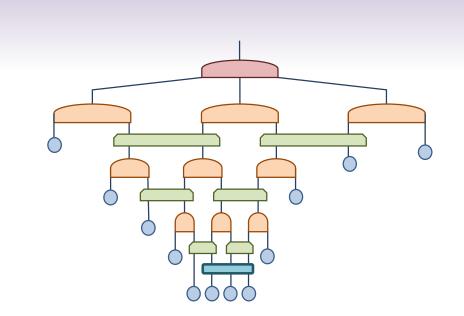
Entangle This IV: Chaos, Order and Qubits Madrid, Sept 2019

Efficient use of tensor networks for tasks in supervised learning



Glen Evenbly



Number-State Preserving Tensor Networks as Classifiers for Supervised Learning G.E., arXiv:1905.06352 (2019)

Before we begin... some advertisements...

Faculty Position - Tenured/Tenure Track Atomic, Molecular and Optical Physics (Georgia Institute of Technology)

The School of Physics of the Georgia Institute of Technology invites applications for a faculty position in Atomic, Molecular and Optical (AMO) Physics and related areas in Quantum Information Sciences (QIS), beginning Fall 2020. Appointments at the Assistant, Associate or Full Professor level will be considered, depending on qualifications.

Postdoc Position – within my group (Georgia Institute of Technology) I am looking for a postdoc to join my group sometime in 2020 for a 2 year term. Applicants should have interest and experience in either tensor networks or some area of quantum info.

Come be my research gremlin in the tensor network mines of Atlanta!

Before we begin... some more advertisements...

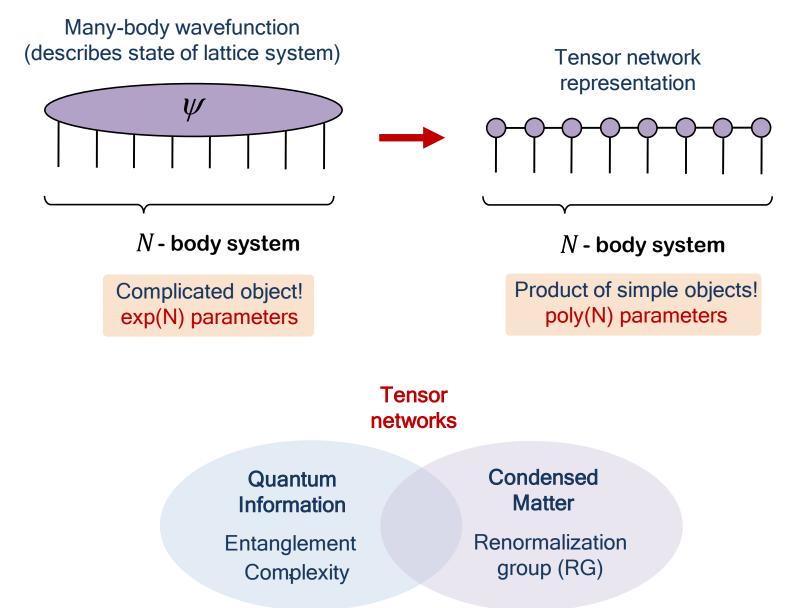
Research website: WWW.tensors.net

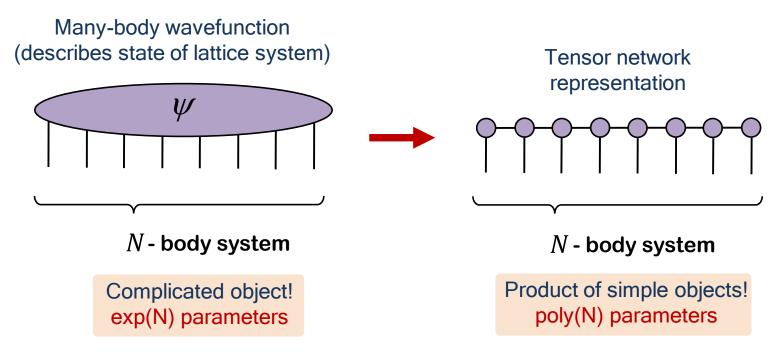
A website designed to help people get started with the practical aspects of implementing tensor network algorithms:

- has tutorials with code examples which detail the basic skills (i.e. contracting a network)
- has example codes of many tensor network algorithms (Exact Diagonalization, DMRG, TEBD, MERA, boundary MERA, TRG, TNR, PEPS)
- all codes are available in MATLAB, Python and Julia languages

I have made an app called "TensorTrace" for designing and implementing tensor networks! Beta version available at:

www.tensortrace.com

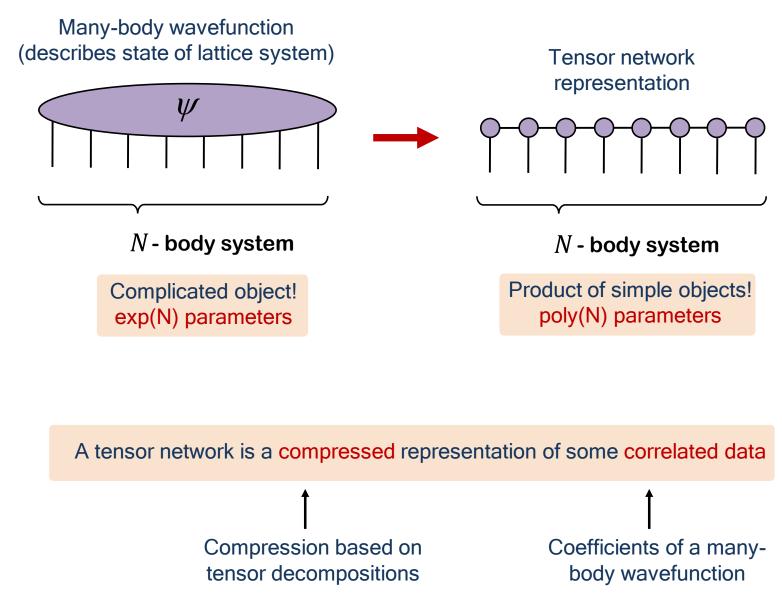


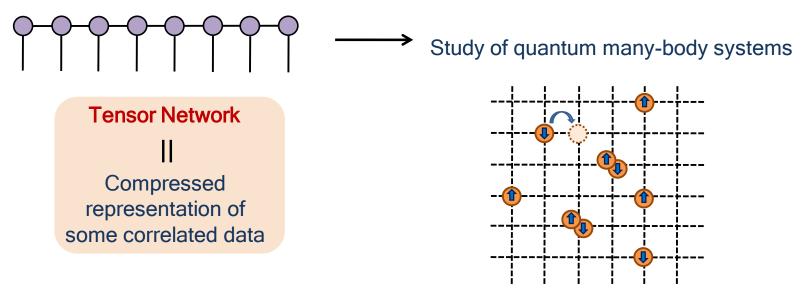


Practical goal: efficient numeric tools for classical simulation of quantum many-body systems

Theoretic goal: better understanding of many-body ground states

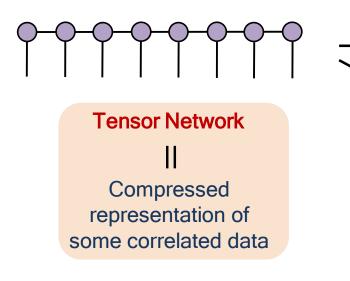
- Classification of phases of matter
- Which classes of quantum system can be efficiently simulated?
- Entanglement structure in many-body systems





Tensor network formalism has a wide variety of uses!

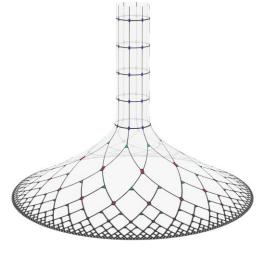
(e.g. interacting fermions on a lattice)

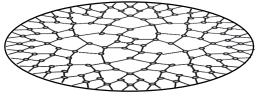


Tensor network formalism has a wide variety of uses!

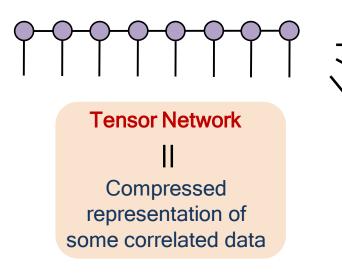
Study of quantum many-body systems

Holography: duality between semi-classical gravity and conformal field theories





(network as a discretization of space-time)

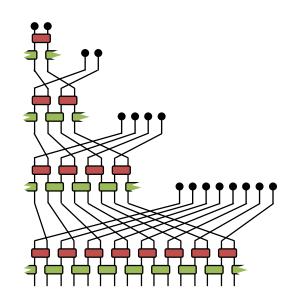


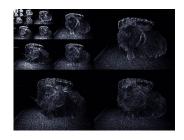
Tensor network formalism has a wide variety of uses!

Study of quantum many-body systems

Holography: duality between semi-classical gravity and conformal field theories

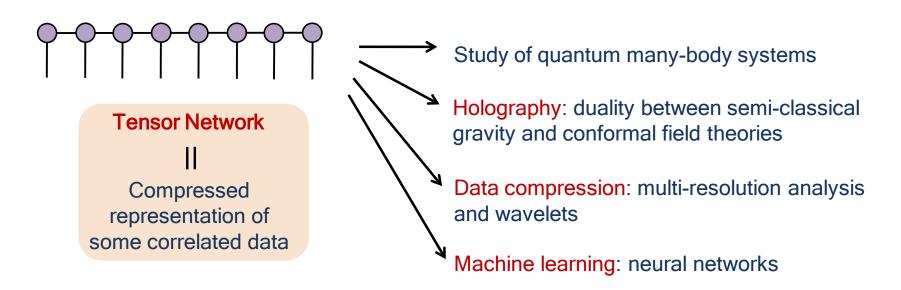
Data compression: multi-resolution analysis and wavelets



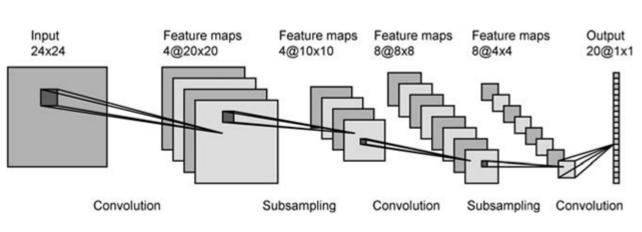




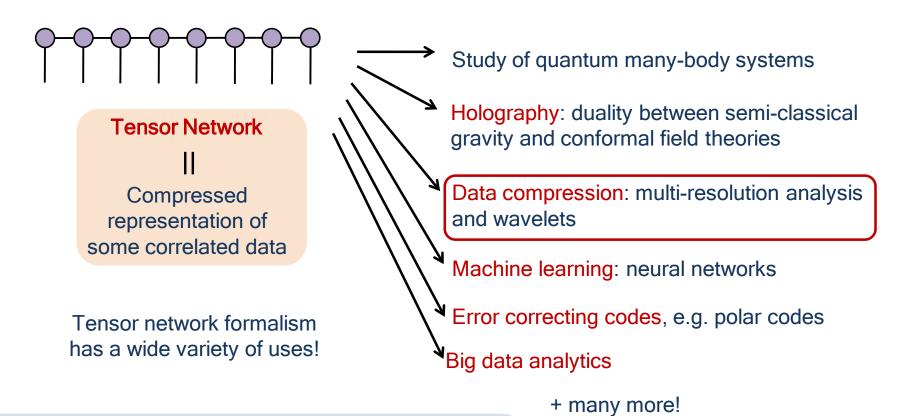
(e.g. image compression)



Tensor network formalism has a wide variety of uses!



(e.g. convolutional neural network)

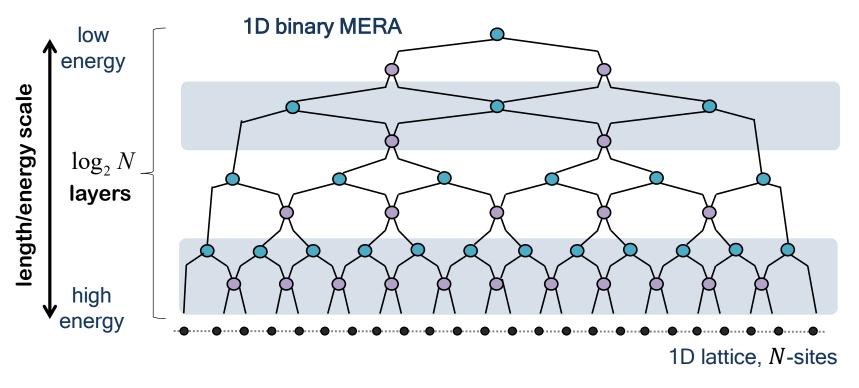


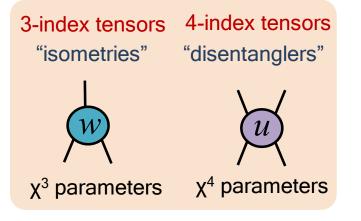
Ideas developed in the context of **entanglement** and efficient representation of quantum **wavefunctions** are useful in many areas outside of physics

> G.E., Steven. R. White, Phys. Rev. Lett 116. 140403 (2016) G.E., Steven. R. White, Phys. Rev. A 97, 052314 (2018) J. Haegeman, B. Swingle, M. Walter, J. Cotlet, G.E., V. Scholz, Phys. Rev. X 8, 111003 (2018)

Multi-scale entanglement renormalization ansatz (MERA)

G. Vidal, PRL 101, 110501 (2008)

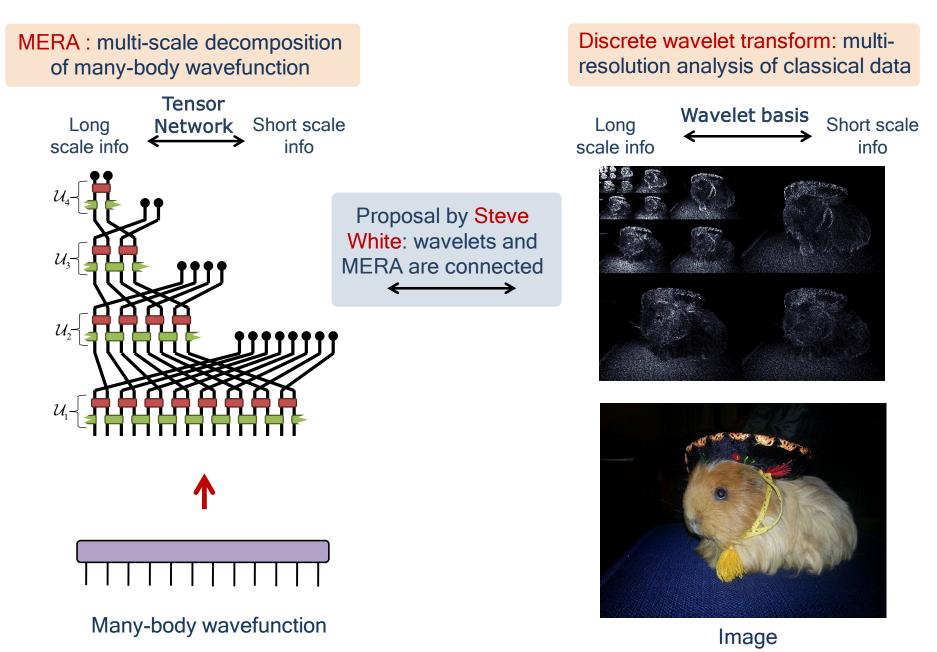




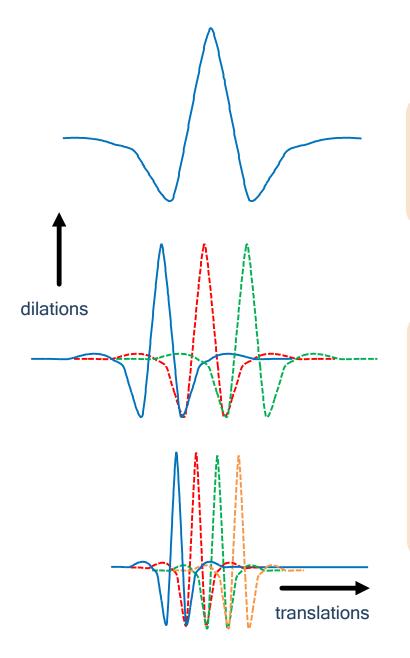
Multi-scale decomposition of the wavefunction:

- lower layers encode short-ranged (high energy) properties of the state
- higher layers encode long-ranged (low energy) properties of the state

Wavelets and tensor networks



Introduction to Wavelets



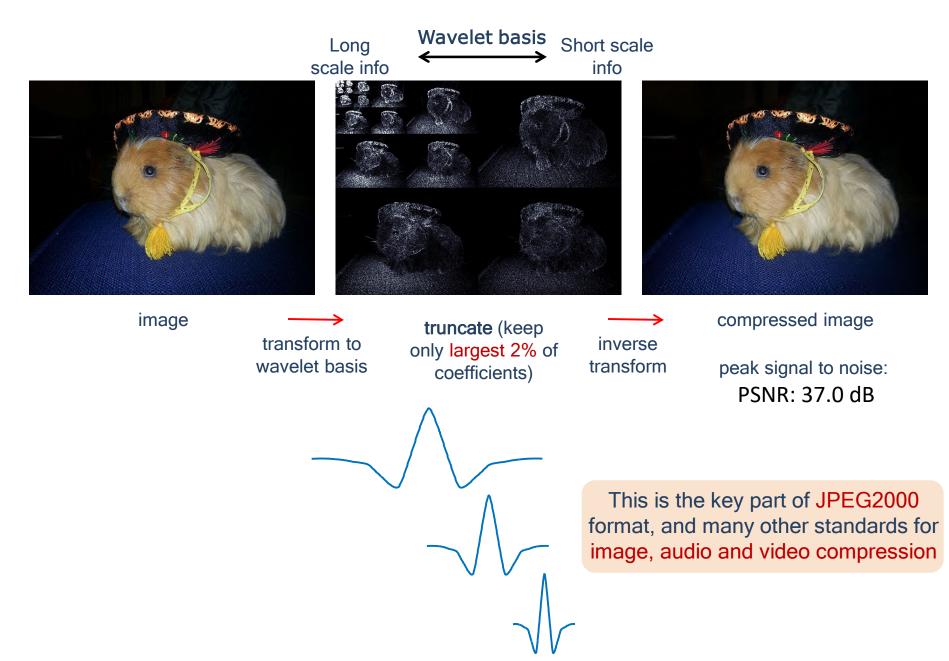
Wavelet basis

- basis consists of translations and dilations of a wavelet function
- is a multi-resolution analysis (MRA)

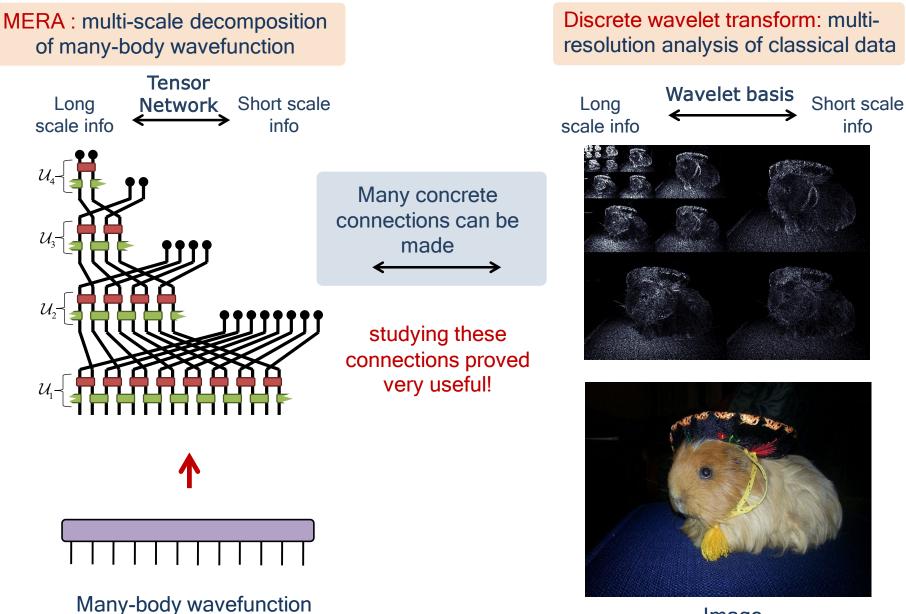
Wavelets are a good compromise between real-space and Fourier-space representations

- compact in real-space and in frequency-space
- developed by math and signal processing communities in late 80's
- applications in signal and image processing, data compression (e.g. JPEG2000 image format)

Image compression with wavelets

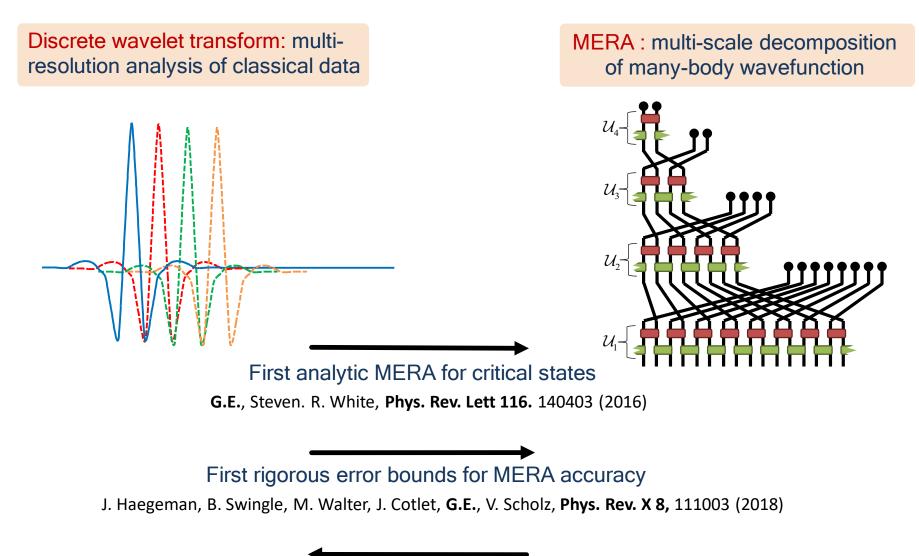


Wavelets and tensor networks



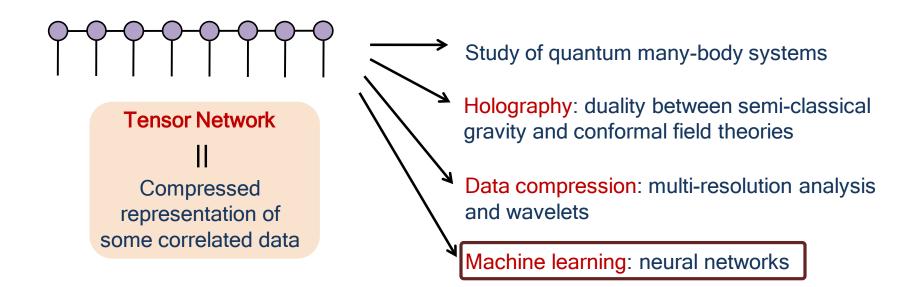
Image

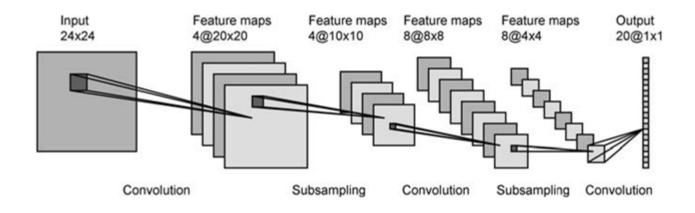
Wavelets and tensor networks



Ideas from tensor networks used to construct new and improved wavelet transformations G.E., Steven. R. White, Phys. Rev. A 97, 052314 (2018)

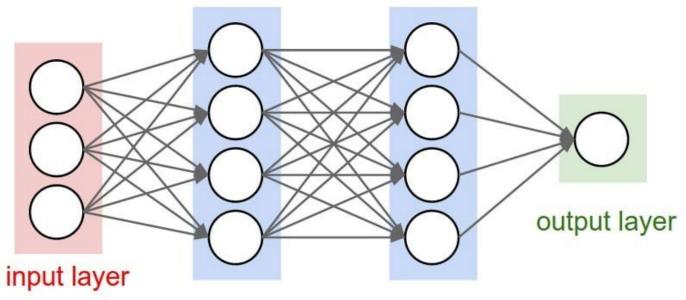
Other Applications of Tensor Networks





Machine Learning and tensor networks

In recent times deep neural networks have been spectacularly successful



hidden layer 1 hidden layer 2

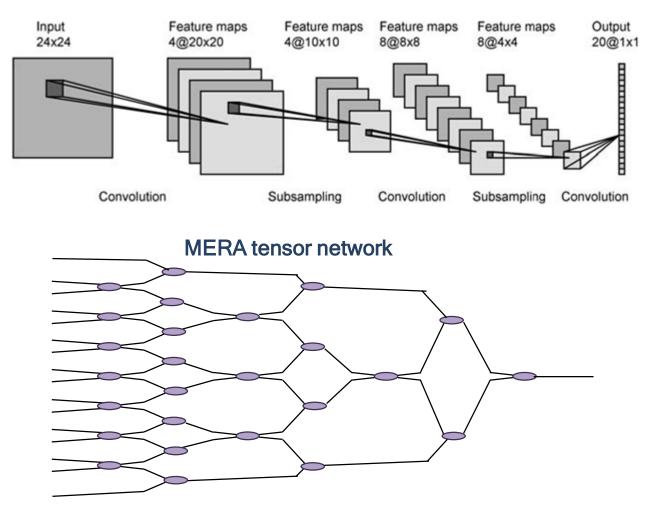
Superficially deep neural networks look very similar to tensor networks. Are there connections?

Can ideas from machine learning be used to improve simulation algorithms for quantum systems?

Can ideas from tensor networks be used to improve machine learning and neural networks?

Machine Learning and tensor networks

Convolutional neural network (CNN)



convolutional neural networks are structurally very similar to MERA tensor network!

Papers using tensor network machine learning

Expressivity & priors of TN based models

- Levine et al., "Deep Learning and Quantum Entanglement: Fundamental Connections with Implications to Network Design" arxiv:1704.01552
- Cohen, Shashua, "Inductive Bias of Deep Convolutional Networks through Pooling Geometry" arxiv:1605.06743
- Cohen et al., "On the Expressive Power of Deep Learning: A Tensor Analysis" arxiv: 1509.05009

Generative Models

- Han et al., "Unsupervised Generative Modeling Using Matrix Product States" arxiv: 1709.01662
- Sharir et al., "Tractable Generative Convolutional Arithmetic Circuits" arxiv: 1610.04167

Supervised Learning

- Novikov et al., "Expressive power of recurrent neural networks", arxiv:1711.00811
- Liu et al., "Machine Learning by Two-Dimensional Hierarchical Tensor Networks: A Quantum Information Theoretic Perspective on Deep Architectures", arxiv: 1710.04833
- Stoudenmire, Schwab, "Supervised Learning with Quantum-Inspired Tensor Networks", arxiv:1605.05775
- Novikov et al., "Exponential Machines", arxiv: 1605.03795

Related uses of tensor networks

Compressing weights of neural nets (& other models)

Yu et al., Advances in Neural Information Processing (2017), arxiv:1711.00073 Izmailov et al., arxiv:1710.07324 (2017) Yang et al., arxiv:1707.01786 (2017) Garipov et al., arxiv:1611.03214 (2016) Novikov et al., Advances in Neural Information Processing (2015) (arxiv:1509.06569)

Large scale linear algebra (PCA/SVD)

Lee, Cichocki, arxiv: 1410.6895 (2014)

Feature extraction & tensor completion

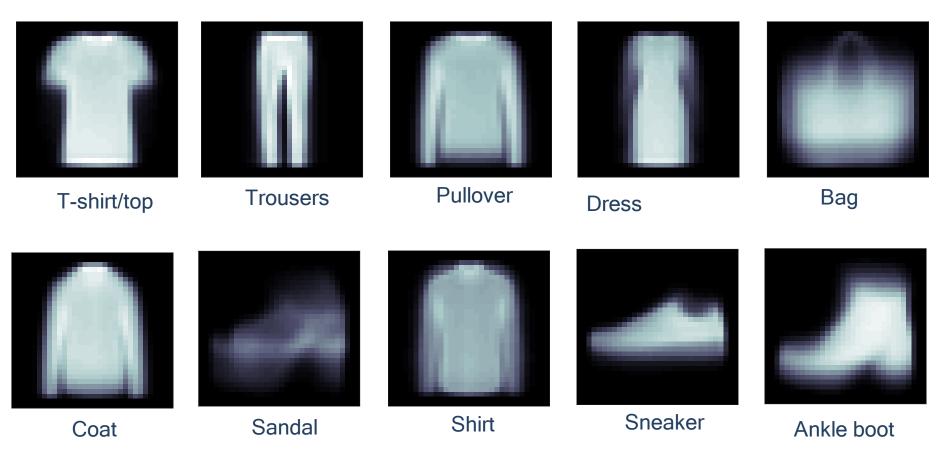
Bengua et al., arxiv:1606.01500, arxiv:1607.03967, arxiv:1609.04541 (2016) Phien et al., arxiv:1601.01083 (2016) Bengua et al., IEEE Congress on Big Data (2015)

Machine learning test problem: Fashion MNIST

Label	Description	Examples	
0	T-Shirt/Top		
1	Trouser		
2	Pullover	a ta	Test Problem: Fashion MNIST database
3	Dress		
4	Coat		10 classes of clothing60,000 training images
5	Sandals	ARRAS AN FOR AND	 10,000 test images
6	Shirt		Goal: train a program to properly
7	Sneaker	NOT CONTRACTOR OF THE STATES	classify the test images
8	Bag		
9	Ankle boots	LLLERERERERERERERERERERERERERERERERERER	

Simplest approach: compare test images again the "average" of all training images in a given category (related to principle component analysis)

Machine learning test problem: Fashion MNIST

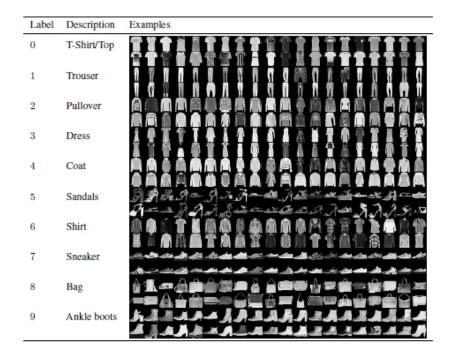


Simplest approach: compare test images again the "average" of all training images in a given category (related to principle component analysis)

• gives 66% correct

More advanced machine learning approaches?

Convolutional Neural Networks



Fashion MNIST test problem: some benchmarks (no preprocessing)

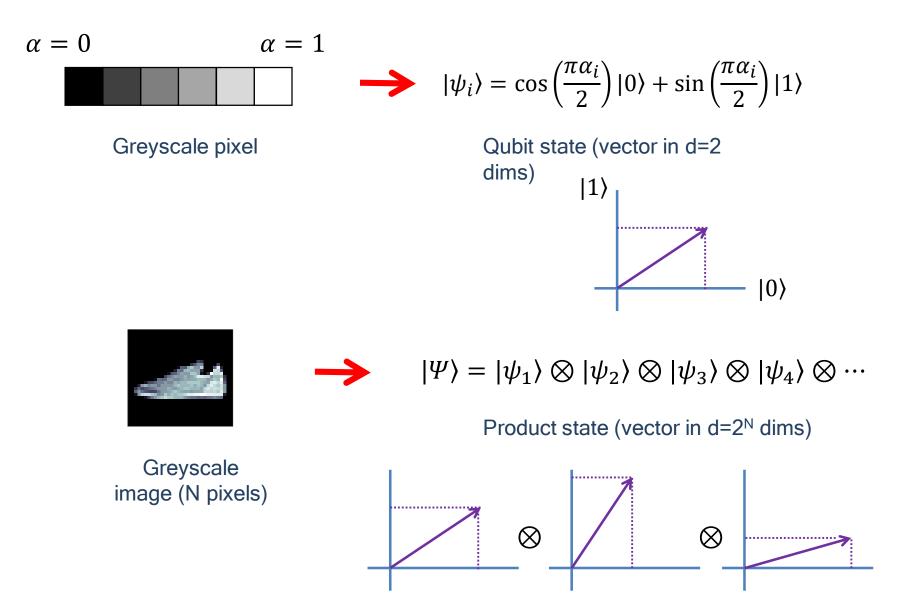
- XGBoost (89.8%)
- AlexNet (89.9%)
- two-layer CNN trained with Keras (87.6%)
- GoogLeNet (93.7%)

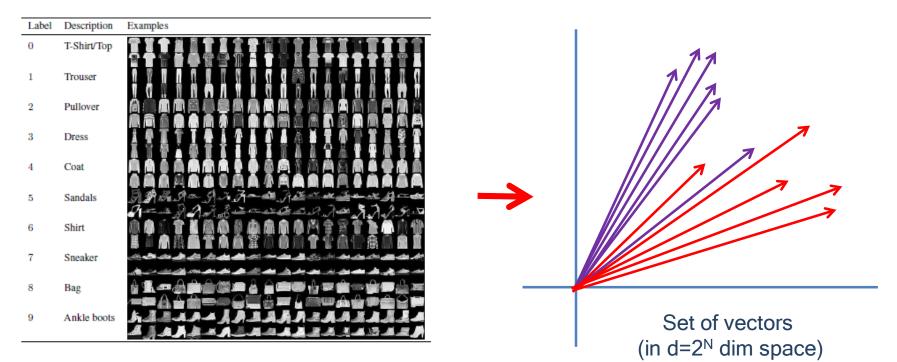
Can tensor network methods be applied to this problem (and other machine learning problems)?

Original study by Miles Stoudenmire

E. M. Stoudenmire, Quantum Sci. and Technol. 3, 034003 (2018)

Reproduced using a similar method by me!

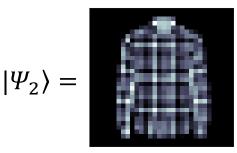


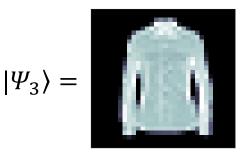


Each test image is a product state on a 2D lattice of qubits:

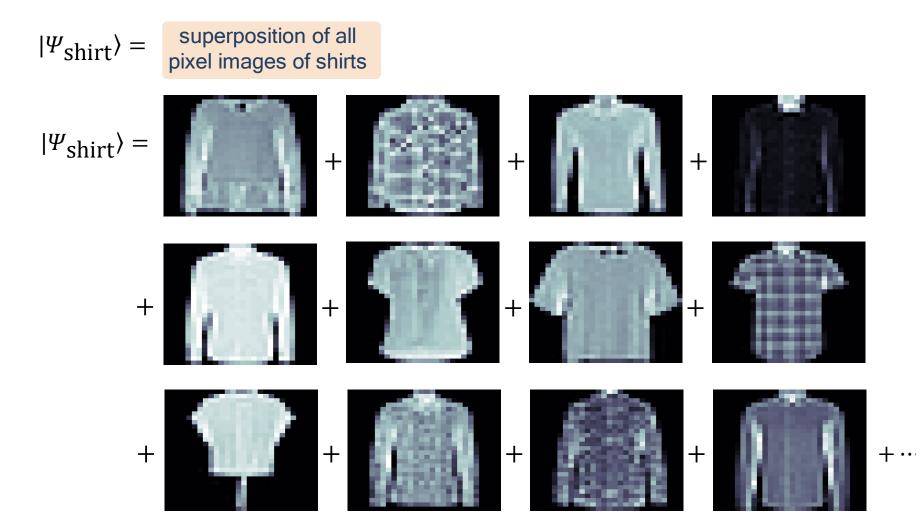
 $|\Psi_1\rangle =$





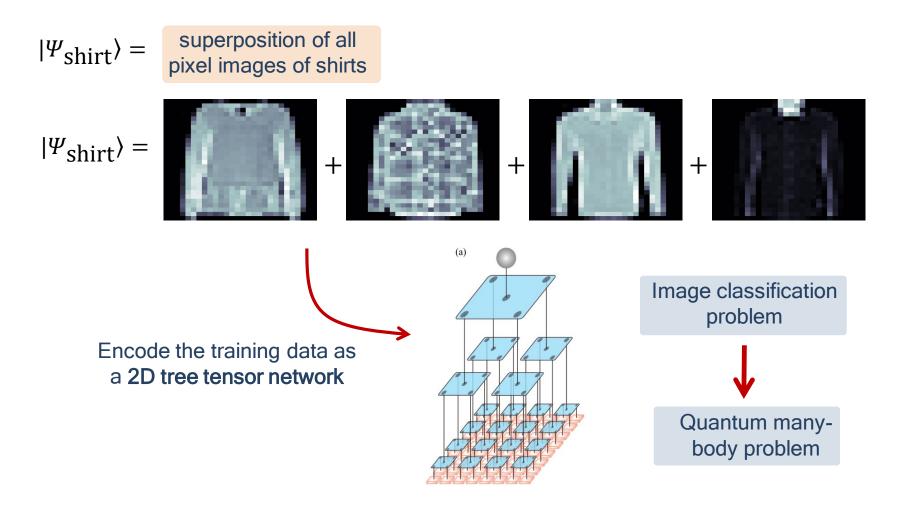


Can we form the (entangled) superposition of all images from a given class?



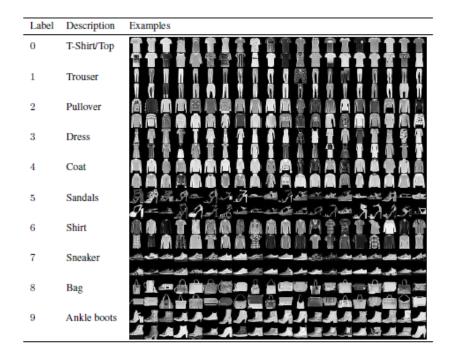
Is this state sufficiently low in entanglement that it can be approximated as a tensor network?

Can tensor network algorithms be adapted to efficiently construct this approximation?



Is this state sufficiently low in entanglement that it can be approximated as a tensor network?

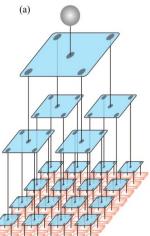
Can tensor network algorithms be adapted to efficiently construct this approximation?



Fashion MNIST test problem: some benchmarks (no preprocessing)

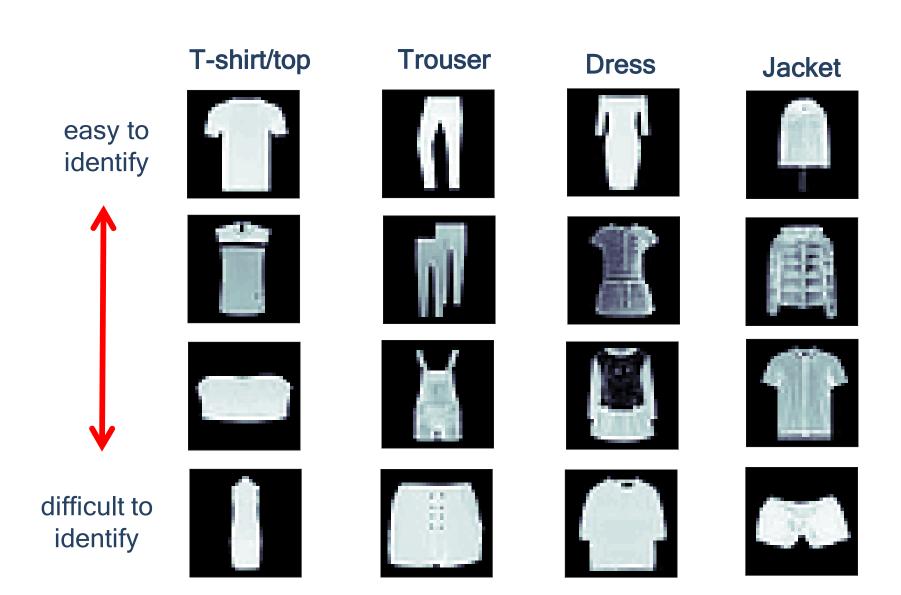
- XGBoost (89.8%)
- AlexNet (89.9%)
- two-layer CNN trained with Keras (87.6%)
- GoogLeNet (93.7%)

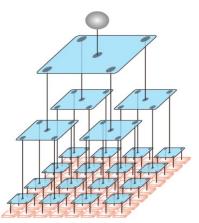
Tree tensor network (4-to-1 blocking scheme)



bond dim χ = 64 training time ~ 60min (laptop)

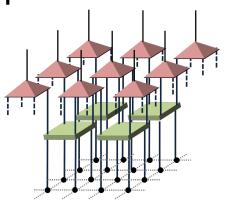
• gives 89.5% correct





Tree tensor network (TTN) + standard tensor network optimization strategies

> Performs quite well in benchmark image classification problem



Can we instead use a multi-scale entanglement renormalization ansatz (MERA)?

Why?

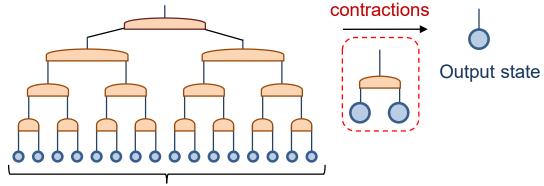
- MERA are expected to greatly outperform a TTN for a 2D problem
- MERA are the natural analogue to convolutional neural networks (CNNs)

There are some problems with trying to use a MERA!

- (1) Computational problem
- (2) Conceptual problem

Tensor networks for machine learning

Classification with a (trained) TTN:



Input sample (product state)



Which category does this belong in?

Contraction of TTN with a product state is efficient!

- classification of samples is
 efficient
- training (or optimization) of TTN can be done efficiently

Tensor networks for machine learning

Classification with a (trained) TTN:

Contractions Output state Input sample (product state)

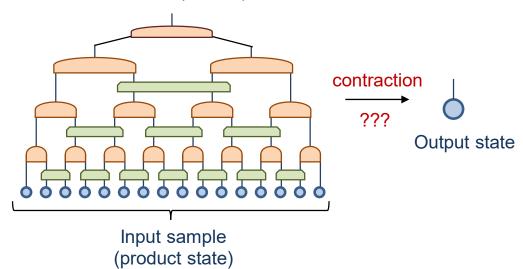
Contraction of TTN with a product state is efficient!

classification of samples is
 efficient

(1) Computational problem

 training (or optimization) of TTN can be done efficiently

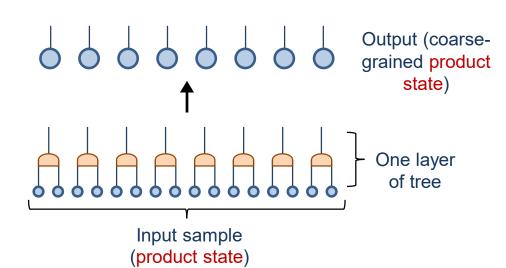
Classification with a (trained) MERA?



Contraction is of MERA with a product state is not efficient!

- classification of samples is not efficient
- training (or optimization) of MERA cannot be done efficiently for large problems

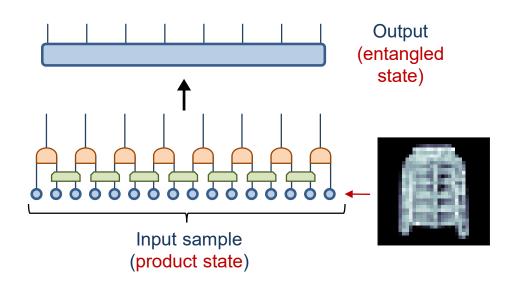
Tensor networks for machine learning



(2) Conceptual problem

TTN maps product states to product states

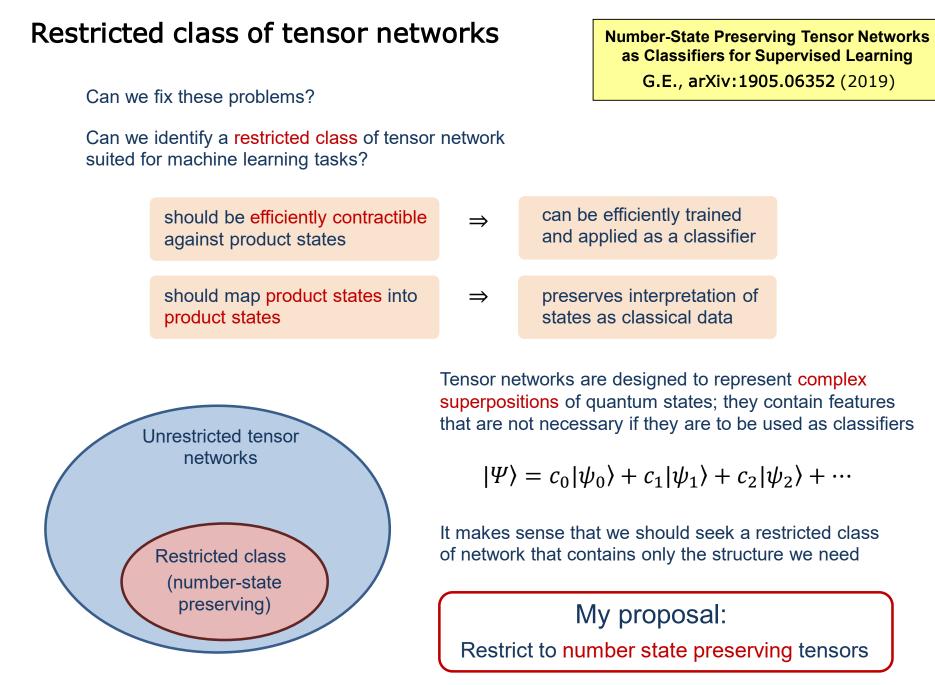
Each intermediate state can still be interpreted classically (i.e. as an image)



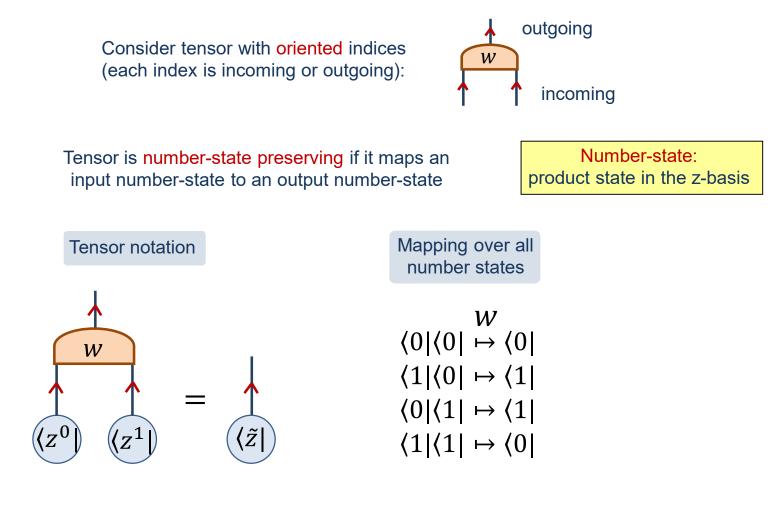
MERA maps product states to entangled states

Cannot relate intermediate states to classical data

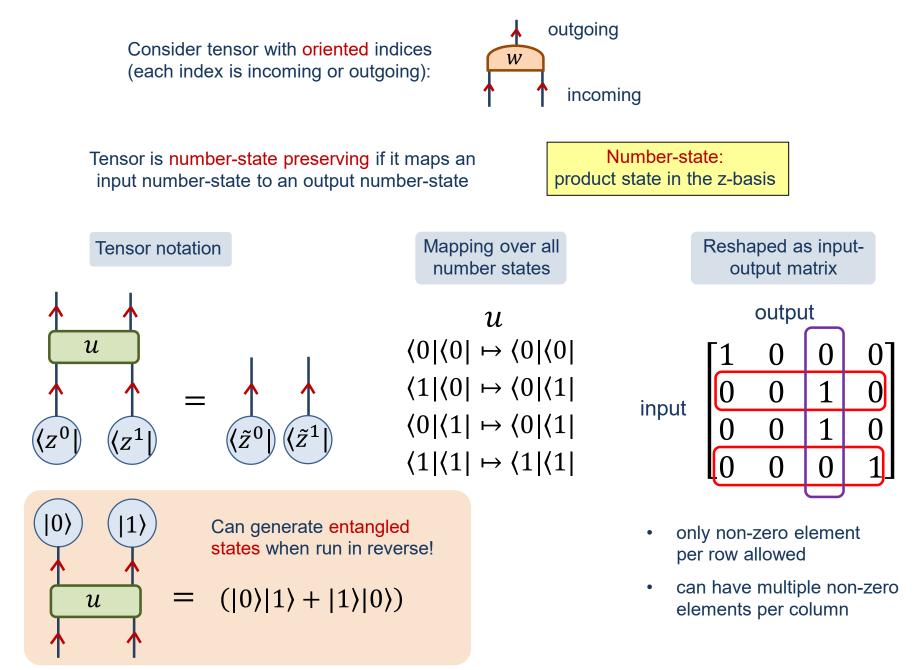
Interpretability has been lost!



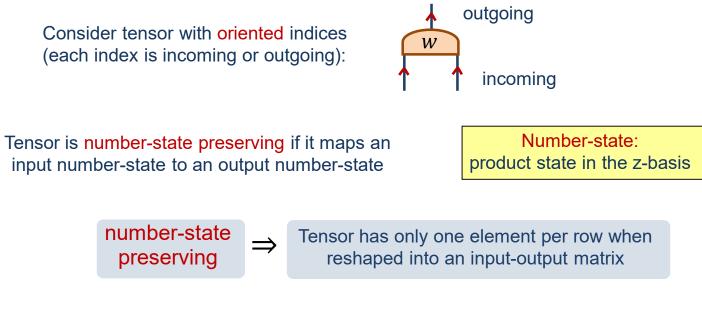
Number state preserving tensors



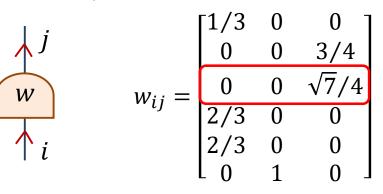
Number state preserving tensors



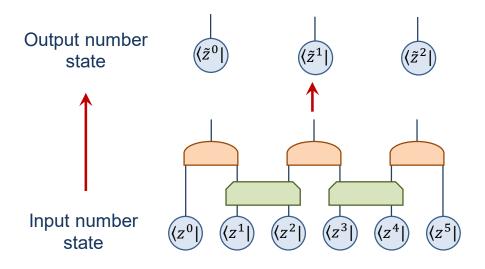
Number state preserving tensors



A final example:



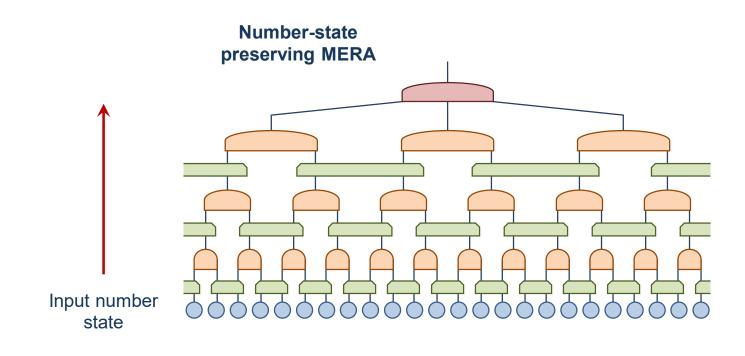
Tensor 'w' is both isometric and number state preserving

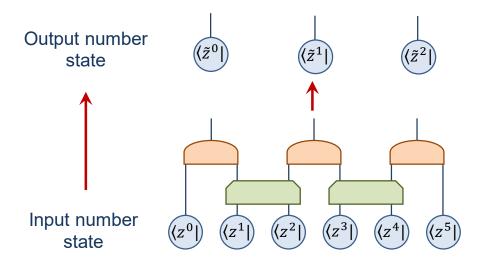


Products of number state preserving tensors are also number state preserving

(similar to how a product of isometric tensors is itself isometric)

We can create number-state preserving versions of existing networks (e.g. MPS and MERA)

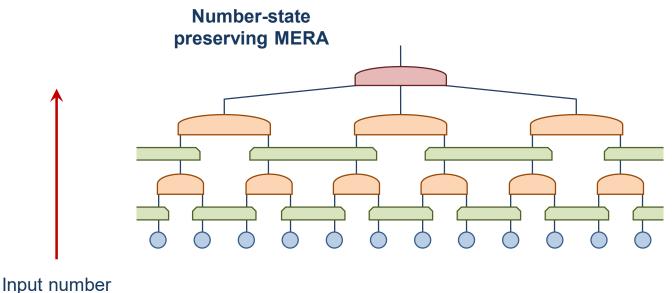




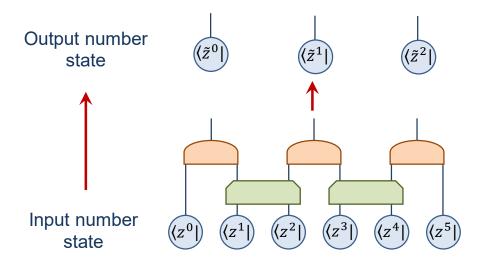
Products of number state preserving tensors are also number state preserving

(similar to how a product of isometric tensors is itself isometric)

We can create number-state preserving versions of existing networks (e.g. MPS and MERA)



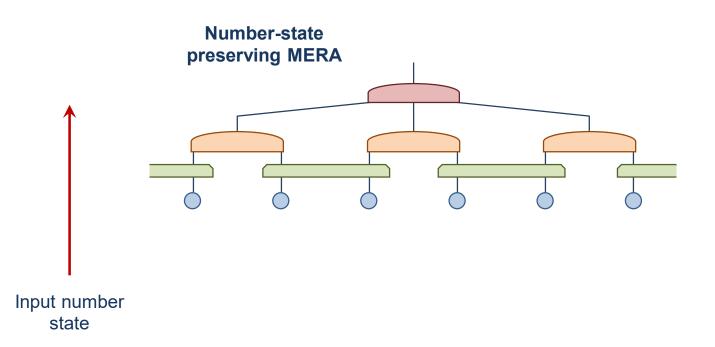
state

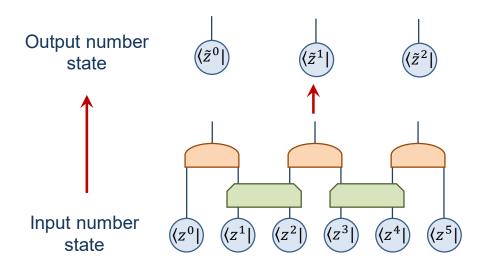


Products of number state preserving tensors are also number state preserving

(similar to how a product of isometric tensors is itself isometric)

We can create number-state preserving versions of existing networks (e.g. MPS and MERA)





Products of number state preserving tensors are also number state preserving

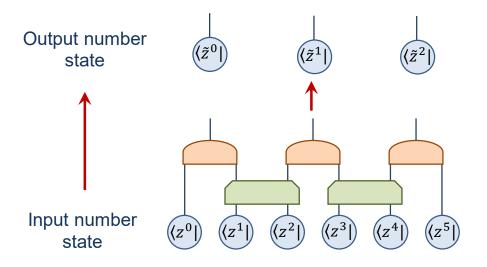
(similar to how a product of isometric tensors is itself isometric)

We can create number-state preserving versions of existing networks (e.g. MPS and MERA)

Number-state preserving MERA







Products of number state preserving tensors are also number state preserving

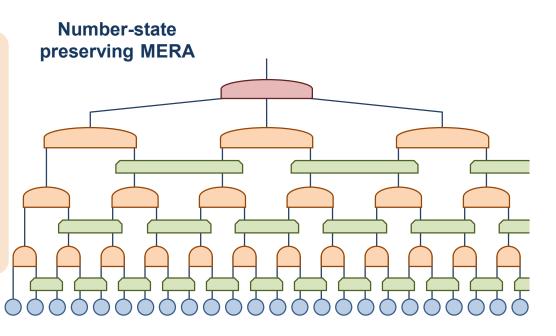
(similar to how a product of isometric tensors is itself isometric)

We can create number-state preserving versions of existing networks (e.g. MPS and MERA)

Useful restriction of tensor networks for machine learning?

Can efficiently be applied as a classifier (for classical data encoded as number states)

Preserves interpretability (intermediate states can still be understood as classical data)



Questions:

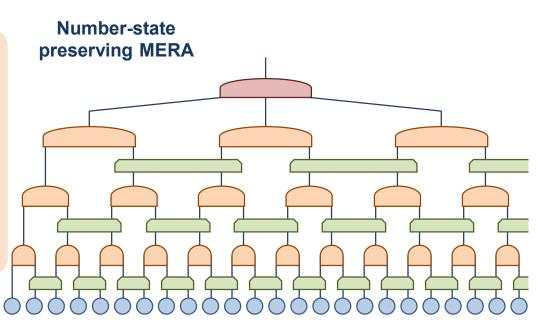
Is this restricted class of network **powerful enough** to interesting things? (i.e. can they describe entangled states?)

Can these networks be **efficiently trained** (or optimized) for machine learning tasks?

Useful restriction of tensor networks for machine learning?

Can efficiently be applied as a classifier (for classical data encoded as number states)

Preserves interpretability (intermediate states can still be understood as classical data)

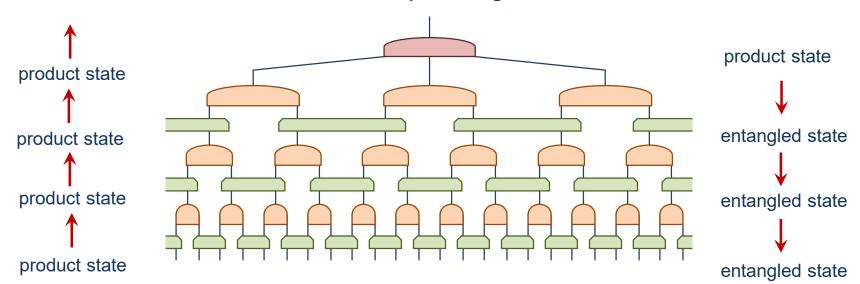




Is this restricted class of network **powerful enough** to interesting things? (i.e. can they describe entangled states?)

Can these networks be **efficiently trained** (or optimized) for machine learning tasks?

Number-state preserving MERA



Number-state preserving MERA are non-trivial! If interpreted as describing a wavefunction ψ on the lattice:

• possess logarithmic scaling of entanglement entropy

 $S_L = k_1 \log(L) + k_2$

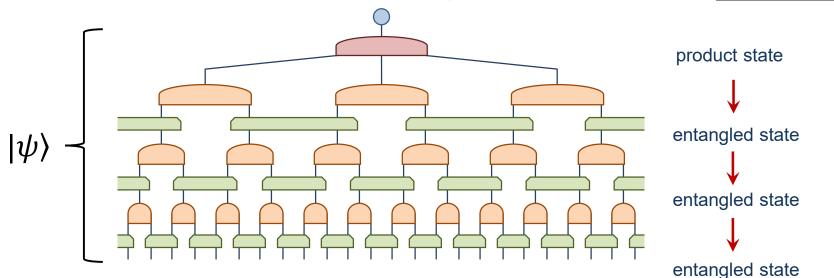
possess polynomial correlation functions

Are they useful for describing quantum critical ground states?

resl

(sometimes

Number-state preserving MERA



Number-state preserving MERA are non-trivial! If interpreted as describing a wavefunction ψ on the lattice:

• possess logarithmic scaling of entanglement entropy

 $S_L = k_1 \log(L) + k_2$

possess polynomial correlation functions

Are they useful for describing quantum critical ground states?



Exact holographic tensor networks for the Motzkin spin chain

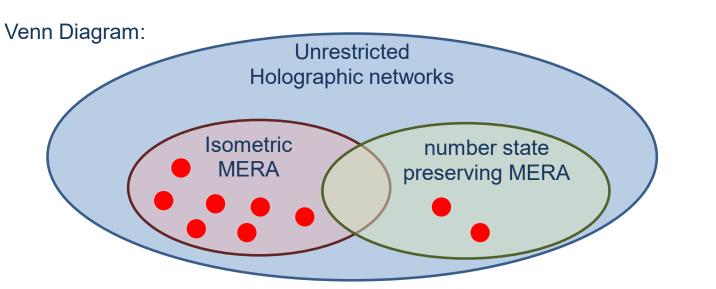
R.N. Alexander, G.E., I. Klich arXiv:1905.06352 (2019)

Motzkin and Fredkin models are described by a local interaction on 1D spin chain (open BC):

$$h_{[j,j+1,j+2]} = (1 + \sigma_j^z) (1 - \vec{\sigma}_{j+1} \cdot \vec{\sigma}_{j+2}) + (1 - \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}) (1 - \sigma_{j+2}^z)$$

- possess unique ground state (but gapless excitations)
- ground states have logarithmic scaling of entanglement entropy

Exact description of ground states as number state preserving MERA!



Number state preserving MERA can describe interesting entangled states!

Open questions:

• What properties differ between isometric MERA and number state preserving MERA?

Critical ground

states

• What types of system can or cannot be described by number state preserving MERA?

Can these networks be efficiently trained (or optimized) for machine learning tasks?

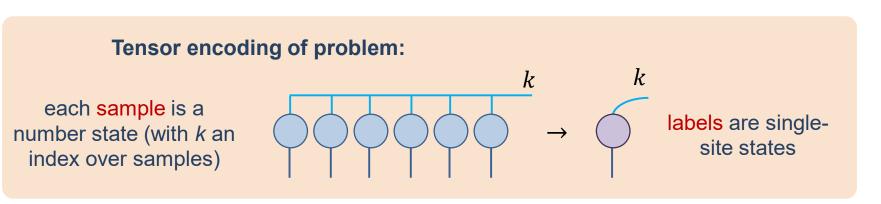
Training tensor networks for classification tasks

Supervised learning task:

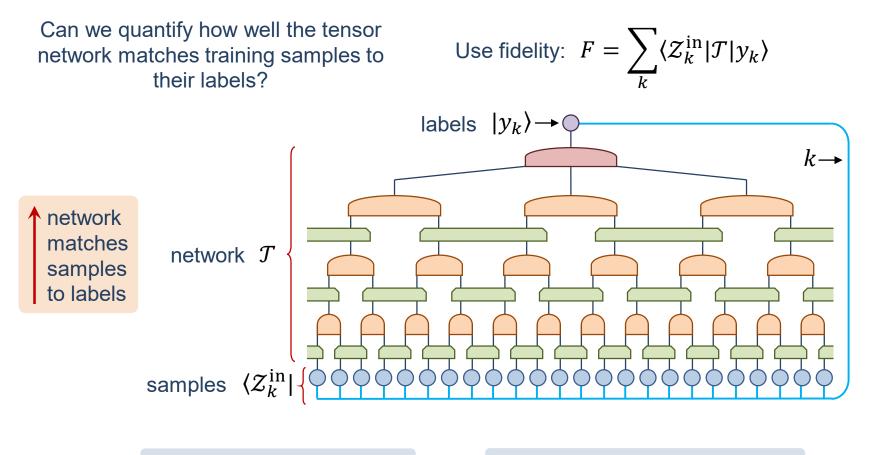
• assume we are given M training samples, each a vector of N integers, together with corresponding labels

samples
$$\left\{ \begin{array}{c} [0,0,1,0,1,0,1,1,0,0] \to 0 \\ [1,0,0,0,1,0,1,1,1,0] \to 1 \\ [0,0,0,0,0,0,0,1,1,0,0] \to 0 \\ [1,0,1,1,1,1,0,1,1,0] \to 1 \end{array} \right\} \text{ labels}$$

Goal: train a tensor network that matches samples to the correct labels



Training tensor networks for classification tasks

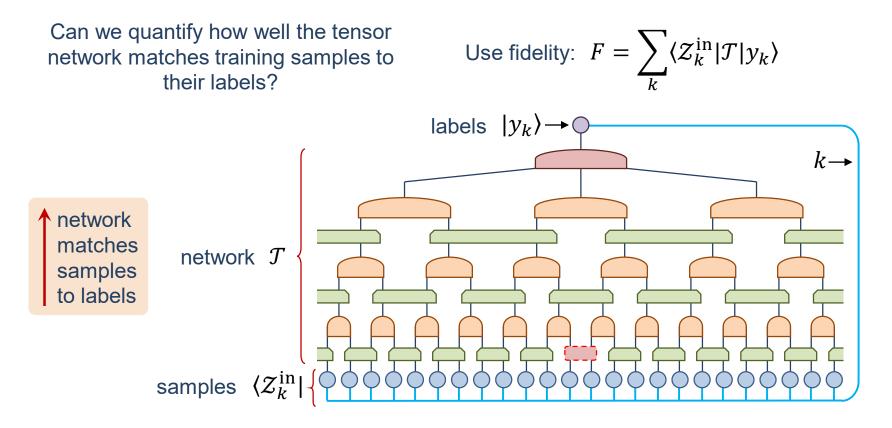


Optimizing the tensors in the network to maximize the fidelity

Use established methods (i.e. variational sweep):

- update one tensor at a time (first computing the tensor environment)
- sweep over all tensors and iterate until converged

Training tensor networks for classification tasks



Can we efficiently compute tensor environments? (or the derivatives of the fidelity w.r.t each tensor

 $\frac{\partial}{\partial u} \langle Z_{\text{product}} | \psi_{\text{MERA}}(u, w) \rangle$

Evaluation of environments

Can we efficiently compute derivatives?

$$\frac{\partial}{\partial u} \langle Z_{\text{product}} | \psi_{\text{MERA}}(u, w) \rangle$$

Simplifications due to numberstate preserving tensors

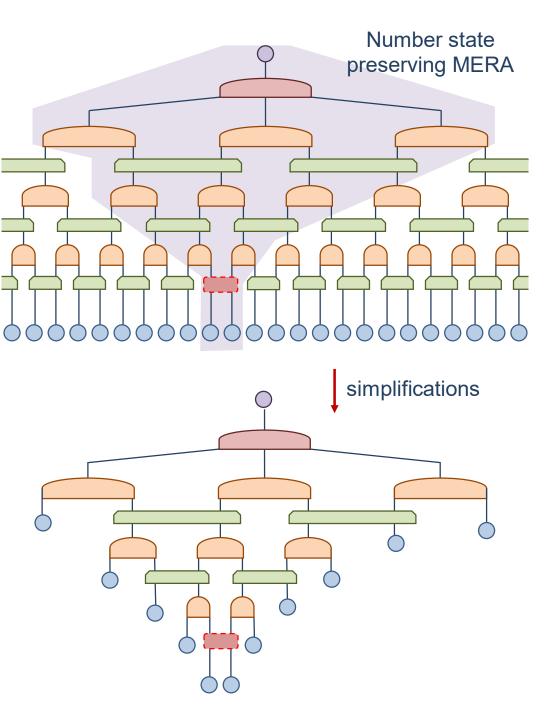
∜

Simplified network has finite tree-width

₩

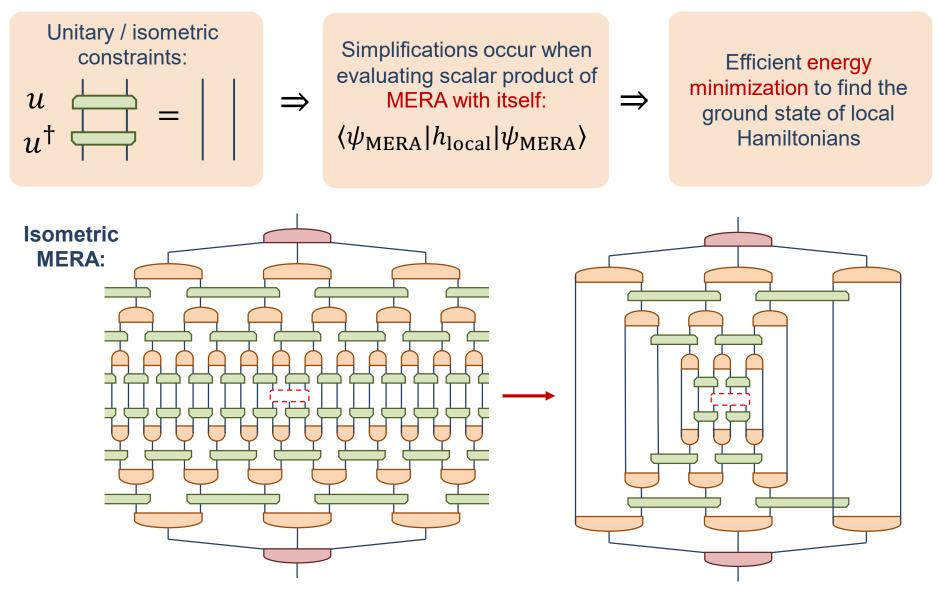
Derivatives can be evaluated at cost: O(log(N))

Network can be trained efficiently



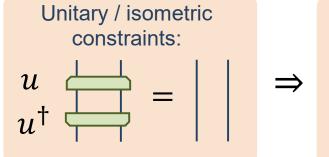
Evaluation of environments

Isometric MERA:



Evaluation of environments

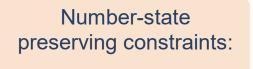
Isometric MERA:



Simplifications occur when evaluating scalar product of MERA with itself: $\langle \psi_{\text{MERA}} | h_{\text{local}} | \psi_{\text{MERA}} \rangle$

Efficient energy minimization to find the ground state of local Hamiltonians

Number state preserving MERA:



Simplifications occur when evaluating scalar product of MERA with a product state $\langle Z_{\text{product}} | h_{\text{local}} | \psi_{\text{MERA}} \rangle$

Efficient training to maximize fidelity against ensemble of classical data

 \Rightarrow

Number state preserving MERA seem to be a natural choice for machine learning tasks!

So far:

- We have proposed a restricted class of tensor network state
- Argued that this class can still possess interesting entanglement
- Argues that this class can be efficiently applied as classifiers

How well do these ideas work in practice? We should crawl before we try to walk. Lets consider a toy supervised learning problem

Number-State Preserving Tensor Networks as Classifiers for Supervised Learning G.E., arXiv:1905.06352 (2019)

Height classification problem:

- Each 'pixel' of a sample is in state: $z \in \{+, 0, -\}$
- Samples are labelled by whether the sum (under regular addition) of all pixels is positive, zero, or negative

samples
$$\begin{cases} [+, 0, -, 0, -, 0, +, +, 0, 0] \rightarrow + \\ [0, +, +, 0, 0, 0, -, -, -, 0] \rightarrow - \\ [-, +, 0 +, +, -, -, 0, -, +] \rightarrow 0 \end{cases}$$
 labels

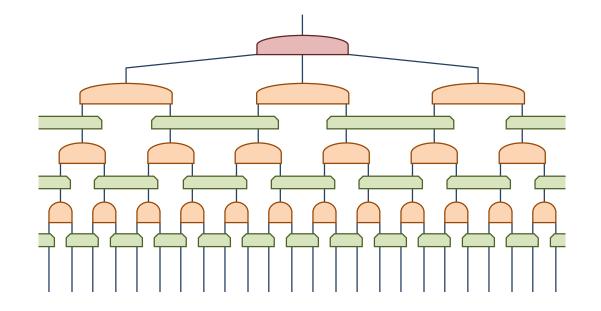
$$\vdots$$
Related to height
models (think of each
sample as a path)

Why this problem? Given an ensemble of samples, the block entropy scales logarithmically:

 \Rightarrow Tree Tensor Network should not work so well

⇒ MERA could work well

- Chain of N = 24 sites (\Rightarrow 3²⁴ basis states)
- Generate 12000 random training samples
- Train 3-level MERA as a classifier (bond dimension chi = 9)
- Initialize disentanglers as identity, initialize other tensors randomly
- After training, generate new samples to test the accuracy as a classifier



Number-State Preserving Tensor Networks as Classifiers for Supervised Learning G.E., arXiv:1905.06352 (2019)

- Chain of N = 24 sites (\Rightarrow 3²⁴ basis states)
- Generate 12000 random training samples
- Train 3-level MERA as a classifier (bond dimension chi = 9)
- Initialize disentanglers as identity, initialize other tensors randomly
- After training, generate new samples to test the accuracy as a classifier

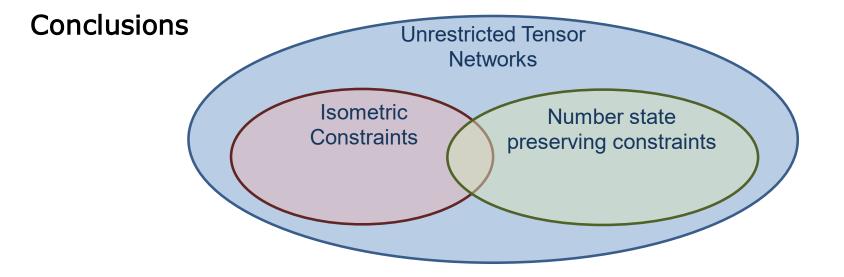


Number-State Preserving Tensor Networks as Classifiers for Supervised Learning G.E., arXiv:1905.06352 (2019)

Number-State Preserving Tensor Networks as Classifiers for Supervised Learning G.E., arXiv:1905.06352 (2019)

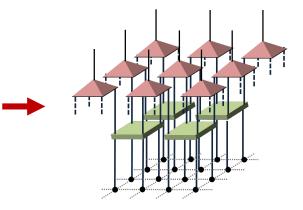
Optimization algorithm generally converges well and can easily be scaled to larger system sizes and higher bond dimensions
Disentanglers have a significant effect (MERA is vastly more accurate than a tree TN)
Good generalization from training to test samples (i.e. we are not just overfitting to the training data)





- number state preserving tensors seems to be a natural restriction for tensor networks when applying to classification problems
- we have efficient training algorithms for this class of network
- performs well in toy classification problems





Can we apply 2D MERA to difficult problems? In progress...

