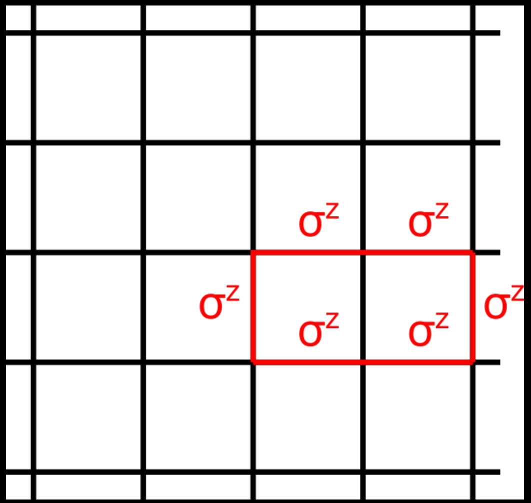
$$n_j = \frac{i}{2\pi} \int dk_x\, dk_y\, \left(\langle \partial_{k_x} u_j | \partial_{k_y} u_j \rangle - \langle \partial_{k_y} u_j | \partial_{k_x} u_j \rangle \right)$$

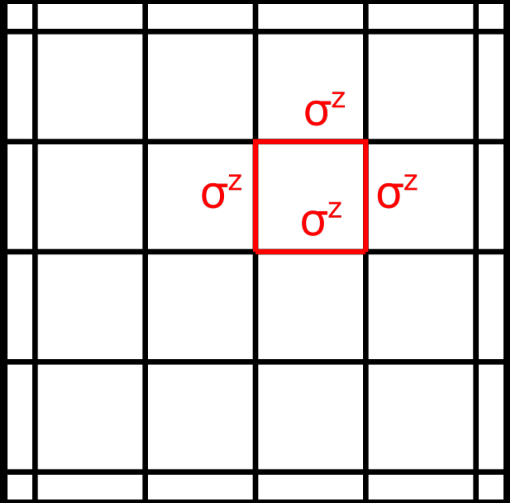
What did the AI learn for Z2 QSL?



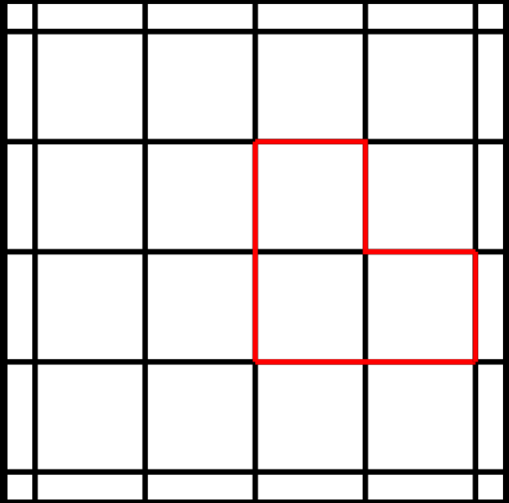
What did the AI learn for Z2 QSL?

1. Full Non-linearity at play!
2. Non-linear products of QLT?





$$(\sigma^z)^2 = 1$$



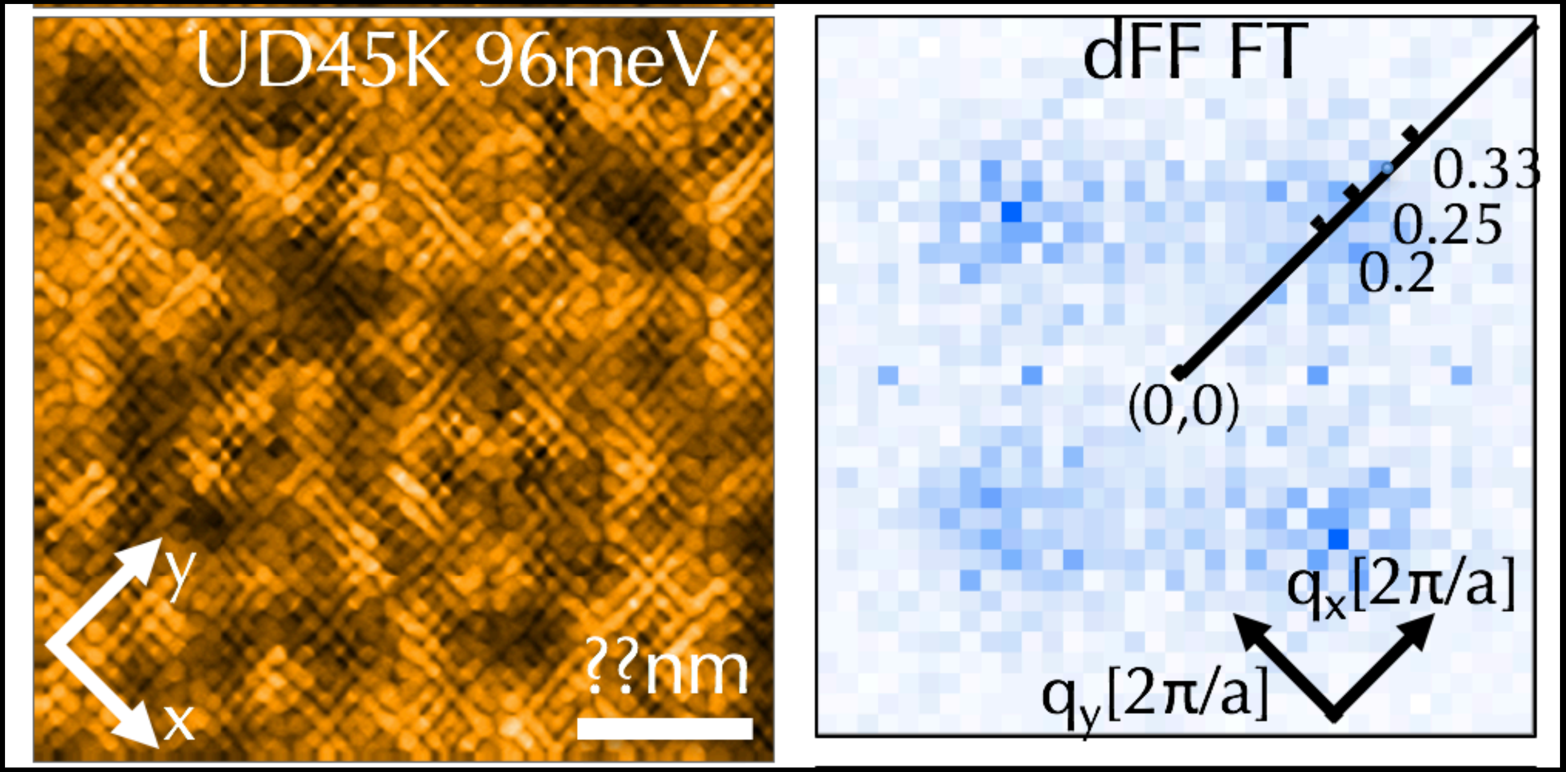
$$W_{C_1} = \prod_{j \in C_1} \sigma_j^z$$

$$W_{C_2} = \prod_{j \in C_2} \sigma_j^z$$

$$W_{C_1} W_{C_2}$$

Non-linearity = Large loops with local info !!

Local Probe Measurements: Dilemma of Large Data set



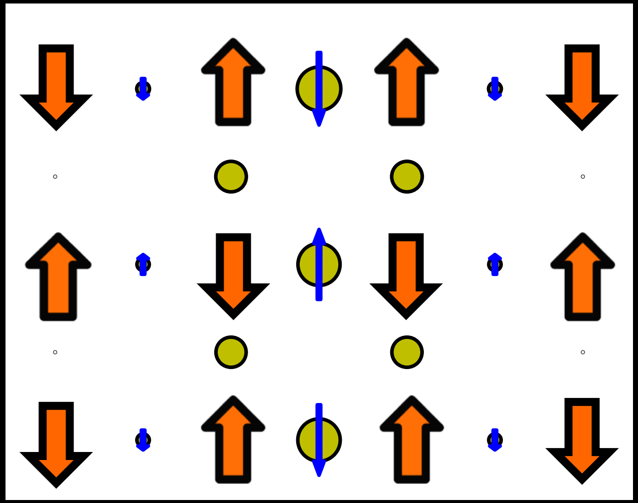
- Local ordering patterns
- How to connect the data to theory?

Questions

1. Origin: r-space or k-space?
2. Nematic?

Strong Coupling Mechanism

- Frustration of AFM order upon doping

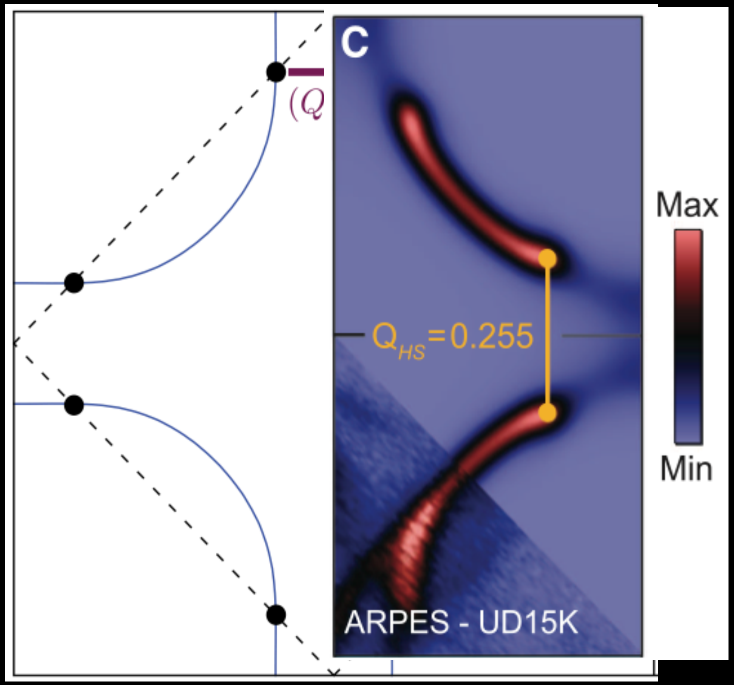


Zaanen, Gunnarson, PRB (1989)
Low, Emery, Fabricious, Kivelson (1994)
Vojta, Sachdev(1999)
White, Scalapino,PRL(1998)
Capponi, Poilblanc (2002)
Corboz, Rice, Troyer, PRL (2014)
Fischer, EAK *et al.*, NJP (2014)

Commensurate Charge Modulation,
period 4a at p=1/8

Weak Coupling Mechnism

- Nesting driven Fermi surface instability

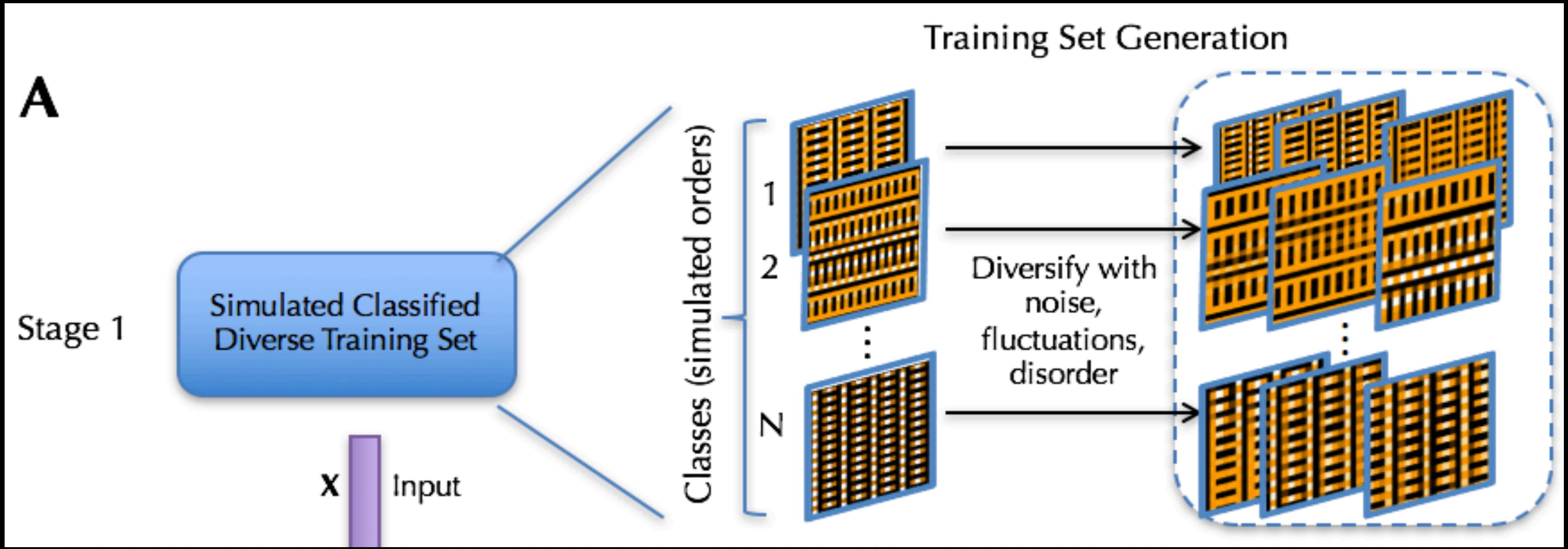


Comin *et al.*, Science(2014)

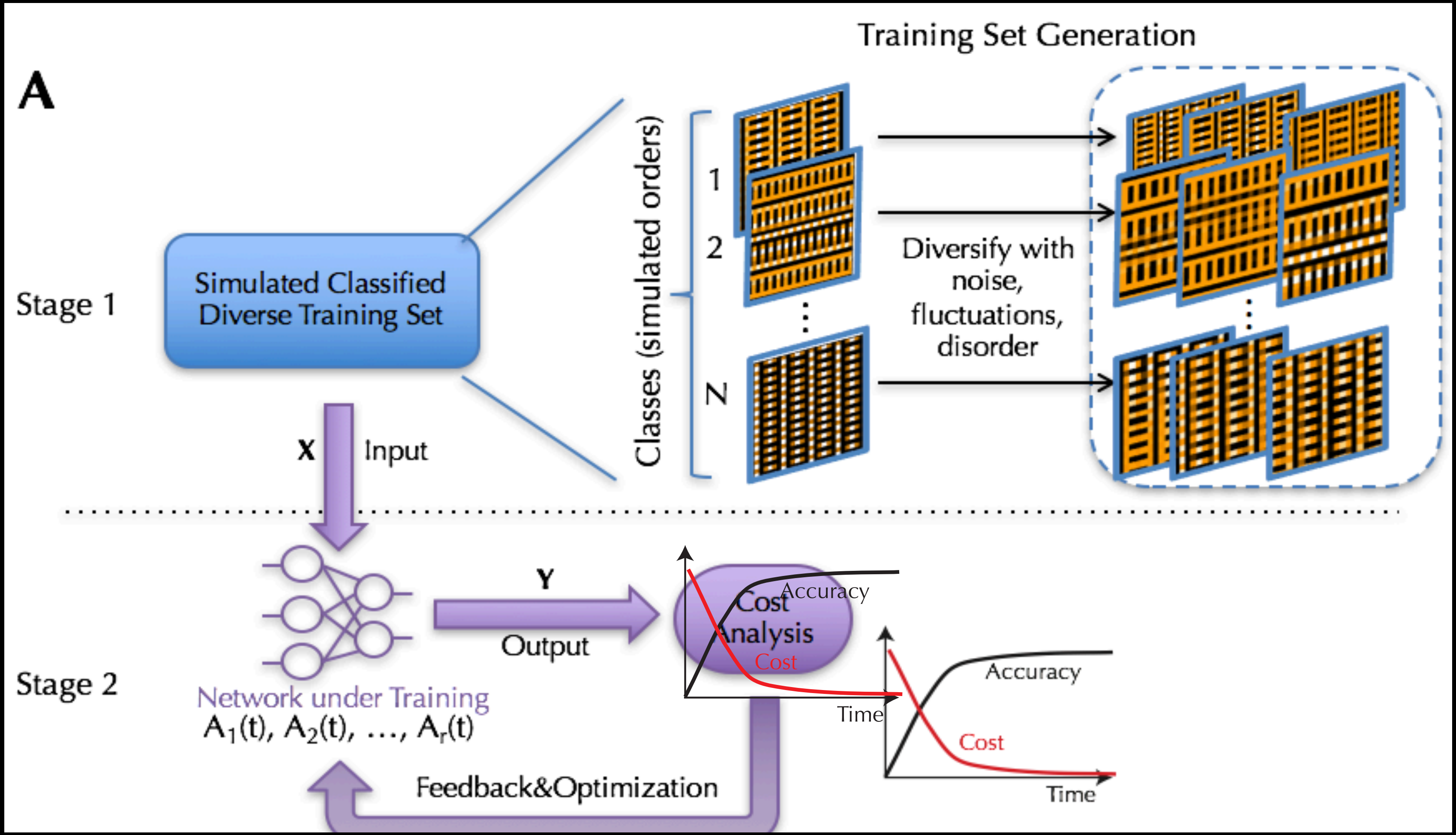
Efitov et al, Nature Physics (2013)
Pepin et al, PRB (2014)
Wang, Chubukov, PRB (2014)
Loder et al, PRL (2011)

Incommensurate,
Q decrease with *p*

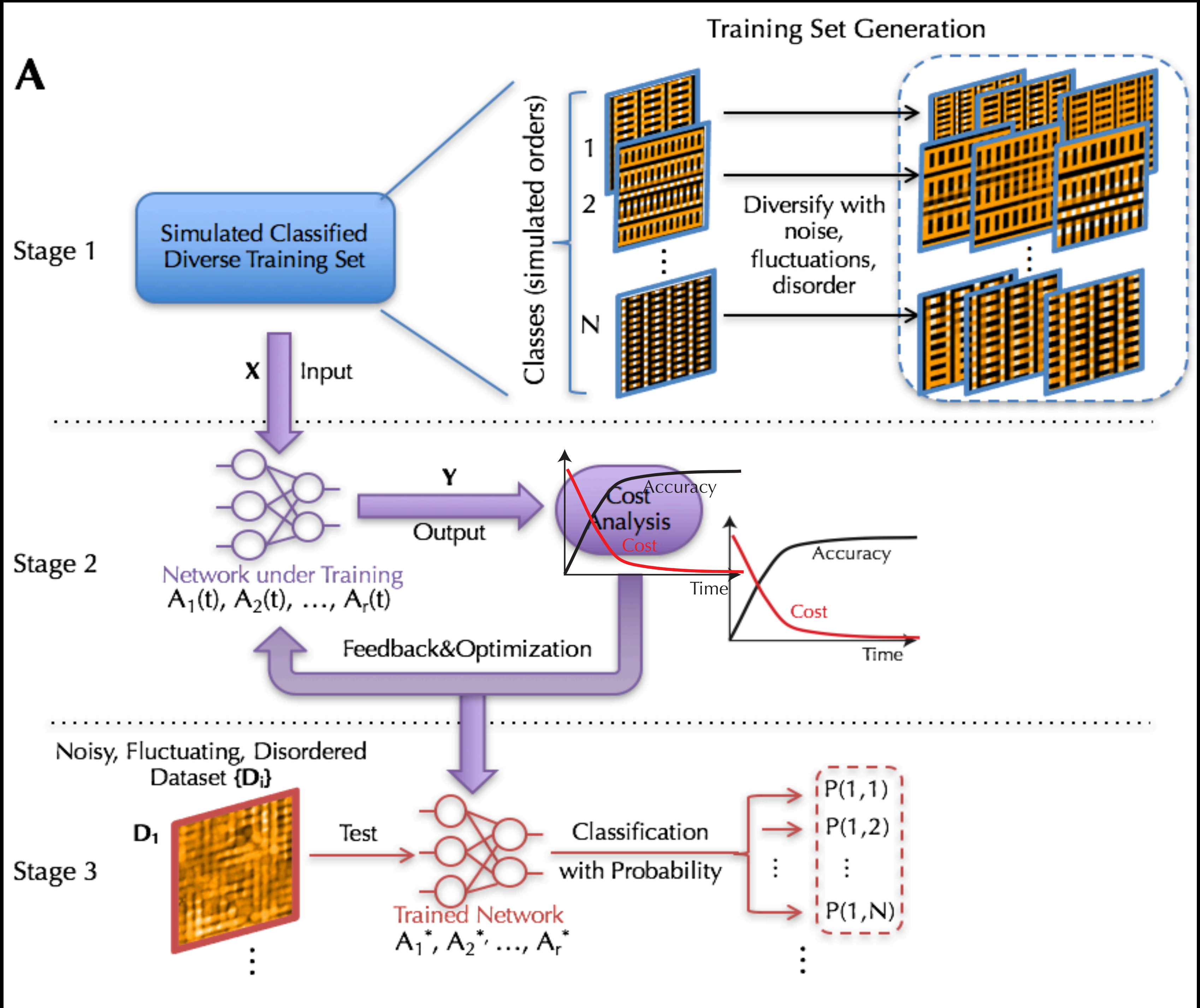
3-stage protocol



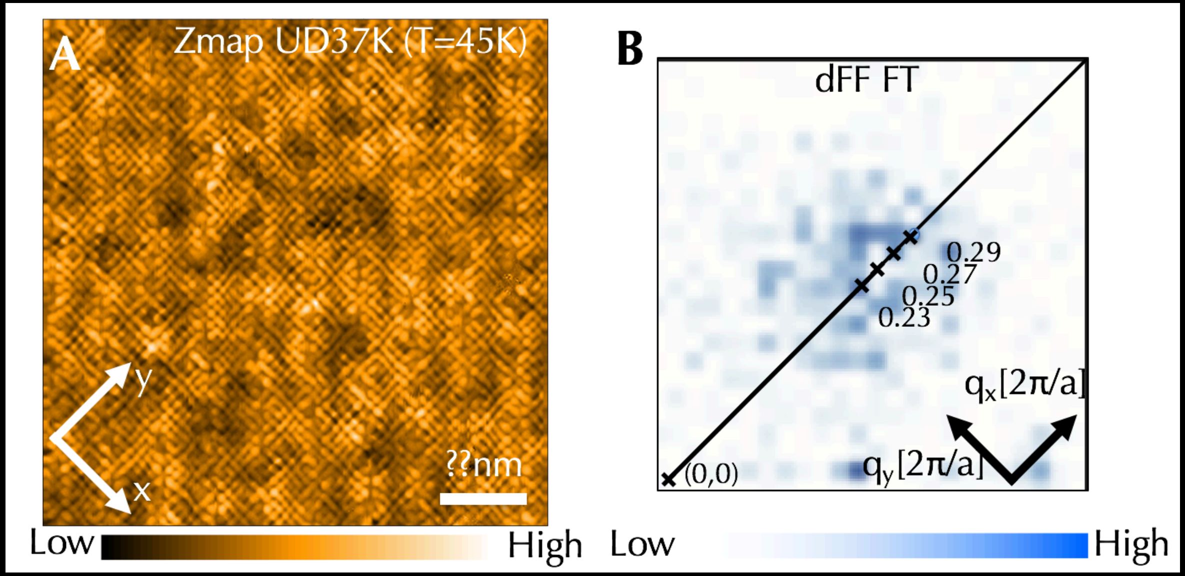
3-stage protocol

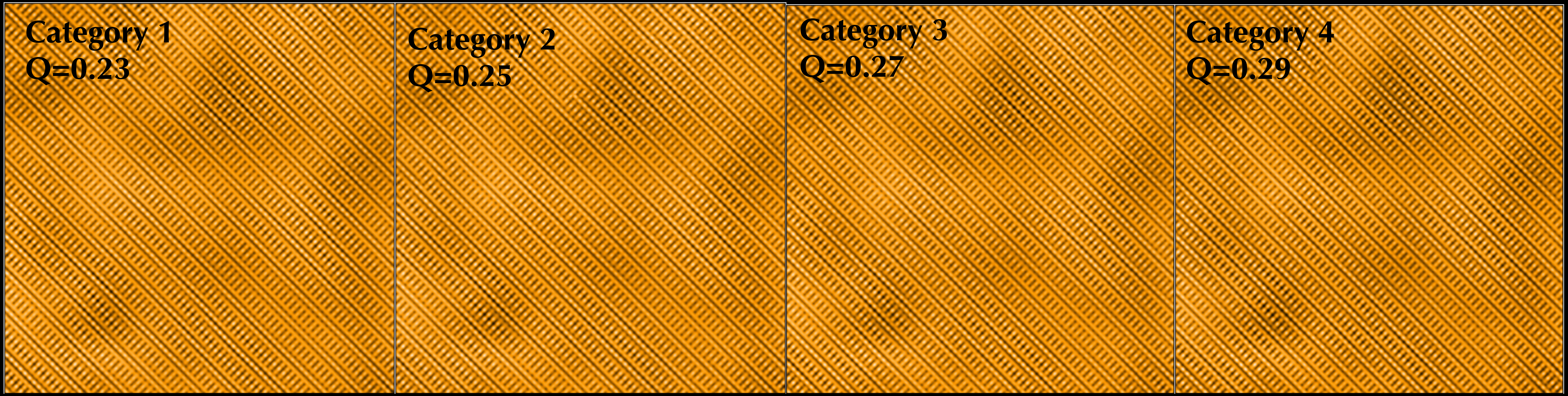


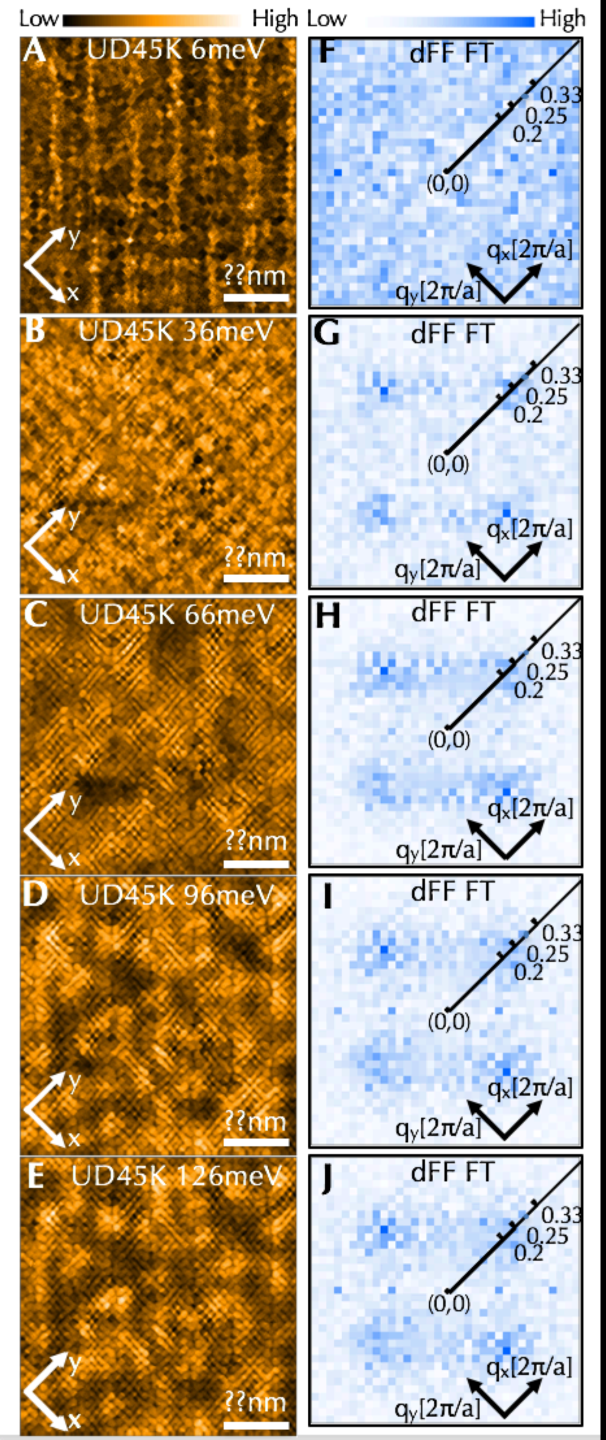
3-stage protocol



Different Hypothesis

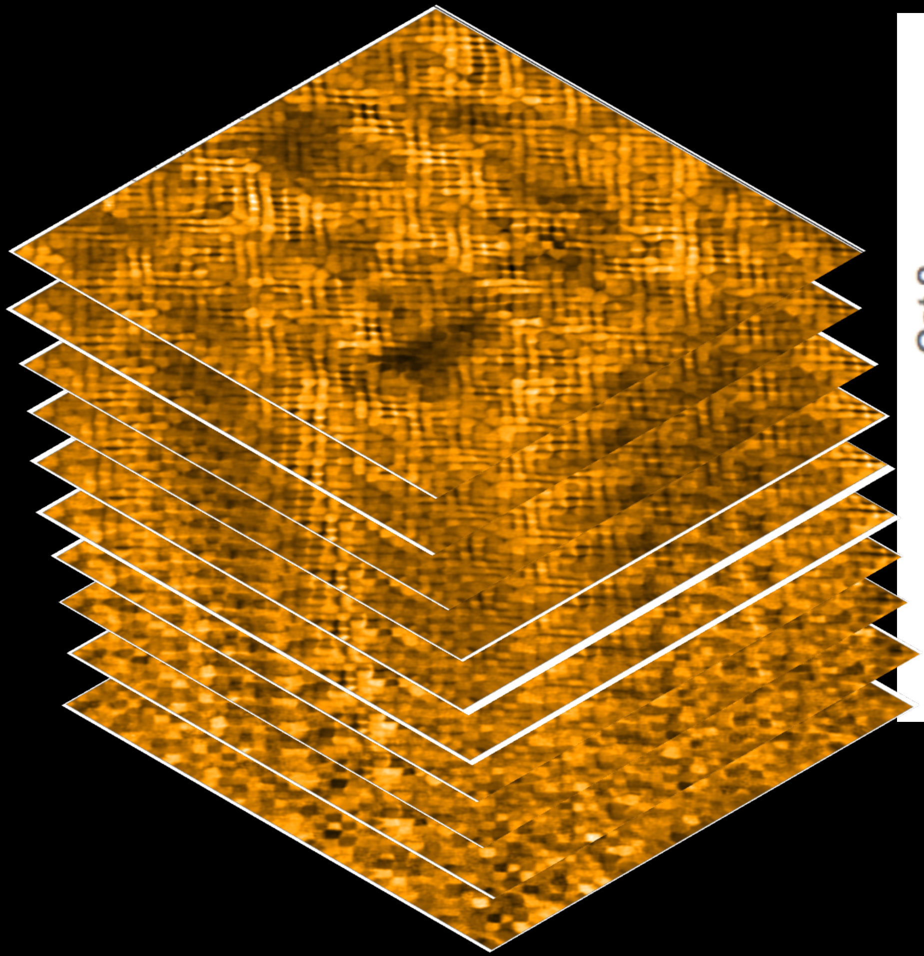


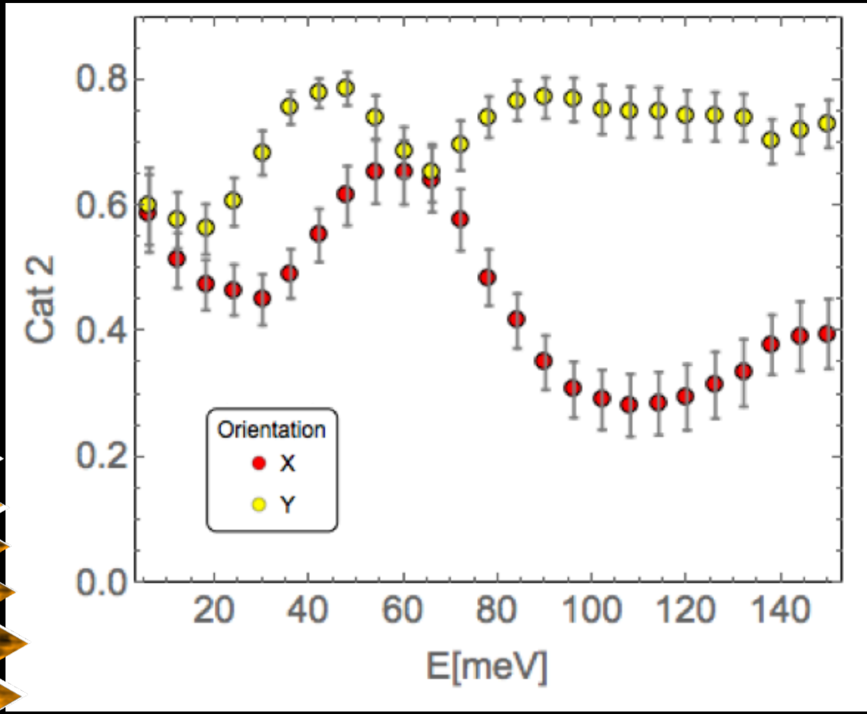


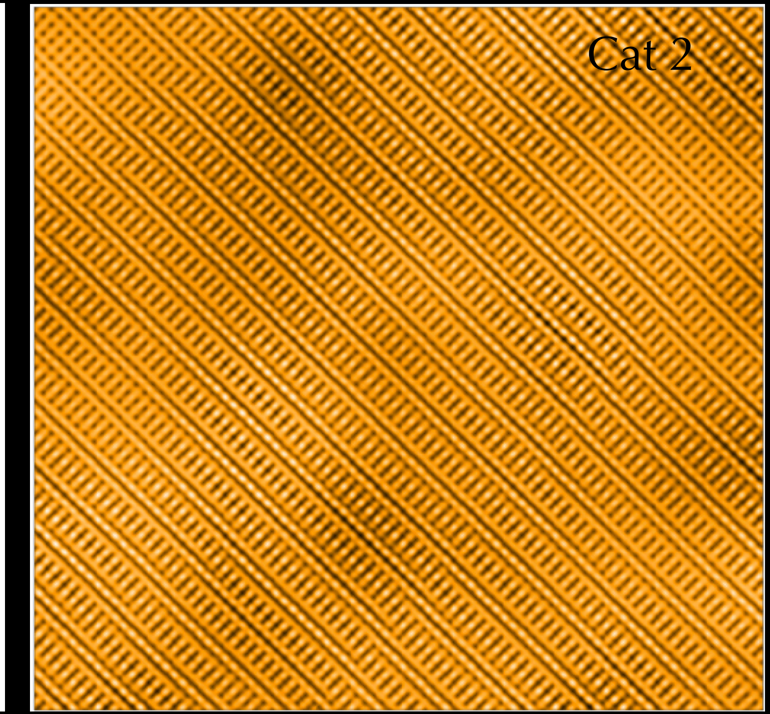


ImageNet Classification with Deep Convolutional Neural Networks

Full 3D data







Global nematic order coupled to modulation amplitude!

With AI,
Learning Quantum Emergence

The journey has just begun….

Acknowledgements

Yi Zhang
(Cornell)

Andrej Mesaros
(CNRS)

K. Fujita
(BNL)

R. Melko
(Waterloo)

E. Khatami
(SJSU

J.C. Davis
(Cornell/BNL)

P. Ginsparg
(Cornell)

K. Winberger
(Cornell)

U.S. DEPARTMENT OF ENERGY