LEARNING AND REPRESENTING QUANTUM STATES WITH PROBABILITY

Juan Carrasquilla
Vector Institute
University of Waterloo
Canada CIFAR AI chair

Machine learning for Quantum Many-Body Physics
KITP, Santa Barbara, CA Jan. 29th 2019

VECTOR INSTITUTE | INSTITUT VECTEUR

CIFAR

UNIVERSITY OF WATERLOO

vectorinstitute.ai | @VectorInst

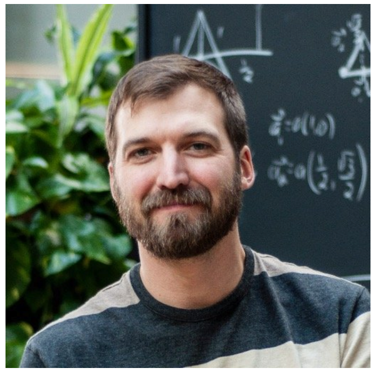
PhD positions and short-term visits

- If you know students interested in working at the intersection between machine learning, condensed matter theory, numerical simulations of quantum many-body systems, and quantum computers
- Possibility to interact and collaborate with ML and quantum computing experts
- Get in touch with me carrasqu@vectorinstitute.ai
- https://vectorinstitute.ai/team/juan-felipe-carrasquilla/

COLLABORATORS

Leandro Aolita
(Universidade Federal do
Rio de Janeiro, ICTP-SAIFR)

Giacomo Torlai
(Flatiron Institute)

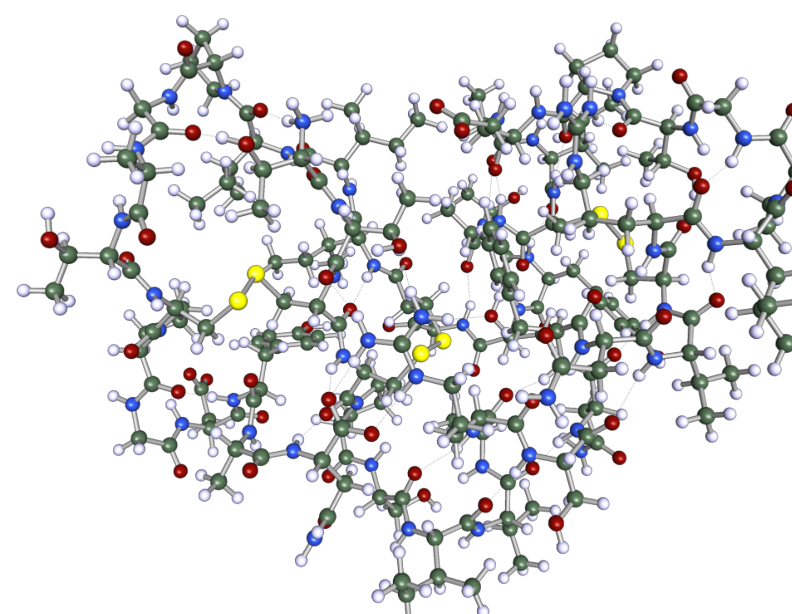


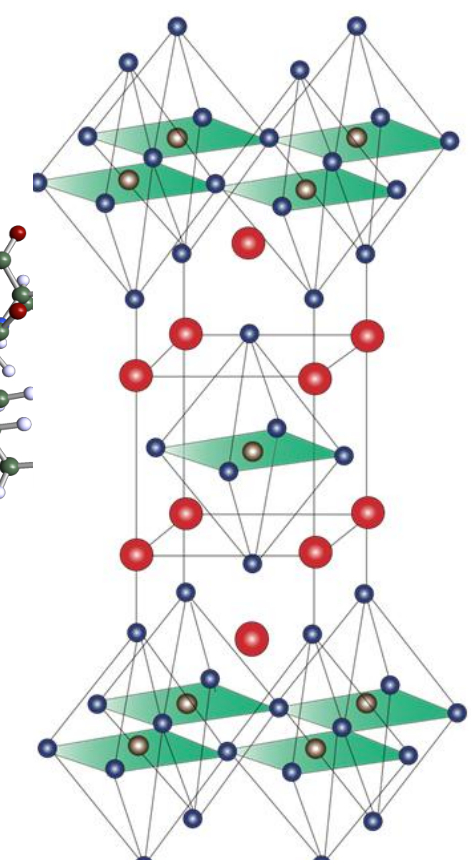
Roger Melko (U.
Waterloo and Perimeter)

THE MANY-BODY PROBLEM IN QUANTUM MECHANICS

- Generic specification of a quantum state requires resources exponentially large in the number of degrees of freedom N
- Today's best supercomputers can solve the wave equation **exactly** for systems with a maximum of ~45 spins.
- Yet, technologically relevant problems in chemistry, condensed matter physics, and quantum computing are much larger than 45.
- Quantum computing

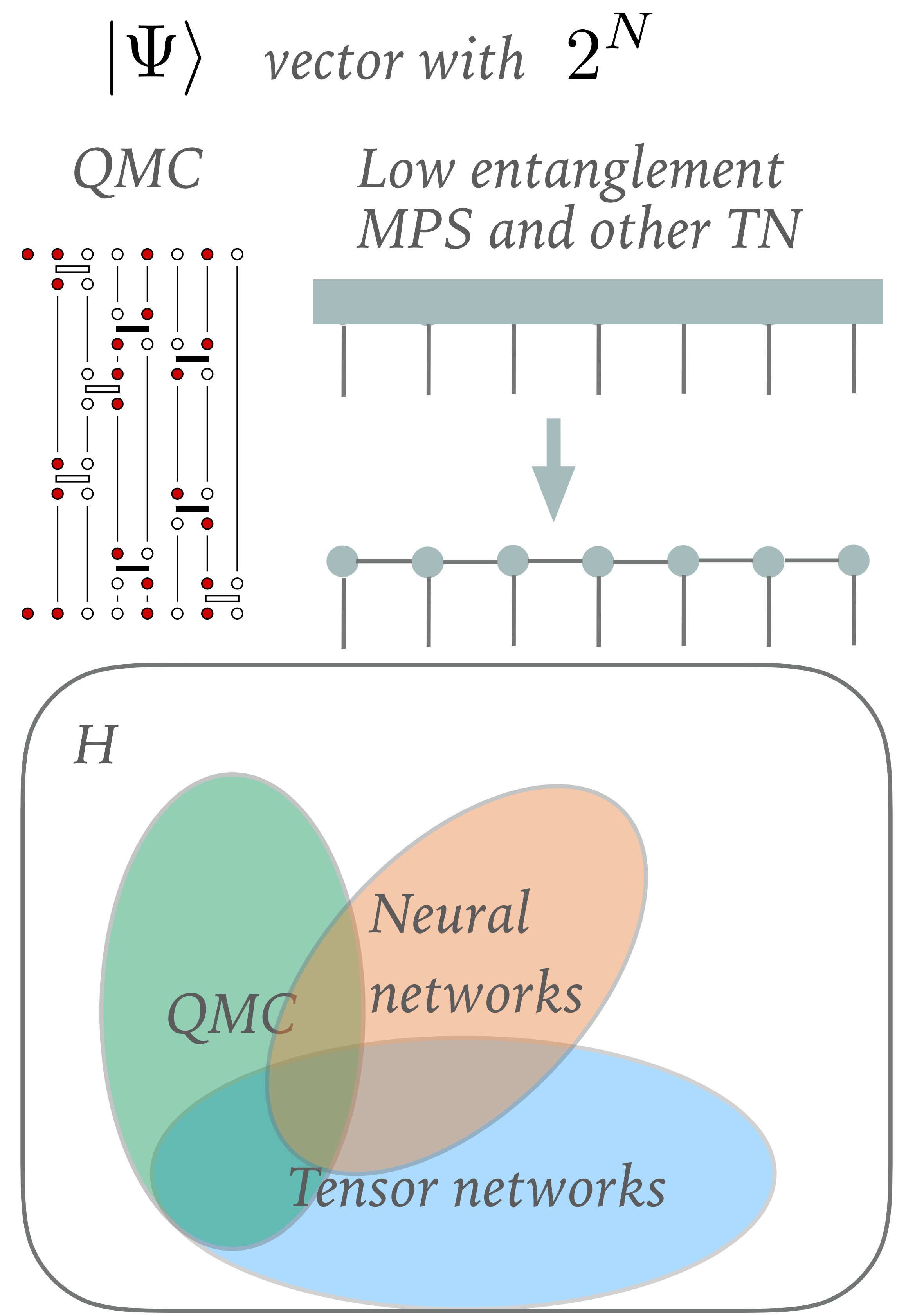
$|\Psi\rangle$ *vector with* 2^N





THERE IS STILL HOPE FOR CLASSICAL ALGORITHMS

- Nature is sometimes compassionate: amount of information smaller than the maximum capacity.
- Quantum Monte Carlo and other numerical methods based on Tensor Networks exploit this fact.
- Machine learning community deals with equally high dimensional problems ($\sim 2^{28x28}$)
- Curse of dimensionality but still successful in wide spectrum of scientific and technologically relevant areas of research.

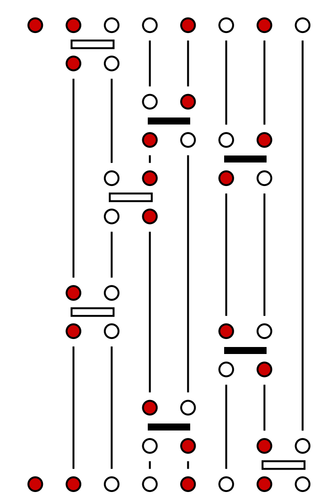


THERE IS STILL HOPE FOR CLASSICAL ALGORITHMS

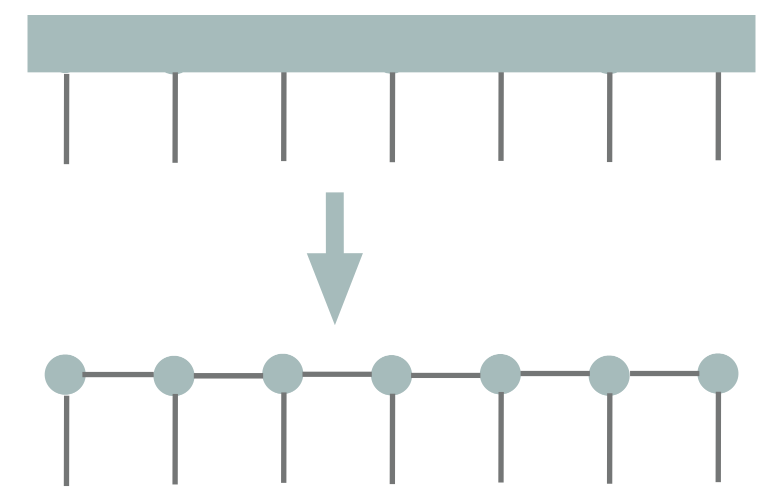
- Nature is sometimes compassionate: amount of information smaller than the maximum capacity.
- Quantum Monte Carlo and other numerical methods based on Tensor Networks exploit this fact.
- Machine learning community deals with equally high dimensional problems ($\sim 2^{28\mathrm{x}28}$)
- Curse of dimensionality but still successful in wide spectrum of scientific and technologically relevant areas of research.

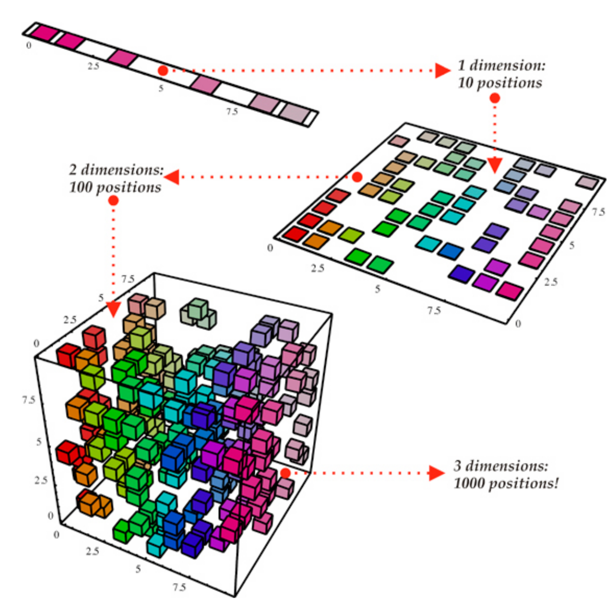
$|\Psi\rangle$ *vector with* 2^N

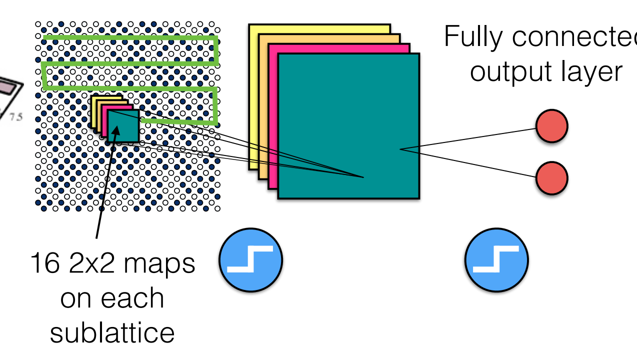
QMC



Low entanglement MPS and other TN







QUANTUM AND CLASSICAL MANY-BODY PHYSICS HAS NOT BEEN THE EXCEPTION

- ML phases of matter/phase transitions (Carrasquilla, Melko 1605.01735, Wang 1606.00318, Zhang, Kim, 1611.01518)
- New ML inspired ansatz for quantum many-body systems (Carleo, Troyer 1606.02318, Deng, Li, Das Sarma, 1701.04844, Deng, Li, Das Sarma 1609.09060, Carrasquilla, Melko 1605.01735)
- Accelerated Monte Carlo simulations (Huang, Wang 1610.02746)
- Quantum state preparation guided by ML (Bukov, Day, Sels, Weinberg, Polkovnikov and Mehta 1705.00565)
- Renormalization group analyses, RBMs, PCA (Bradde, Bialek 1610.09733, Koch-Janusz, Ringel 1704.06279,Mehta, Schwab,1410.3831)
- Quantum state tomography based on RBMs (Torlai, Mazzola, Carrasquilla, Troyer, Melko, Carleo, 1703.05334)
- ML based decoders for topological codes (Torlai, Melko 1610.04238, Varsamopoulos, Criger, Bertels, 1705.00857)
- Supervised Learning with Quantum-Inspired Tensor Networks (Stoudenmire, Schwab 1605.05775, Novikov, Trofimov, Oseledets, 1605.03795)
- Quantum Boltzmann machines (Amin, Andriyash, Rolfe, Kulchytskyy, Melko, 1601.02036, Kieferova, Wiebe, 1612.05204,)
- Quantum machine learning algorithms to accelerate learning (Biamonte, Wittek, Pancotti, Rebentrost, Wiebe, Lloyd, 1611.09347)

And many more ***https://physicsml.github.io/pages/papers.html***

LEARNING QUANTUM STATES AND QUANTUM STATE TOMOGRAPHY

QUANTUM STATE TOMOGRAPHY

Quantum state tomography is the process of reconstructing the quantum state by **measurements** on the system. It "is the gold standard for verification and benchmarking of quantum devices"*

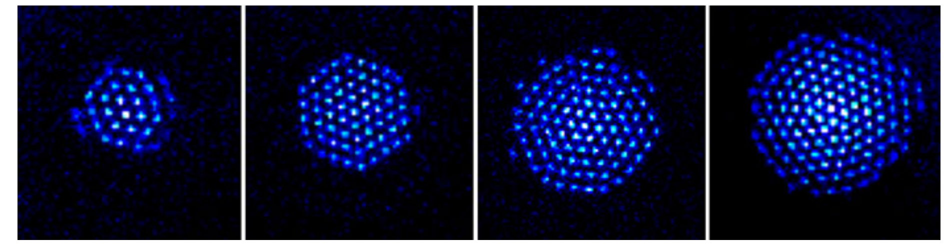
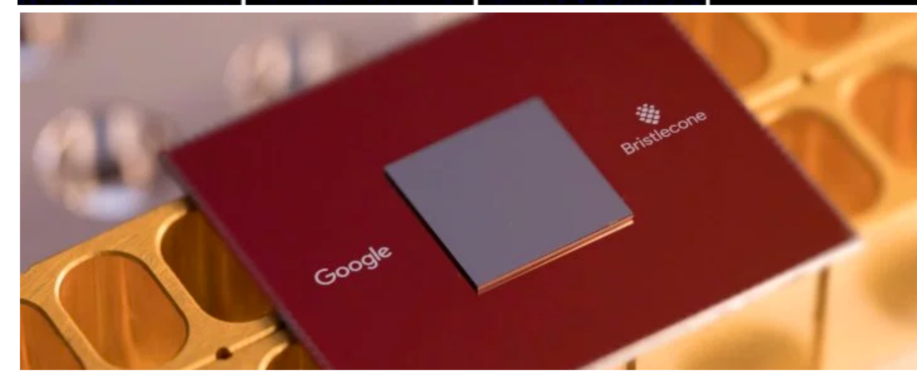
Useful for:

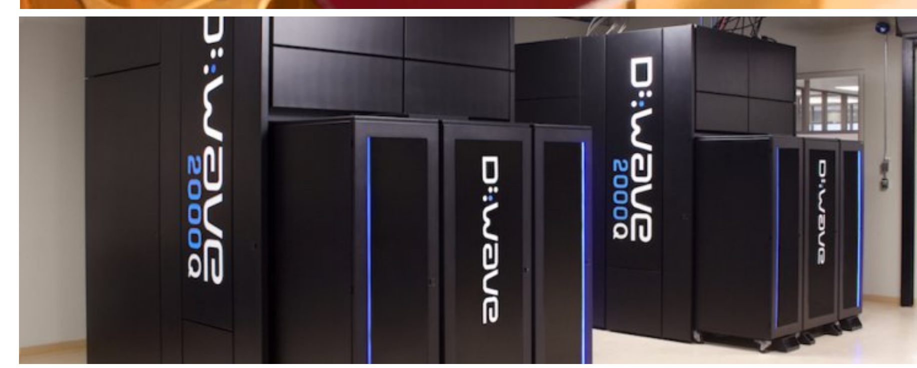
- Characterizing optical signals
- Diagnosing and detecting errors in state preparation, e.g. states produced by quantum computers reliably.
- Entanglement verification

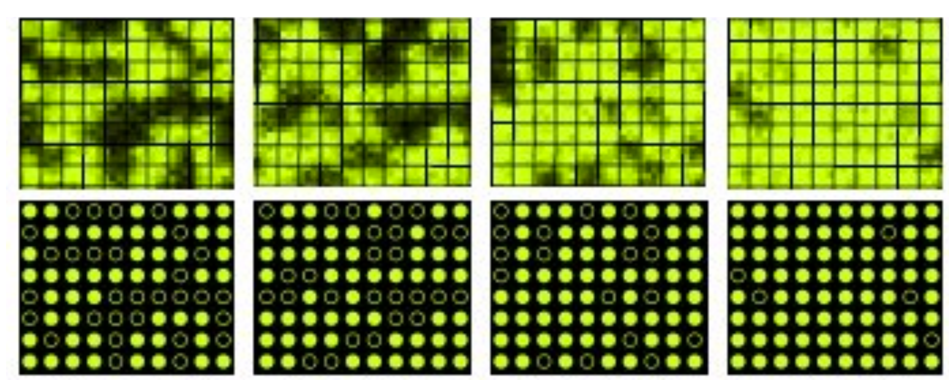
* Efficient quantum state tomography. Marcus Cramer, Martin B. Plenio, Steven T. Flammia, Rolando Somma, David Gross, Stephen D. Bartlett, Olivier Landon-Cardinal, David Poulin & Yi-Kai Liu. Nature Communications volume **1**, Article number: 149

NEED TO GO BEYOND STANDARD QUANTUM STATE TOMOGRAPHY

- Progress in controlling large quantum systems.
- Availability of arbitrary measurements performed with great accuracy.
- The bottleneck limiting progress in the estimation of states: curse of dimensionality.





SYNTHETIC QUANTUM DEVICES ARE GROWING FAST

nature.com > nature > articles > article

nature International journal of science

Article | Published: 29 November 2017

Probing many-body dynamics on a 51-atom quantum simulator

Hannes Bernien, Sylvain Schwartz, Alexander Keesling, Harry Levine, Ahmed Omran, Hannes Pichler, Soonwon Choi, Alexander S. Zibrov, Manuel Endres, Markus Greiner, Vladan Vuletić & Mikhail D. Lukin

Nature **551**, 579–584 (30 November 2017) | Download Citation

nature.com > nature > letters > article

nature International journal of science

Letter | Published: 29 November 2017

Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator

J. Zhang, G. Pagano, P. W. Hess, A. Kyprianidis, P. Becker, H. Kaplan, A. V. Gorshkov, Z.-X. Gong & C. Monroe

Nature **551**, 601–604 (30 November 2017) | Download Citation

nature.com > nature > letters > article

nature International journal of science

Letter | Published: 22 August 2018

Observation of topological phenomena in a programmable lattice of 1,800 qubits

Andrew D. King, Juan Carrasquilla, […] Mohammad H. Amin

Nature **560**, 456–460 (2018) | Download Citation

PHYSICAL REVIEW X

Highlights Recent Subjects Accepted Collections Authors Referees Search Press About Staff

Open Access

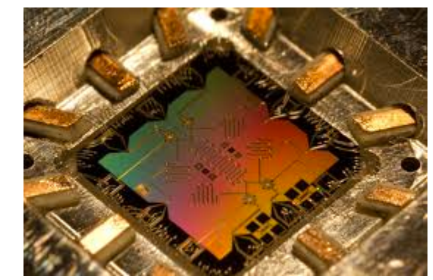
Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator

Cornelius Hempel, Christine Maier, Jonathan Romero, Jarrod McClean, Thomas Monz, Heng Shen, Petar Jurcevic, Ben P. Lanyon, Peter Love, Ryan Babbush, Alán Aspuru-Guzik, Rainer Blatt, and Christian F. Roos

Phys. Rev. X **8**, 031022 – Published 24 July 2018

QUANTUM STATE TOMOGRAPHY

Required ingredients



- A quantum system that can be prepared repeatedly
- Set of **measurements**.
- A training procedure and a model (full density matrix, MPS, MPO, neural networks)
- Certification

A typical state tomography protocol prepares many copies of ρ which are measured in diverse ways, and finally the outcomes of those measurements (data) are analyzed to produce an estimate ρ*.

* Efficient quantum state tomography. Marcus Cramer, Martin B. Plenio, Steven T. Flammia, Rolando Somma, David Gross, Stephen D. Bartlett, Olivier Landon-Cardinal, David Poulin & Yi-Kai Liu. Nature Communications volume 1, Article number: 149

TRADITIONALLY QST REQUIRES EXPONENTIAL RESOURCES

Examples

- Linear inversion method requires inverting a large matrix and results in an explicit representation of the density matrix

$$P(\mathbf{a}) = \mathrm{Tr}\,\rho M^{\mathbf{a}}$$ experimental histogram → $$p_{\mathrm{hist}}(a)$$

$$\hat{\rho} = \sum_{a,a'} T^{-1}_{a,a'} p_{\mathrm{hist}}(a') M^{(a)}$$

- Issues: Exponential scaling both in the representation and inversion problem
- Potentially unphysical density matrices $\hat{\rho}$

On the Measurement of Qubits. Daniel F. V. James, Paul G. Kwiat, William J. Munro, Andrew G. White. Physical Review A 64, 052312 (2001)

TRADITIONALLY QST REQUIRES EXPONENTIAL RESOURCES

Examples

- Maximum likelihood estimation. Requires an explicit "physical" density matrix → representation scales poorly

$$L(\hat{\rho}) = \prod_a P(a)^{f_a}$$

Maximize probability of observed data with respect to a parametrization of $\hat{\rho}$

- Issues: Exponential scaling in the parametrization
- Estimation of errors due to finite statistics in the measurements is difficult

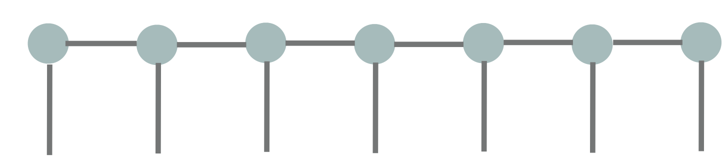
On the Measurement of Qubits. Daniel F. V. James, Paul G. Kwiat, William J. Munro, Andrew G. White. Physical Review A 64, 052312 (2001)

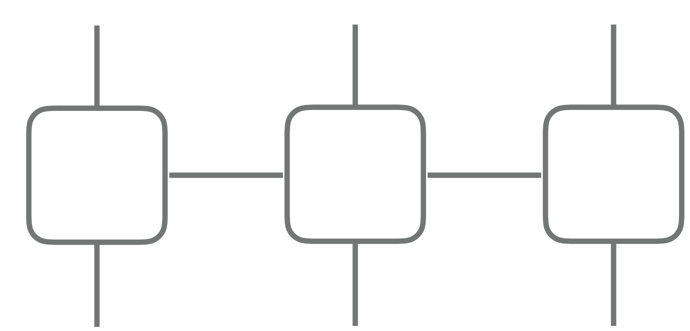
HOW TO MAKE QST EFFICIENT?

- Introduce a parametrization of the quantum state with good scaling if non-trivial structural information on the quantum systems under consideration is utilized: MPS[1] and MPO[2] tomography

[1] **Efficient quantum state tomography**. Marcus Cramer, Martin B. Plenio, Steven T. Flammia, Rolando Somma, David Gross, Stephen D. Bartlett, Olivier Landon-Cardinal, David Poulin & Yi-Kai Liu. Nature Communications volume **1**, Article number: 149

[2] **A scalable maximum likelihood method for quantum state tomography** T Baumgratz1, A Nüßeler, M Cramer and M B Plenio. New Journal of Physics, Volume 15, December 2013

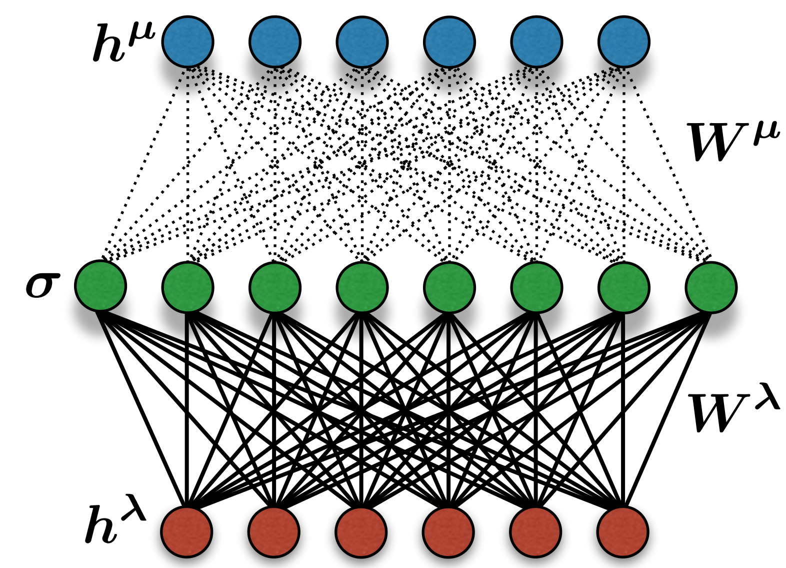




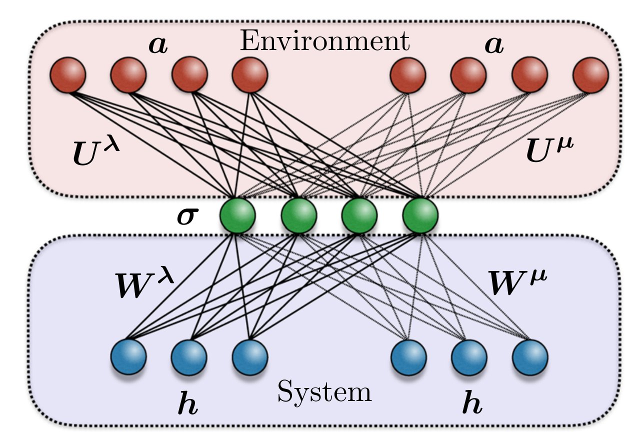
HOW TO MAKE QST EFFICIENT?

- Introduce a parametrization of the quantum state with good scaling if non-trivial structural information on the quantum systems under consideration is utilized: Restricted Boltzmann machines both for pure[3] states and mixed states[4]

[3] **Neural-network quantum state tomography.** G. Torlai, G. Mazzola, J. Carrasquilla, M. Troyer, R. Melko, and G. Carleo, Nat. Phys. 14, 447 (2018).



[4] **Latent Space Purification via Neural Density Operators**. Giacomo Torlai and Roger G. Melko. Phys. Rev. Lett. 120, 240503 (2018)*

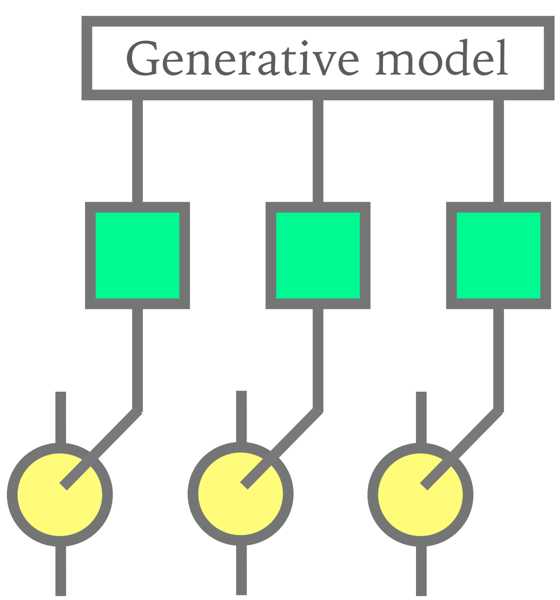


*Has exponential scaling

IN THIS TALK

- ~~Parametrize the quantum state~~ We parametrize the Born's rule in terms of generative models. Measurements: informationally complete positive operator valued measures (POVM)
- Use this idea to learn states from synthetic measurements mimicking experimental data

$$\rho_{\text{model}} = (\mathbf{T}^{-1} P_{\text{model}})^T \mathbf{M}$$



MEASUREMENTS: POSITIVE OPERATOR-VALUED MEASURE (POVM)

- POVM elements $\mathbf{M} = \{M^{(a)} \mid a \in \{1, ..., m\}\}$
- Positive semidefinite operators
- $\sum_i M^{(a)} = \mathbb{1}$

EXAMPLE: MEASUREMENT IN THE COMPUTATIONAL BASIS

$$M^{(0)} = |0\rangle\langle 0| \quad M^{(1)} = |1\rangle\langle 1| \quad \mathbb{I} = |0\rangle\langle 0| + |1\rangle\langle 1|$$

STATE $|\Psi\rangle = a|0\rangle + b|1\rangle$

$$\left.\begin{aligned} p(0) &= \langle\Psi|M^{(0)}|\Psi\rangle = |a|^2 \\ p(1) &= \langle\Psi|M^{(1)}|\Psi\rangle = |b|^2 \end{aligned}\right\}$$

BORN RULE: PROVIDES A LINK BETWEEN QUANTUM THEORY AND EXPERIMENT

MEASUREMENTS: POSITIVE OPERATOR-VALUED MEASURE (POVM)

POVM ELEMENTS $\mathbf{M} = \{M^{(a)} \mid a \in \{1, ..., m\}\}$ $\sum_i M^{(a)} = \mathbb{1}$

$P(\mathbf{a}) = \mathrm{Tr}\,\rho M^{\mathbf{a}}$ Born rule. Defines a distribution over the generalized measurements => link between quantum theory and experimental outcome

INFORMATIONALLY COMPLETE POVM

- The measurement statistics $P(\mathbf{a})$ contains all of the information about the state.
- If m is at least $D^2=2^{2N}$ and M span the entire Hilbert space

$$O = \sum_{\mathbf{a}} O(a) M^{(a)}$$

- Relation between ρ and distribution $P(\mathbf{a})$ can be inverted.

MEASUREMENTS: POSITIVE OPERATOR VALUED MEASURES (POVM)

CONSTRUCTING POVMS: TAKE A SINGLE QUBIT POVM AND MAKE A TENSOR PRODUCT OF MANY

Pauli measurement for one qubit

$$\begin{aligned}\boldsymbol{M}_{\text{Pauli}} := \{ & M^{(0)} := p(3) \times |0\rangle\langle 0|\,, M^{(1)} := p(3) \times |1\rangle\langle 1|\,, \\ & M^{(+)} := p(1) \times |+\rangle\langle +|\,, M^{(-)} := p(1) \times |-\rangle\langle -|\,, \\ & M^{(r)} := p(2) \times |r\rangle\langle r|\,, M^{(l)} := p(2) \times |l\rangle\langle l|\,\},\end{aligned}$$

For multiqubit systems $\boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes$

we will consider

$$\boldsymbol{M} = \left\{ M^{(a_1)} \otimes M^{(a_2)} \otimes \ldots M^{(a_N)} \right\}_{a_1, \ldots a_N}$$

Experimental realization: pick a random direction with probability 1/3, then measure in that direction

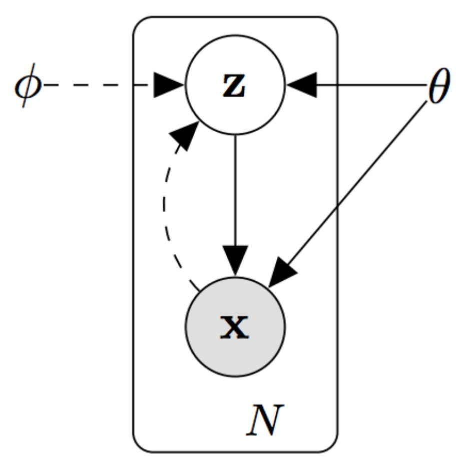
Easy to implement in gate-based QC (Qiskit, Cirq, Rigetti, etc.)

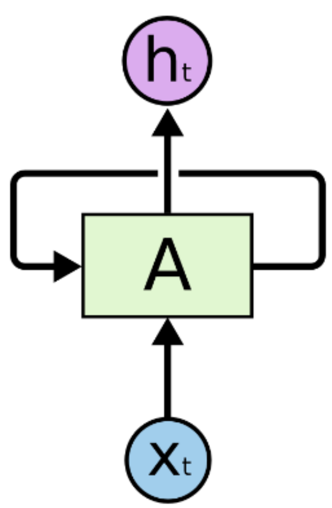
KEY INSIGHT: PARAMETRIZE STATISTICS AND INVERT

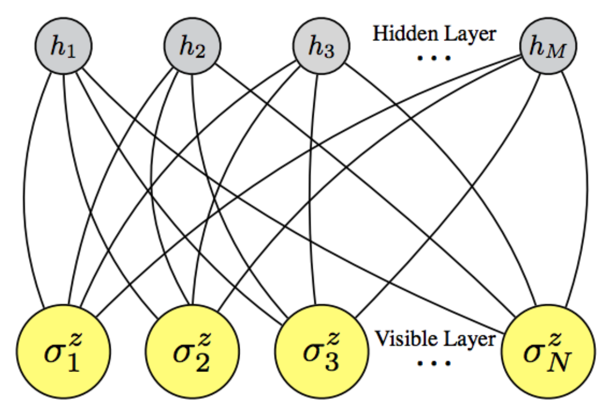
$$P(\mathbf{a}) = \mathrm{Tr}\,\rho M^{\mathbf{a}}$$

=> Unsupervised learning of P(a)

$$P_{\text{model}}(\mathbf{a}) \longrightarrow$$ VAE, RBM, GAN, autoregressive models, etc







Goodfellow et al. Deep Learning (2016)

Check out tomorrow's chalkboard talk: Michael Albergo 🔥

WHAT ARE THESE MODELS TYPICALLY USED FOR?

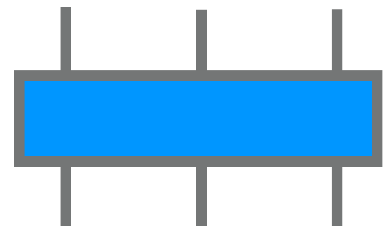
$P_{\text{model}}(\mathbf{a})$ ⟶ **VAE, RBM, GAN, autoregressive models, etc**

- Understand probability distributions defined over high-dimensional data
- Language translation $P(\text{English}|\text{French})$
- Image generation
- Density estimation
- Anomaly/novelty detection

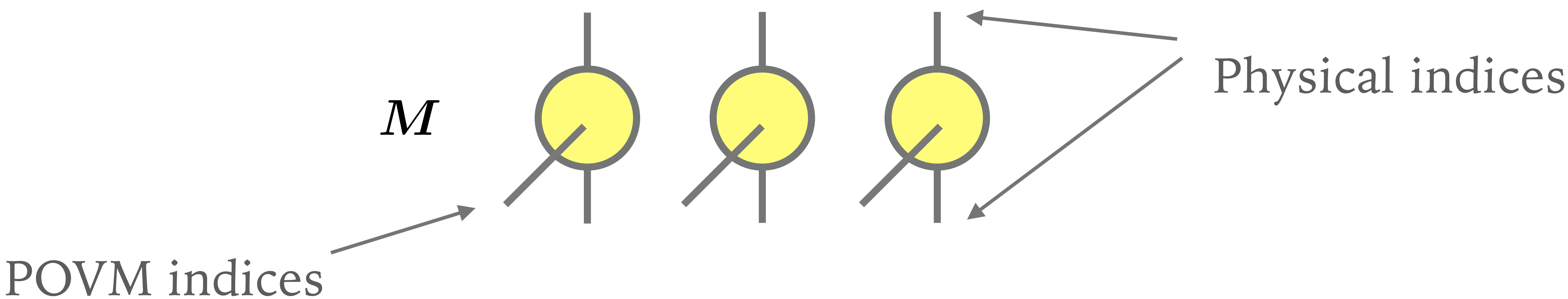
Source	When asked about this, an official of the American administration replied: "The United States is not conducting electronic surveillance aimed at offices of the World Bank and IMF in Washington."
PBMT	Interrogé à ce sujet, un responsable de l'administration américaine a répondu : "Les Etats-Unis n'est pas effectuer une surveillance électronique destiné aux bureaux de la Banque mondiale et du FMI à Washington".
GNMT	Interrogé à ce sujet, un fonctionnaire de l'administration américaine a répondu: "Les États-Unis n'effectuent pas de surveillance électronique à l'intention des bureaux de la Banque mondiale et du FMI à Washington".
Human	Interrogé sur le sujet, un responsable de l'administration américaine a répondu: "les Etats-Unis ne mènent pas de surveillance électronique visant les sièges de la Banque mondiale et du FMI à Washington".

GRAPHICAL NOTATION

Density matrix ρ



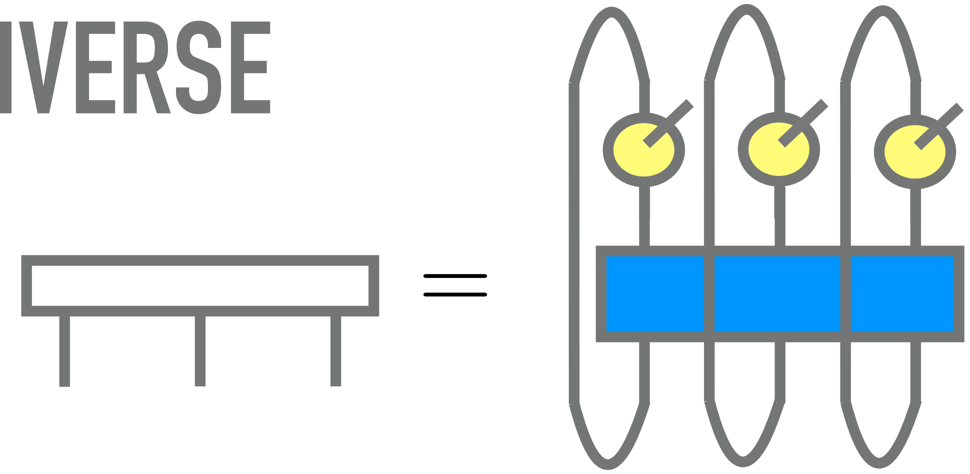
Statistics of measurement $P(\mathbf{a})$



$$\boldsymbol{M} = \left\{M^{(a_1)} \otimes M^{(a_2)} \otimes \ldots M^{(a_N)}\right\}_{a_1,\ldots a_N}$$

GRAPHICAL NOTATION AND INVERSE

Born rule $P(\mathbf{a}) = \mathrm{Tr}\, \rho M^{\mathbf{a}}$



If the POVM is informationally complete then

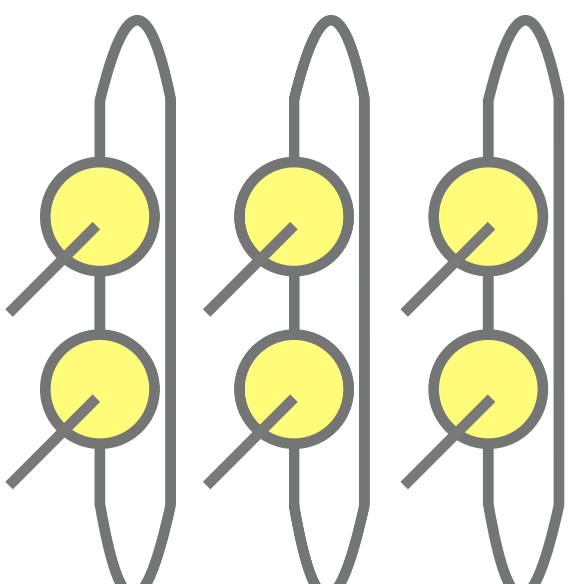
$$\rho = \sum_a O_\rho(a) M^{(a)}$$

Insert this relation into Born's rule $P(a) = \sum_{a'} O_\rho(a') Tr[M^{(a)} M^{(a')}] = \sum_{a'} O_\rho(a') T_{a'a}$

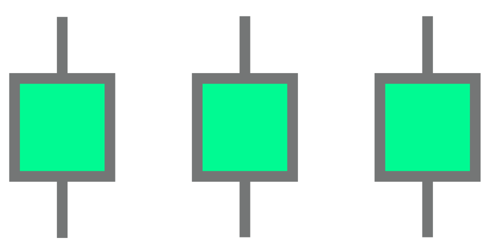
$$\rho = \sum_{a,a'} T^{-1}_{a,a'} P(a') M^{(a)}$$

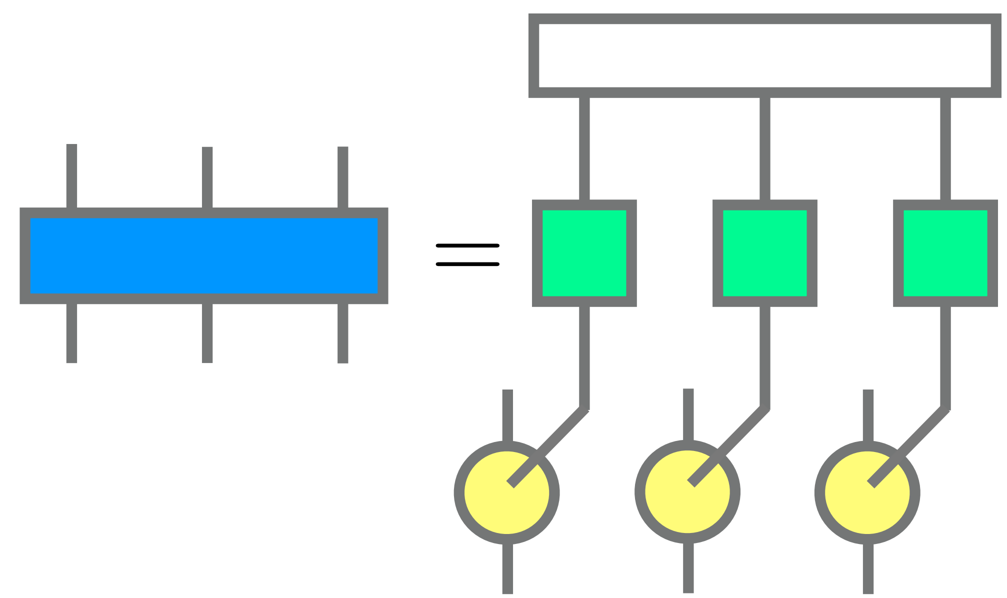
$$\rho = \sum_{a,a'} T^{-1}_{a,a'} P(a') M^{(a)}$$

$T_{\alpha,\beta} = \mathrm{Tr}\ M^\alpha M^\beta$



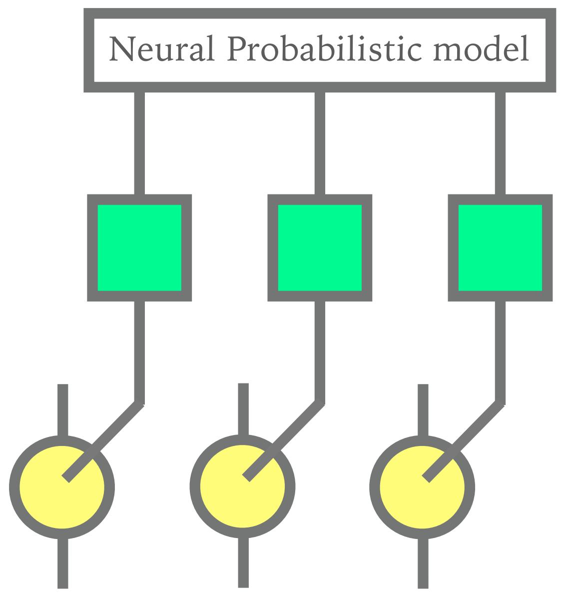
$\mathbf{T}^{-1}$





LEARNING MIXED STATES USING POSITIVE OPERATOR VALUED MEASURE

$$\rho_{\text{model}} = (\mathbf{T}^{-1} P_{\text{model}})^{T} \mathbf{M}$$



The statistics of the measurements is given by **Born rule**

quantum state

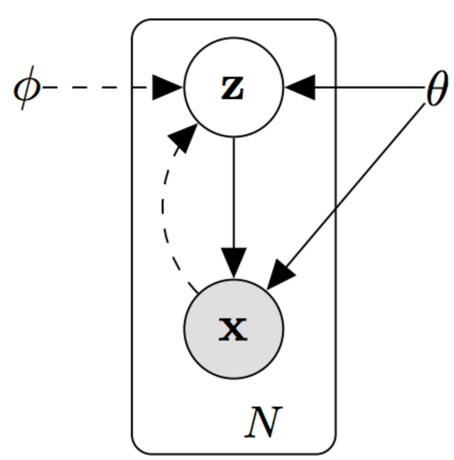
$$P(\mathbf{a}) = \mathrm{Tr}\, \rho M^{\mathbf{a}}$$

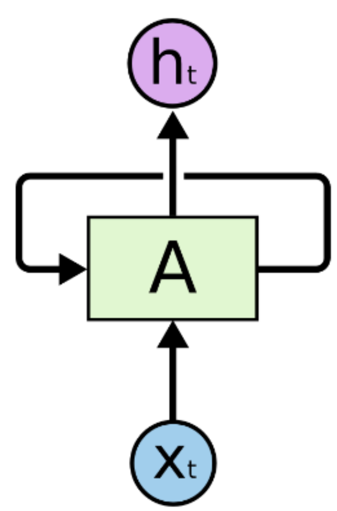
Statistics of the measurements

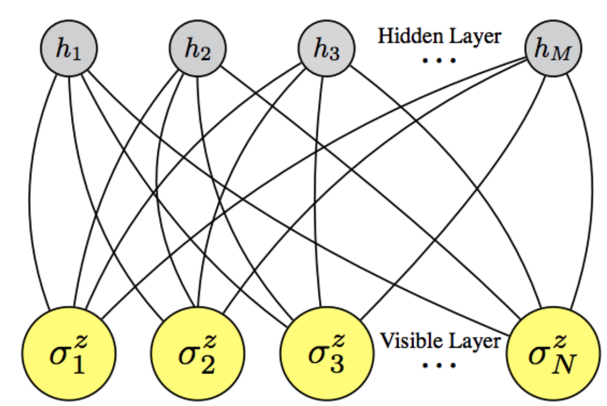
Measurements

=> Unsupervised learning of P(a)

$$P_{\text{model}}(\mathbf{a}) \longrightarrow$$ **VAE, RBM, GAN, autoregressive models, any model**



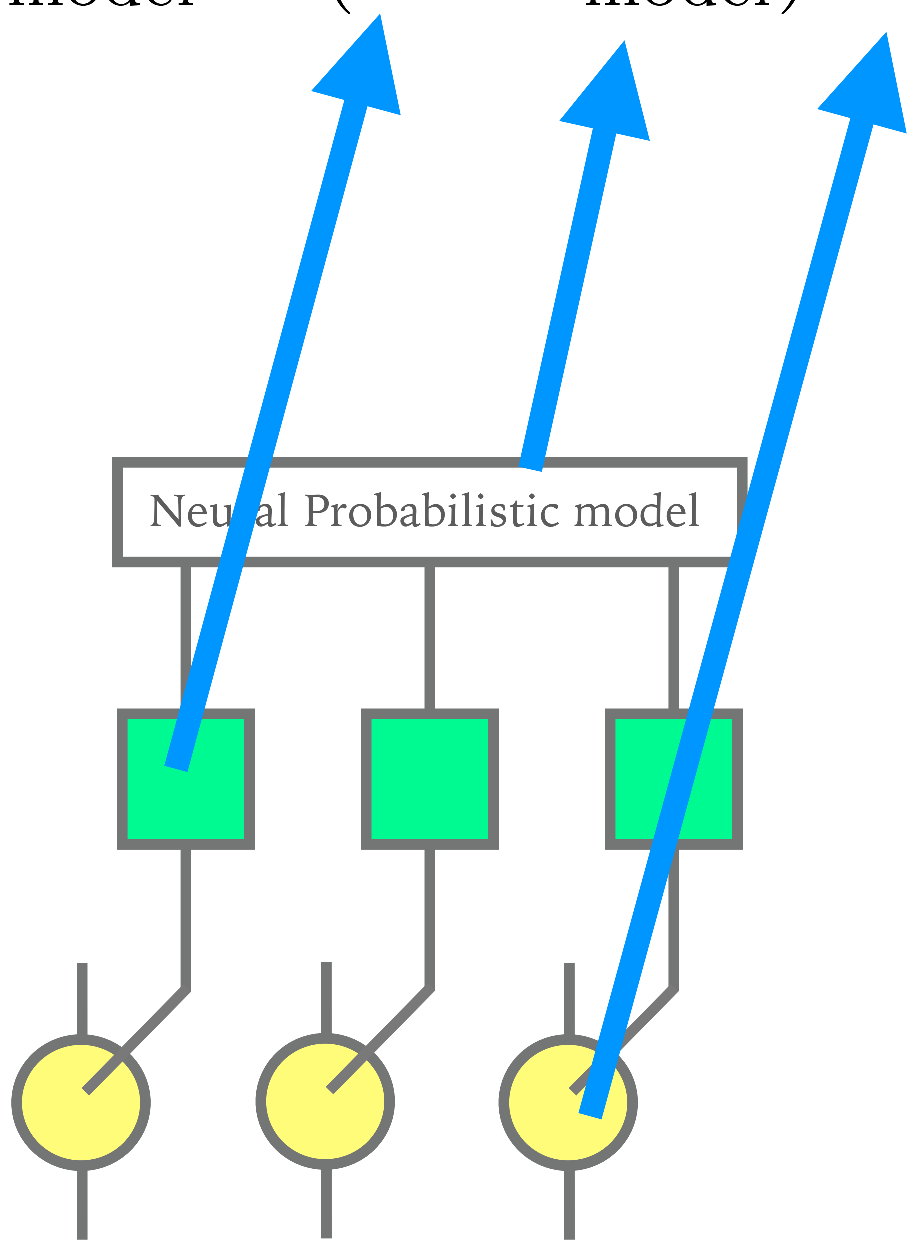




Goodfellow et al. Deep Learning (2016)

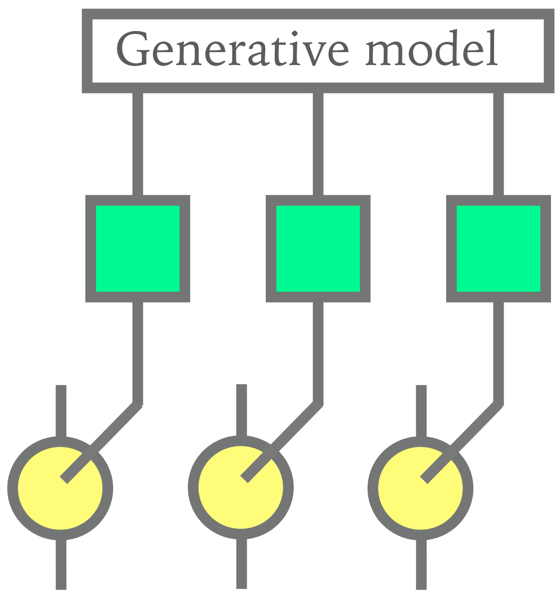
BORN RULE IS A LINEAR RELATION AND CAN BE INVERTED

$$\rho_{\text{model}} = (\mathbf{T}^{-1} P_{\text{model}})^T \mathbf{M}$$



MODEL FOR THE DENSITY MATRIX

$$\rho_{\text{model}} = (\mathbf{T}^{-1} P_{\text{model}})^T \mathbf{M}$$



- Factorization of the state in terms of a probability distribution and a set of tensors
- All the entanglement and potential complexity of the state comes from the structure of the P(a)
- P(a) is approximated by powerful neural network probabilistic models

CERTIFICATION: FIDELITY, CLASSICAL FIDELITY, CORRELATION FUNCTIONS

- Fidelity
- Classical fidelity in POVM space
- Kullback–Leibler divergence in POVM space
- Correlation functions

$$F(\rho,\sigma) = \mathrm{Tr}\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right]^2$$

$$KL(P_{\mathrm{model}}|P) = -\sum_a P(a)\log\frac{P_{model}(a)}{P(a)}$$

$$F_{\mathrm{Classical}} = \sum_a \sqrt{P(a)P_{model}(a)}$$

LEARNING MIXED STATES USING POVM: PROCEDURE

- Prepare a desired quantum state repeatedly
- Perform generalized measurements
- Reconstruct P(a) using unsupervised learning
- "Invert" $\rho = \sum_{a,a'} T^{-1}_{a,a'} P(a') M^{(a)}$
- Perform some sort of certification via fidelity or classical fidelity or measure correlation functions etc.

Combines the idea of MLE with linear inversion in one method (observables/certification)

RESULTS

GHZ + NOISE, GROUND STATES OF QUANTUM SYSTEMS APPROXIMATED BY MPS STATES

RESULTS ON SYNTHETIC DATASETS FOR GHZ STATES

Pure GHZ

$$|\Psi_0\rangle \equiv \alpha\,|0\rangle^{\otimes N} + \beta\,|1\rangle^{\otimes N}$$

$$\begin{aligned}\varrho_0 &\coloneqq |\Psi_0\rangle\langle\Psi_0| \\ &= |\alpha|^2\,|0\rangle\langle 0|^{\otimes N} + |\beta|^2\,|1\rangle\langle 1|^{\otimes N} + \left(\alpha\beta^*\,|0\rangle\langle 1|^{\otimes N} + \text{ h.c.}\right)\end{aligned}$$

GHZ with

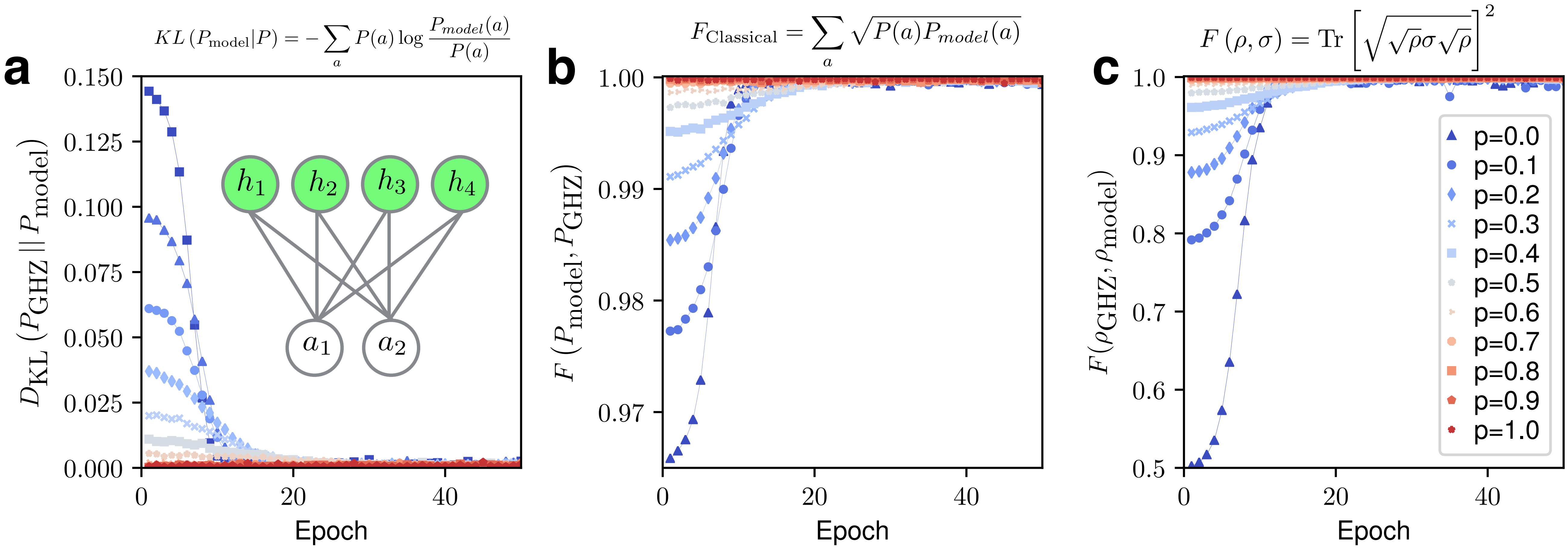
Locally depolarized

generalized GHZ

$$\mathcal{E}_i\varrho_0 = (1-p)\,\varrho_0 + \frac{p}{3}\left(\sigma_i^{(1)}\,\varrho_0\,\sigma_i^{(1)} + \sigma_i^{(2)}\,\varrho_0\,\sigma_i^{(2)} + \sigma_i^{(3)}\,\varrho_0\,\sigma_i^{(3)}\right)$$

states : a model of a decohering qubit where with probability $1 - p$ the qubit remains intact, while with probability p an “error” occurs.

LEARNING 2 QUBIT LOCALLY DEPOLARIZED GHZ



This result is obtained by parametrizing the P(a) with an RBM with multinomial visible units (4 states per qubit for the corresponding to the outcomes of the POVMs)

$$v_i = 0, 1, 2, 3, 4$$

$$h_j = 0, 1$$

Restricted Boltzmann Machines for Collaborative Filtering. Salakhutdinov, Mnih, Hinton. 2007

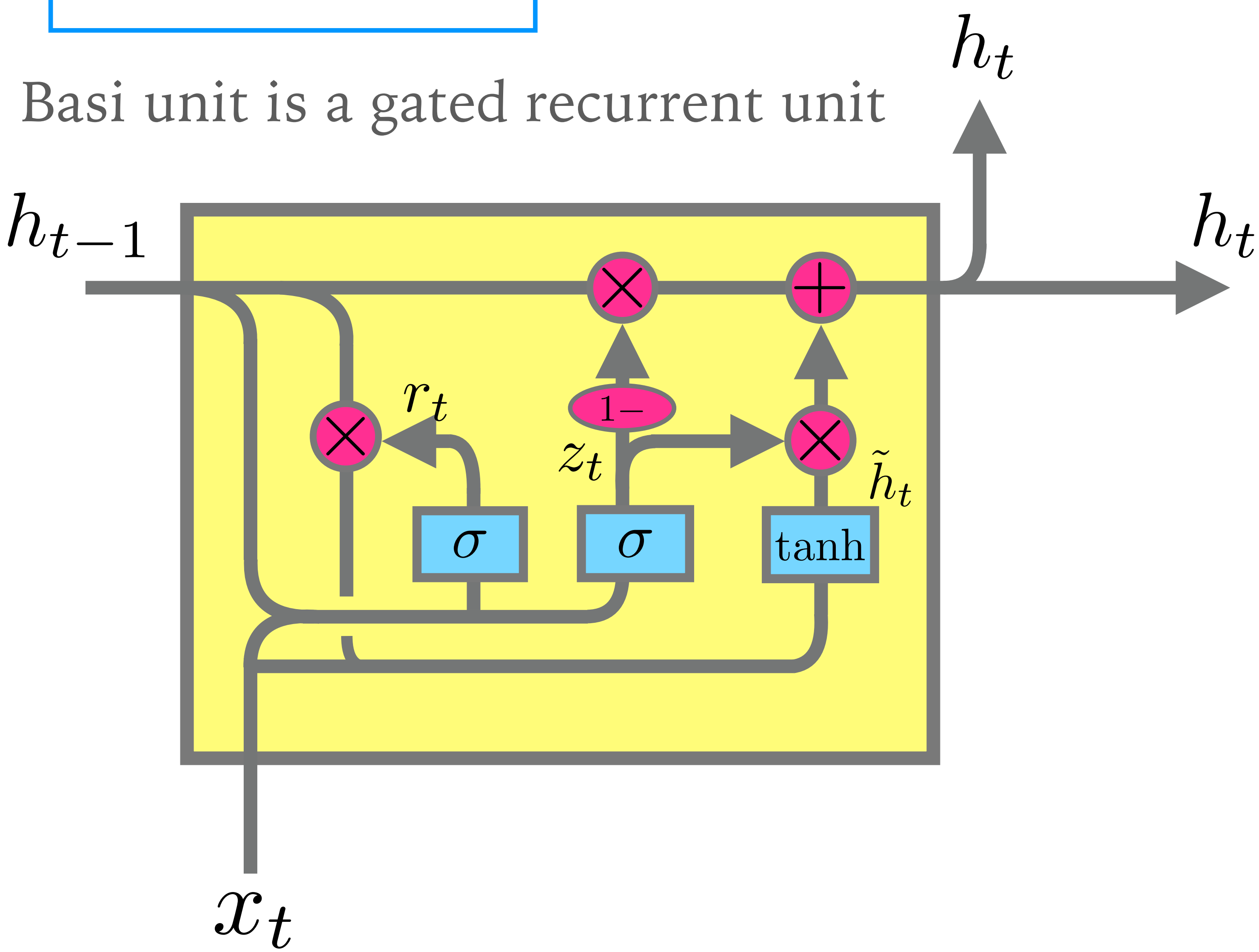
RECURRENT NEURAL NETWORK MODEL AND RESULTS

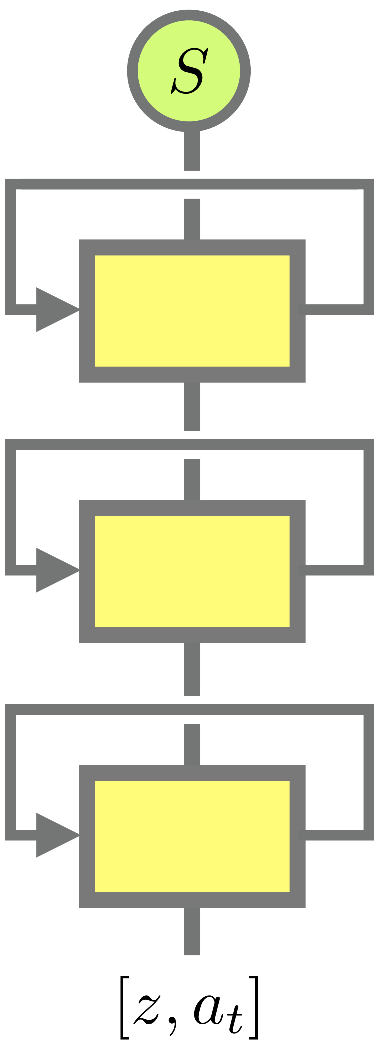
GHZ results

40 qubit p=0
Fc = 0.9992(4)
80 qubits p =0.01
Fc = 0.9988(1)
KL = 0.0050(2)

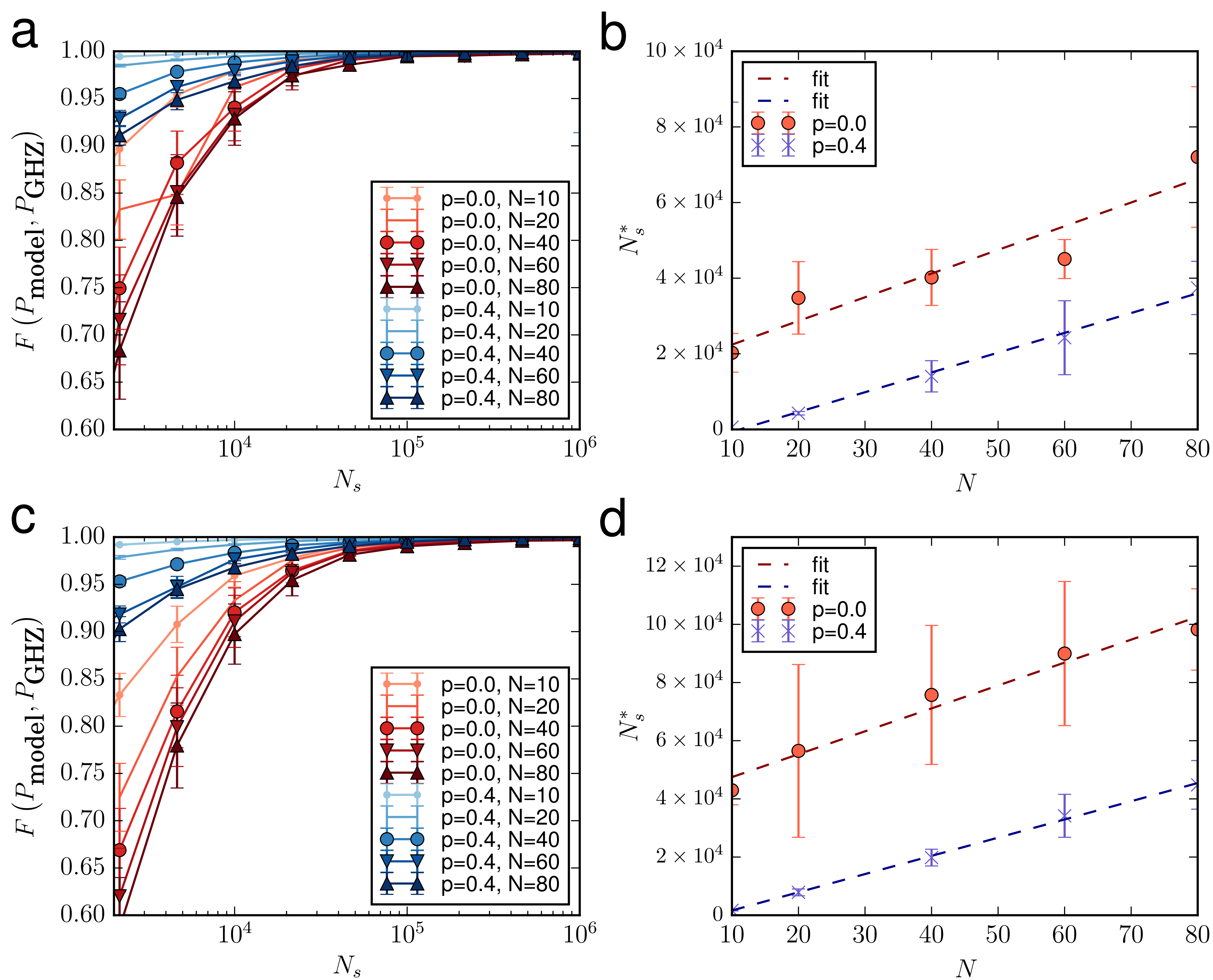
Full model stacks three of these units and adds a softmax dense layer at each time step

Basi unit is a gated recurrent unit



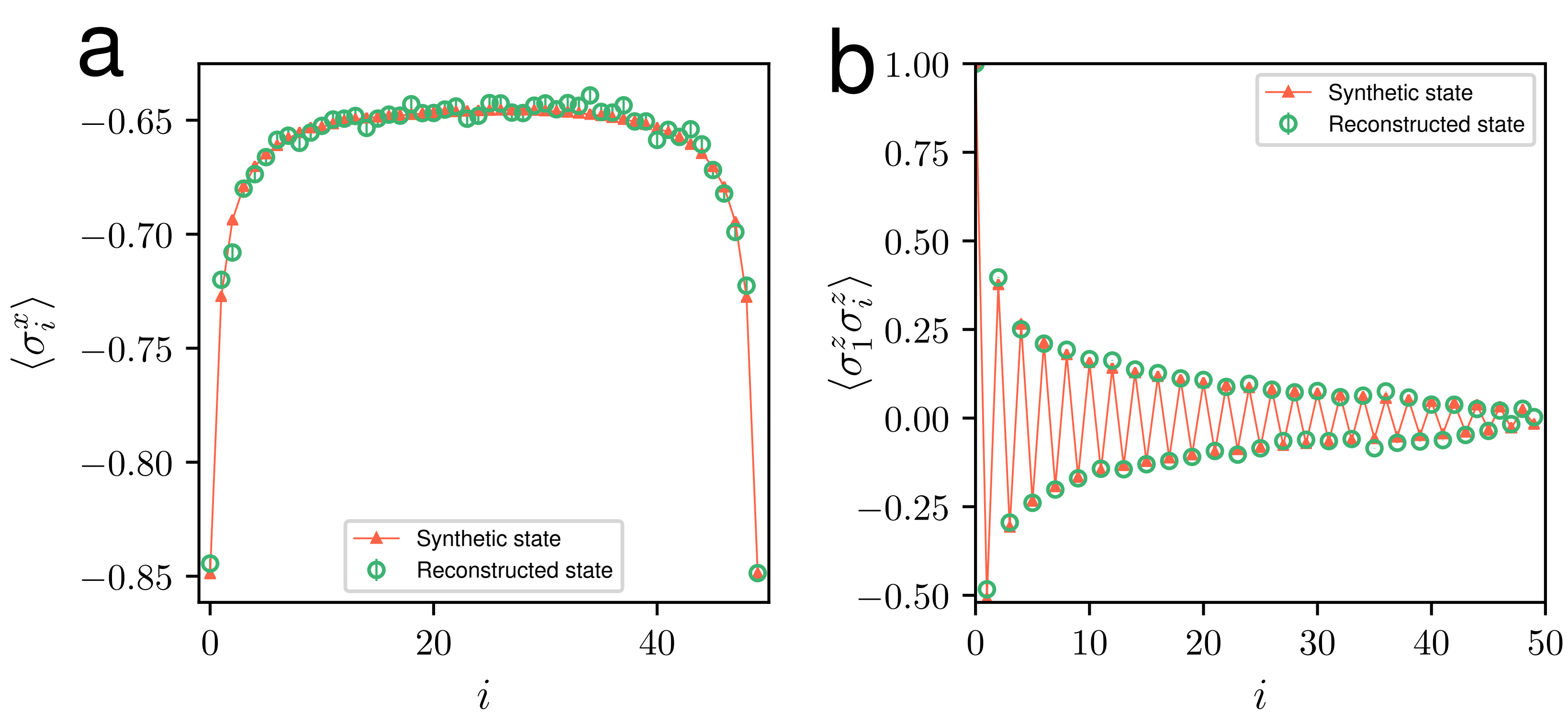


NUMERICAL INVESTIGATION OF THE SAMPLE COMPLEXITY OF LEARNING



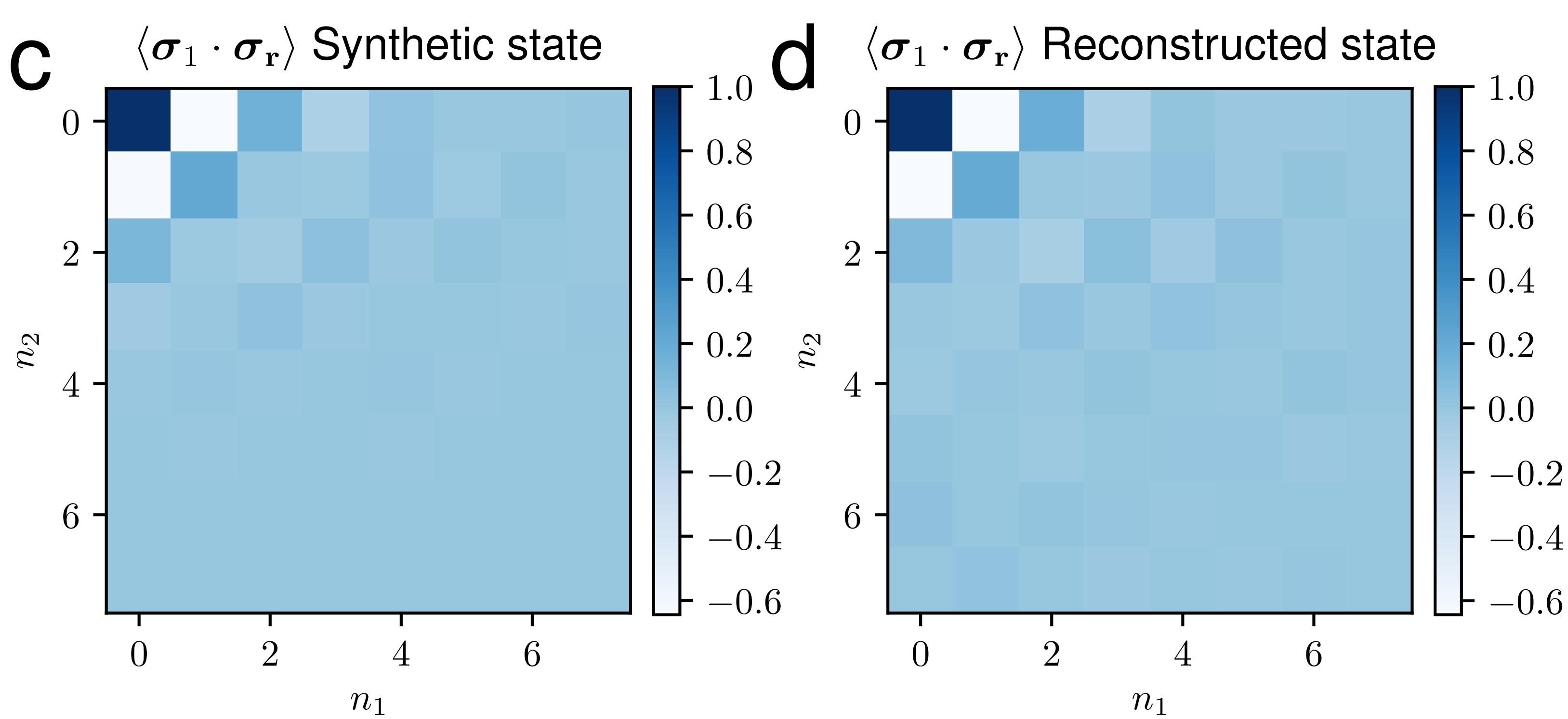
Favorable scaling. arXiv:1810.10584 Carrasquilla, Torlai, Melko, Aolita

GROUND STATES OF LOCAL HAMILTONIANS

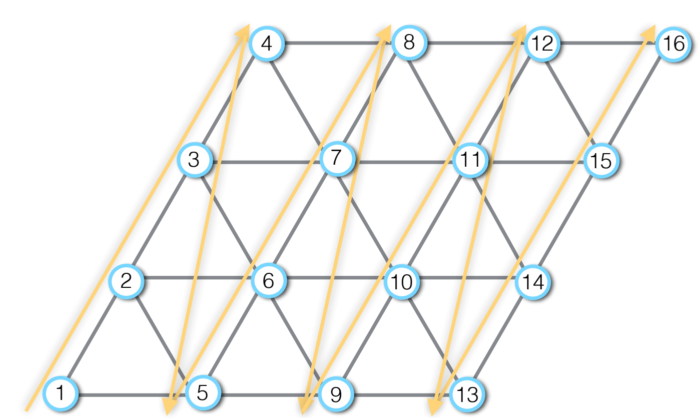


$\mathcal{H} = J \sum_{ij} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x$

N=50 spins. P(a) is a deep (3 layer GRU) recurrent neural network language model.

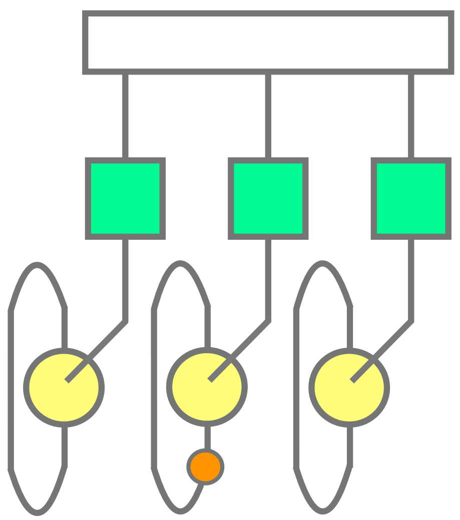


$$H = J \sum_{i,j} \boldsymbol{\sigma}_i . \boldsymbol{\sigma}_j$$

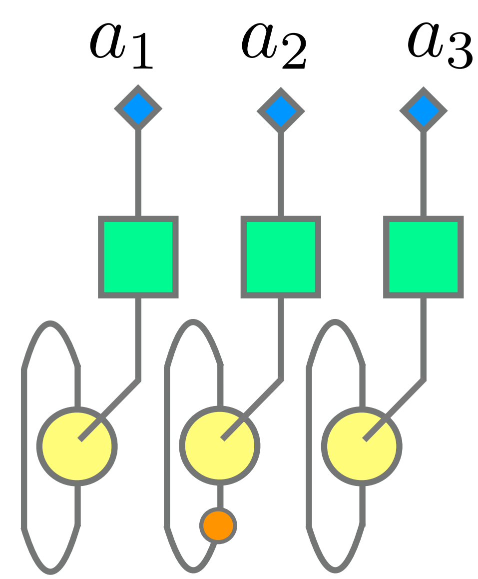


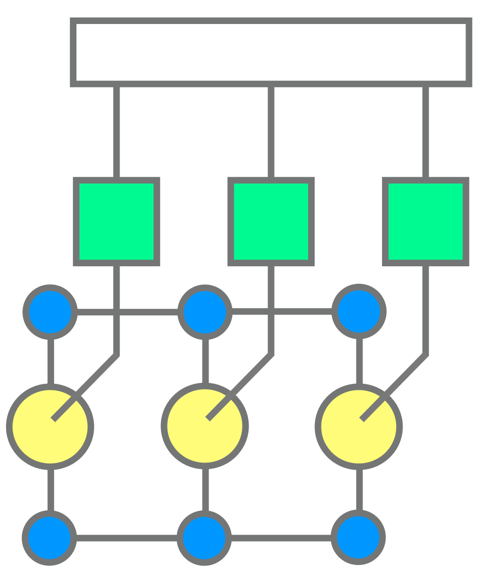
arXiv:1810.10584 Carrasquilla, Torlai, Melko, Aolita

OBSERVABLES AND FIDELITY W.R.T. AN MPS

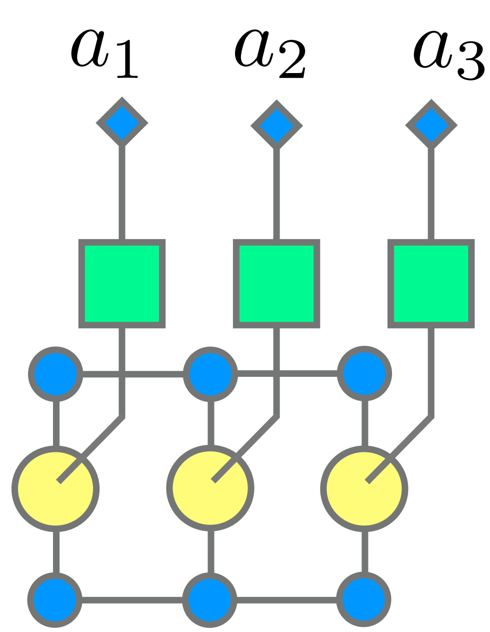


$$\approx \frac{1}{N_s} \sum_{\boldsymbol{a} \sim \boldsymbol{P}_{\mathrm{model}}}$$





$$\approx \frac{1}{N_s} \sum_{\boldsymbol{a} \sim \boldsymbol{P}_{\mathrm{model}}}$$

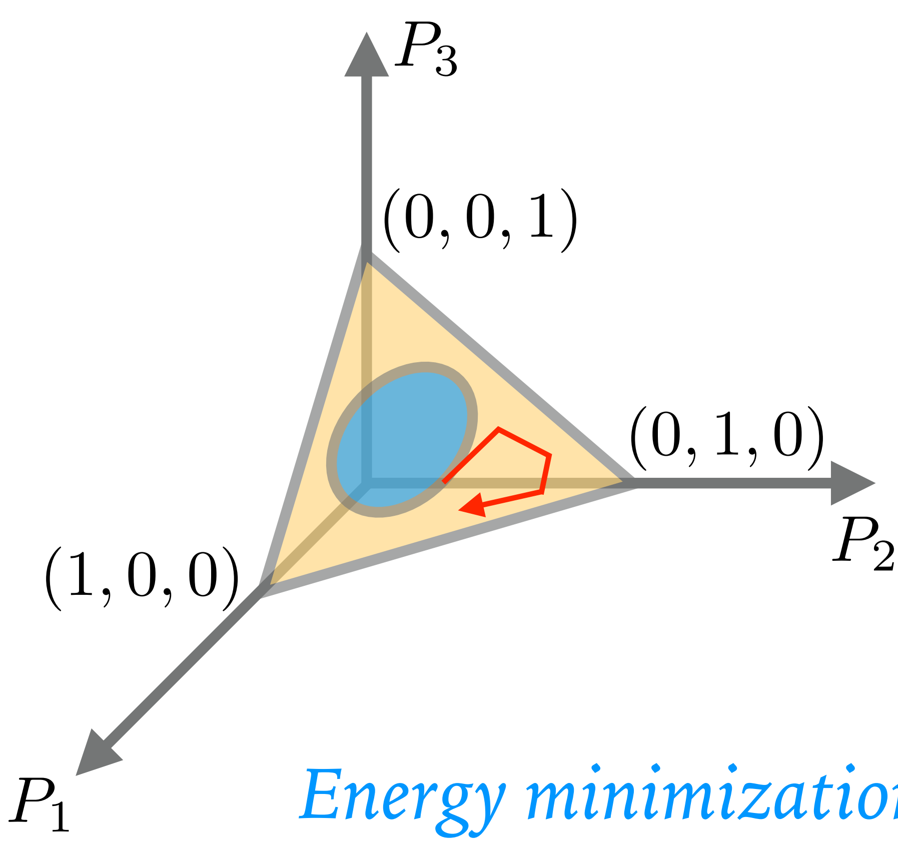


REGULARIZATION ISSUES

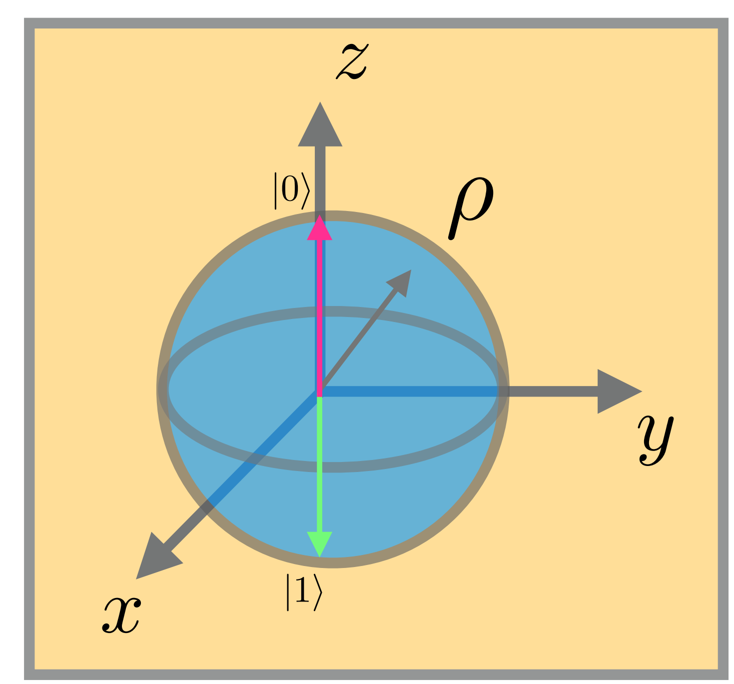
Requisite to specifying a quantum state through P(a), one must have an understanding of the allowed probabilities since not every choice of P(a) will give rise to positive semi-definite density matrix.

Requires regularization that is tricky to perform for large systems

For this tomography problem in particular we just use a lot of data



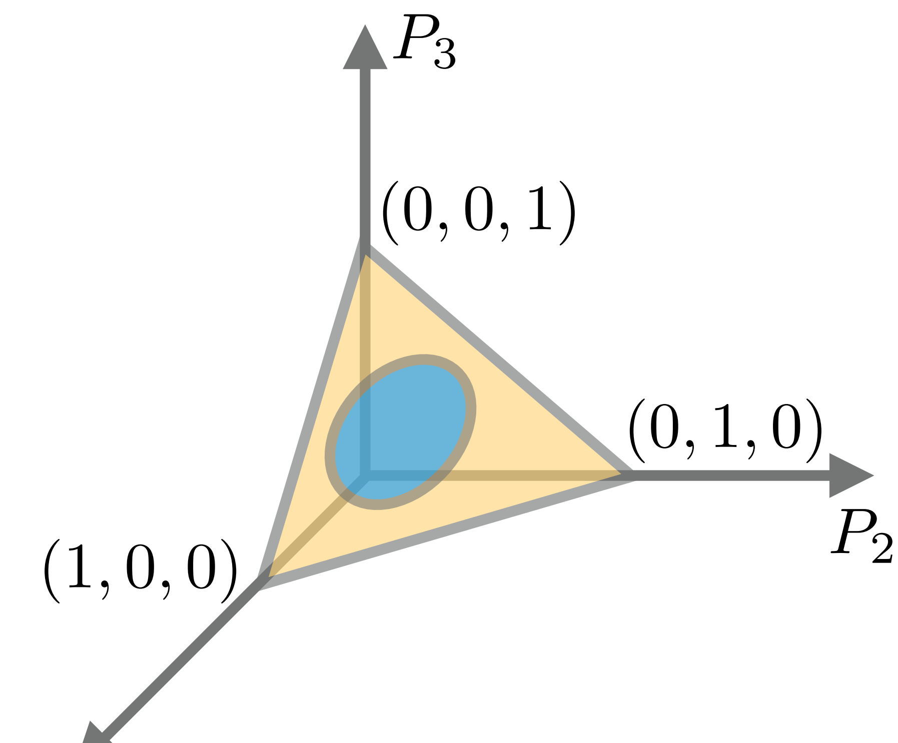
$$\rho = \sum_{a,a'} T^{-1}_{a,a'} P(a') M^{(a)}$$



Energy minimization is not variational. How to fix this?

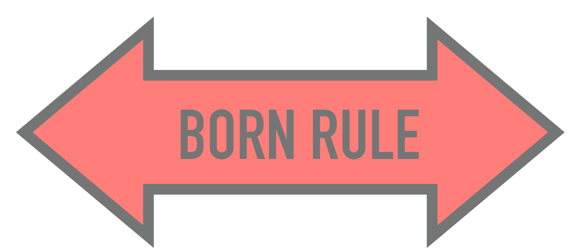
THE STANDARD SIMPLEX AND QUANTUM STATES

In probability, the points of the standard *n*-simplex in (*n* + 1)-space are the space of possible parameters (probabilities) of the categorical distribution on *n* + 1 possible outcomes.

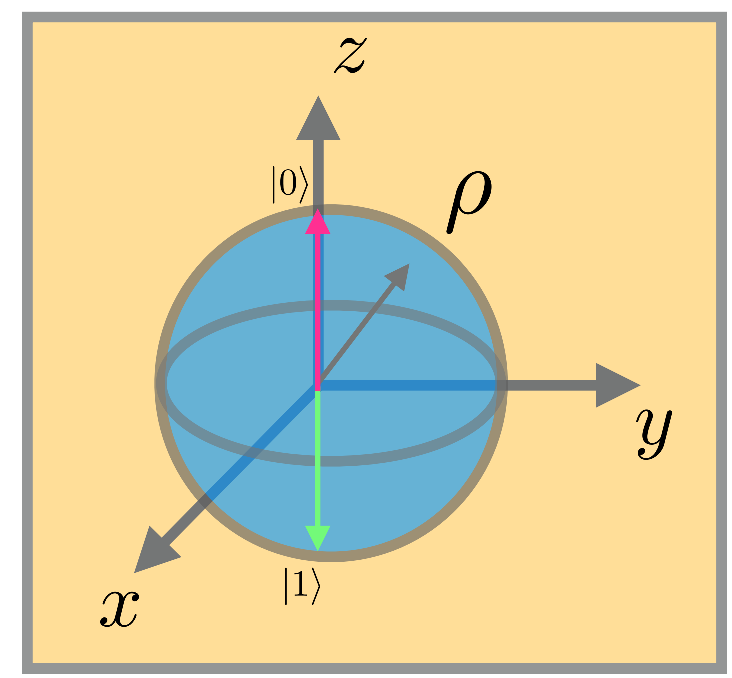


$$P_1 + P_2 + P_3 = 1$$

$$P\left(\mathbf{a}\right) = \mathrm{Tr}\, \rho M^{\mathbf{a}}$$



$$\rho = \sum_{a,a'} T^{-1}_{a,a'} P(a') M^{(a)}$$



$\{x \in \mathbb{R}^{k+1} : x_0 + x_1 + \ldots + x_k = 1, x_i \geq 0, i = 0, 1, \ldots k\}$ "All convex bodies behave a bit like Euclidean balls." Keith Ball

THE STANDARD SIMPLEX AND QUANTUM STATES

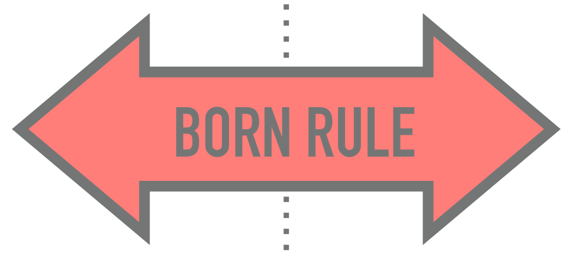
$$i\frac{\partial P(\mathbf{a}'')}{\partial t} = \sum_{\mathbf{a},\mathbf{a}'} T^{-1}_{\mathbf{a},\mathbf{a}'} P(\mathbf{a}') \mathrm{Tr}\left([H, M^{(\mathbf{a}'')}]\right)$$

$$P_U(\mathbf{a}'') = \sum_{\mathbf{a}'} P(\mathbf{a}') O_{\mathbf{a}',\mathbf{a}''}$$

$$O_{\mathbf{a}'\mathbf{a}''} = \sum_{\mathbf{a}} \mathrm{Tr}(U M^{(\mathbf{a})} U^\dagger M^{(\mathbf{a}'')}) T^{-1}_{\mathbf{a},\mathbf{a}'}$$

$$i\frac{\partial \rho}{\partial t} = [H, \rho]$$

$$\rho_U = U \rho U^\dagger$$



Unitary matrices U

Generalization of stochastic matrices:

Somewhat stochastic matrices:

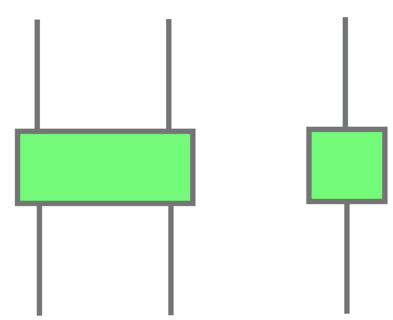
https://arxiv.org/abs/0709.0309

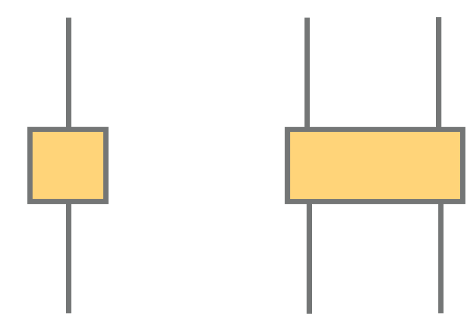
Somewhat stochastic matrices

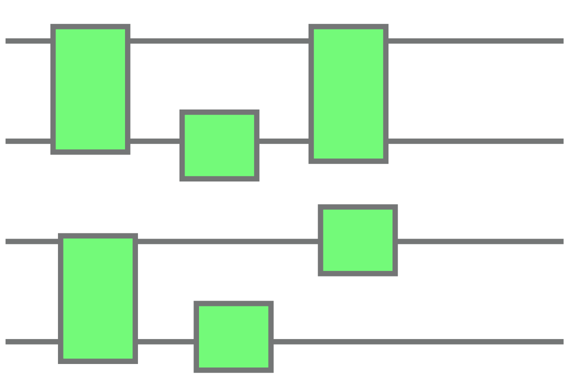
Branko Ćurgus, Robert I. Jewett

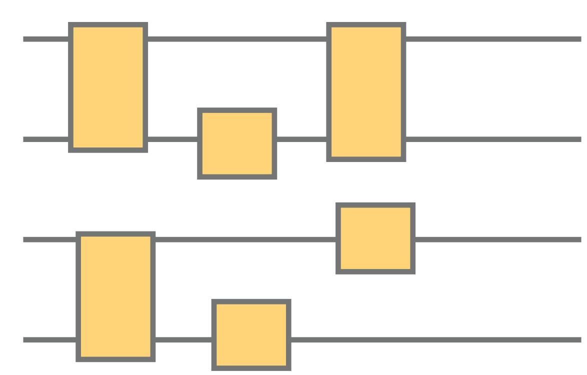
(Submitted on 3 Sep 2007)

The standard theorem for regular stochastic matrices is generalized to matrices with no sign restriction on the entries. The condition that column sums be equal to 1 is kept, but the regularity condition is replaced by a condition on the ℓ_1-distances between columns.





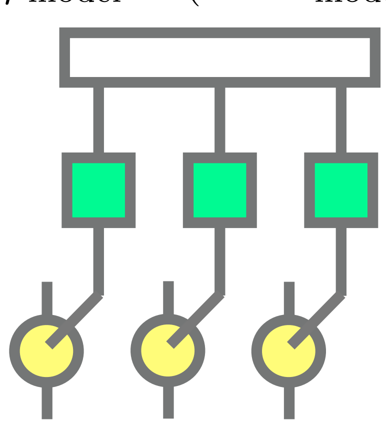




CONCLUSION

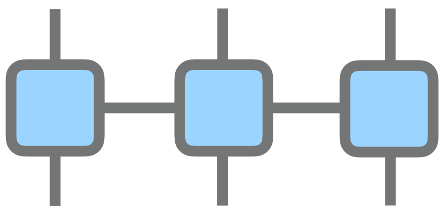
- We are starting to explore a machine learning perspective on many-body problems in classical and quantum physics.
- We have performed QST based on neural networks which enable us to study of 2- and potentially 3-dimensional quantum systems and quantum devices
- I believe there are a lot of opportunities for us physicists.
  ⟨ PHYSICS | MACHINE LEARNING ⟩

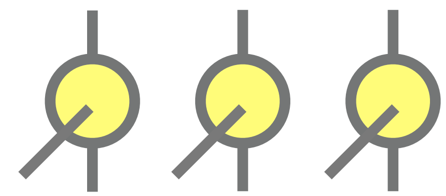
$$\rho_{\text{model}} = (\mathbf{T}^{-1} P_{\text{model}})^T \mathbf{M}$$



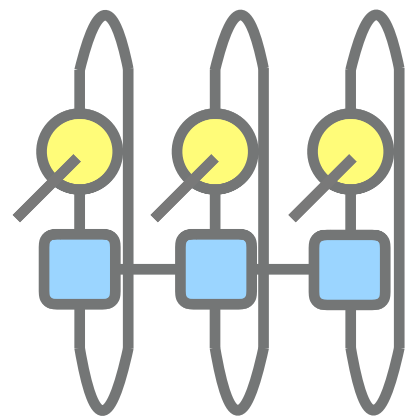
FOR LARGER GHZ STATES USE MPS/MPO

GENERATING **SYNTHETIC** DATA FOR BIG SYSTEMS EFFICIENTLY USING TENSOR NETWORKS

ρ 

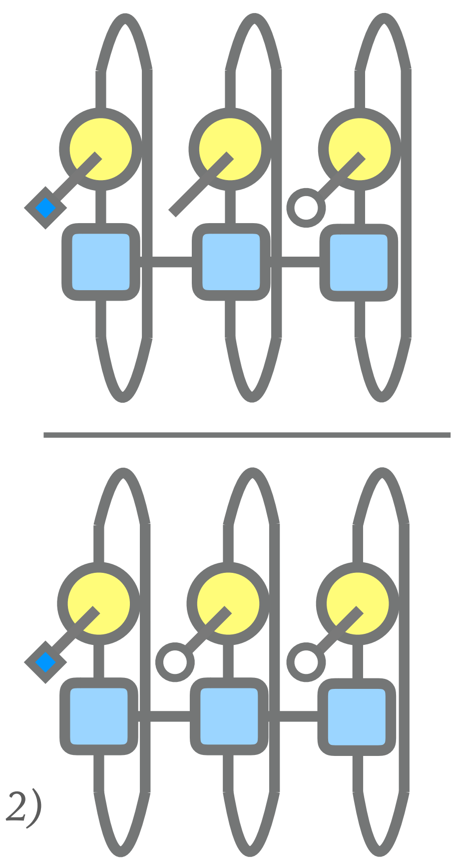
$\mathbf{M}$ 

$$P\left(\mathbf{a}\right) = \mathrm{Tr}\, \rho M^{\mathbf{a}}$$



Can be sampled in polynomial time exactly (zipper algorithm)

$$P(a_i|a_{<i}) = \frac{\sum_{a_{j>i}} P(\mathbf{a})}{\sum_{a_{j\geq i}} P(\mathbf{a})}$$

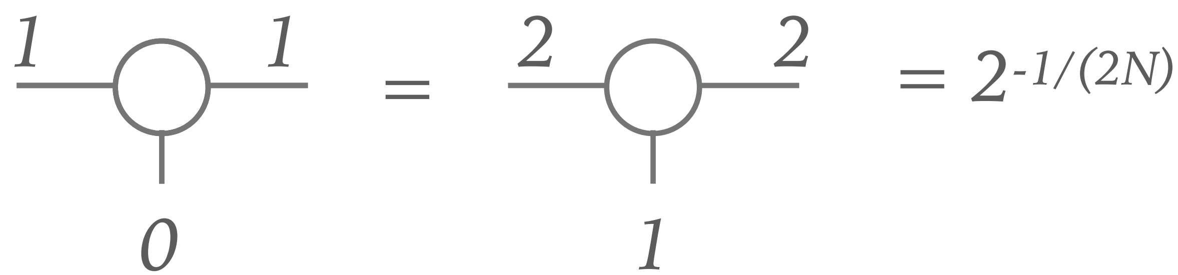


$$P(a_2|a_1)$$

AJ Ferris and G. Vidal. PRB 85, 165146 (2012)

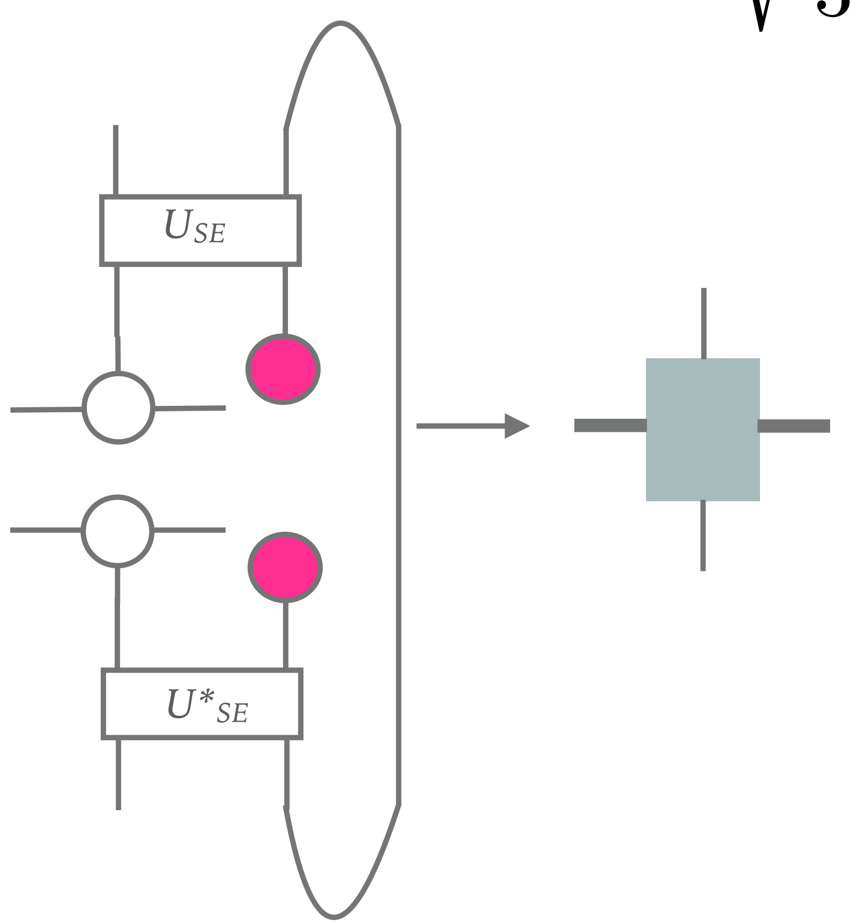
FOR LARGER GHZ STATES USE MPS/MPO

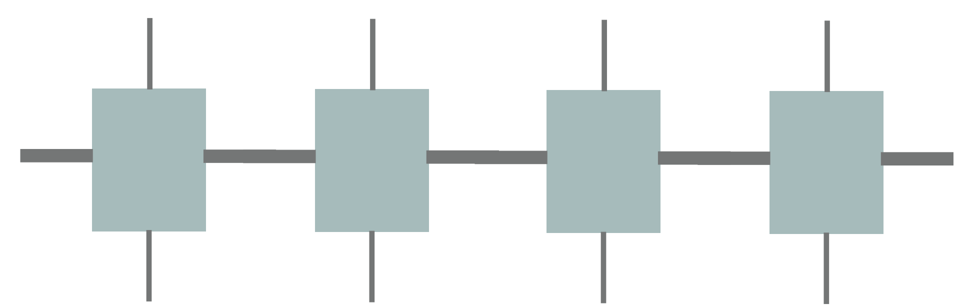
Pure GHZ = MPS



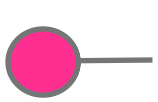
Locally depolarized GHZ

$$U_{SE} = \mathbb{1}_S \otimes |0\rangle\langle 0|_E + \sqrt{\frac{p}{3}}\,(\sigma^x_S \otimes |1\rangle\langle 0|_E + \sigma^y_S \otimes |2\rangle\langle 0|_E + \sigma^z_S \otimes |3\rangle\langle 0|_E)$$





Locally depolarized GHZ = MPO

 = (1 0 0 0)

Preskill's notes http://www.theory.caltech.edu/people/preskill/ph219/

DEPOLARIZING CHANNEL

3.4.1 Depolarizing channel

The *depolarizing channel* is a model of a decohering qubit that has particularly nice symmetry properties. We can describe it by saying that, with probability $1-p$ the qubit remains intact, while with probability p an "error" occurs. The error can be of any one of three types, where each type of error is equally likely. If $\{|0\rangle, |1\rangle\}$ is an orthonormal basis for the qubit, the three types of errors can be characterized as:

1. Bit flip error: $\begin{smallmatrix}|0\rangle\mapsto|1\rangle\\|1\rangle\mapsto|0\rangle\end{smallmatrix}$ or $|\psi\rangle \mapsto \boldsymbol{\sigma}_1|\psi\rangle, \boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$,

2. Phase flip error: $\begin{smallmatrix}|0\rangle\mapsto|0\rangle\\|1\rangle\mapsto-|1\rangle\end{smallmatrix}$ or $|\psi\rangle \mapsto \boldsymbol{\sigma}_3|\psi\rangle, \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$,

3. Both: $\begin{smallmatrix}|0\rangle\mapsto+i|1\rangle\\|1\rangle\mapsto-i|0\rangle\end{smallmatrix}$ or $|\psi\rangle \mapsto \boldsymbol{\sigma}_2|\psi\rangle, \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

If an error occurs, then $|\psi\rangle$ evolves to an ensemble of the three states $\boldsymbol{\sigma}_1|\psi\rangle, \boldsymbol{\sigma}_2|\psi\rangle, \boldsymbol{\sigma}_3|\psi\rangle$, all occurring with equal likelihood.

Unitary representation. The depolarizing channel mapping qubit A to A can be realized by an isometry mapping A to AE, where E is a four-dimensional environment, acting as

$$\begin{aligned} \boldsymbol{U}_{A\to AE} : |\psi\rangle_A \mapsto & \sqrt{1-p}\ |\psi\rangle_A \otimes |0\rangle_E \\ & + \sqrt{\frac{p}{3}} \left(\boldsymbol{\sigma}_1|\psi\rangle_A \otimes |1\rangle_E + \boldsymbol{\sigma}_2|\psi\rangle_A \otimes |2\rangle_E + \boldsymbol{\sigma}_3|\psi\rangle_A \otimes |3\rangle_E \right). \end{aligned} \tag{3.83}$$

Preskill's notes http://www.theory.caltech.edu/people/preskill/ph219/

NEUMARK'S DILATION THEOREM

How one can implement a general quantum measurement by performing a unitary on the system of interest and an ancilla, followed by a von Neumann measurement of the ancilla.

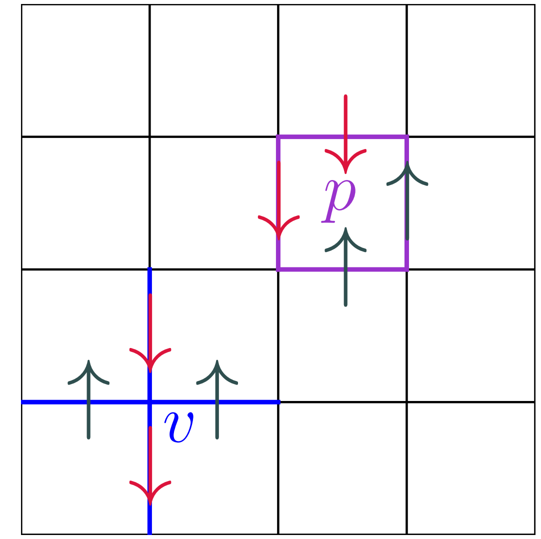
$$P(a) = \mathrm{Tr}\rho M^{(a)} = \mathrm{Tr}\left[\mathbf{I}_s \otimes |a\rangle\langle a|_p U_{sp}\rho \otimes |0\rangle\langle 0|_p U_{sp}^\dagger\right]$$

- Requires projective measurements in only one basis set

Experimental schemes see: Phys. Rev. A 86, 062107 (2012), Phys. Rev. A 83, 051801(R) (2011), Phys. Rev. A 91, 042101 (2015)

KITAEV'S QUANTUM ERROR CORRECTING CODE WITH CONVOLUTIONAL NEURAL NETWORKS

KITAEV'S TORIC CODE GROUND STATE

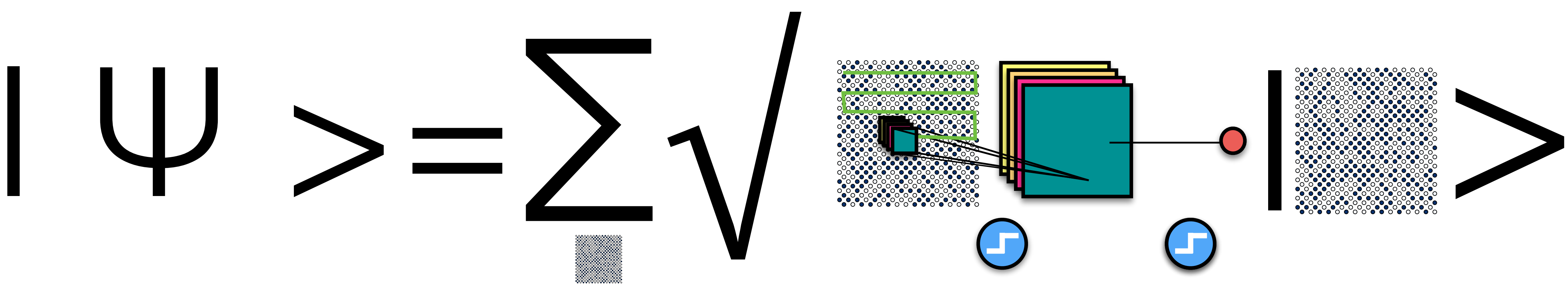


$$H = -J_p \sum_p \prod_{i\in p} \sigma_i^z - J_v \sum_v \prod_{i\in v} \sigma_i^x$$

$$|\Psi_{\mathrm{TC}}\rangle \propto \lim_{\beta\to\infty} \sum_{\sigma_1,\ldots,\sigma_N} e^{\frac{\beta}{2} J \sum_p \prod_{i\in p} \sigma_i^z} |\sigma_1, \ldots, \sigma_N\rangle$$

PEPS : *F. Verstraete, M. M. Wolf, D. Perez-Garcia, J. I. Cirac Phys. Rev. Lett. 96, 220601 (2006).*

$$O_{\mathrm{cold}}(\sigma_1, \ldots, \sigma_N) \propto \lim_{\beta\to\infty} \exp \beta J \sum_p \prod_{i\in p} \sigma_i^z$$



J. Carrasquilla and R. G. Melko. Nature Physics 13, 431–434 (2017)
Dong-Ling Deng et al Phys. Rev. X 7, 021021 (2017)
Jing Chen, Song Cheng, Haidong Xie, Lei Wang, Tao Xiang arXiv:1701.04831 RBMs

SYNTHETIC QUANTUM DEVICES ARE GROWING FAST

nature
International journal of science

Letter | Published: 22 August 2018

Observation of topological phenomena in a programmable lattice of 1,800 qubits

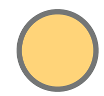
Andrew D. King, Juan Carrasquilla, […] Mohammad H. Amin

Nature **560**, 456–460 (2018) | Download Citation

- "These are really rather beautiful pieces of science," says physicist Seth Lloyd of MIT
- "This work presents the cleanest data for a KT transition that I have seen in any quantum simulator to date. It is the most advanced use I have to date seen of a superconducting quantum simulator." Matthias Troyer of ETH and Microsoft
- "This paper represents a breakthrough in the simulation of physical systems which are otherwise essentially impossible," said 2016 Nobel laureate Dr. J. Michael Kosterlitz.
- "**They haven't addressed at all whether it's a quantum system they've got,**" says physicist Graeme Smith of the JILA research center in Boulder

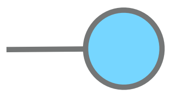
NOTATION SLIDE

S



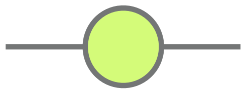
Scalar

V_i



Vector

$W_{i,j}$



Matrix

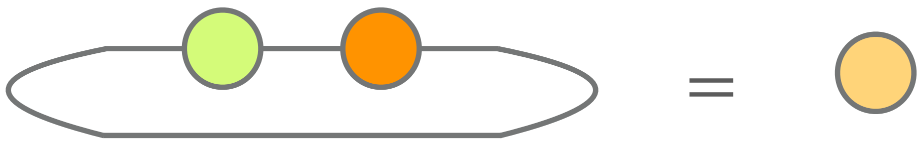
$$C_k = \sum_j W_{k,j} V_j$$

Matrix vector Multiplication

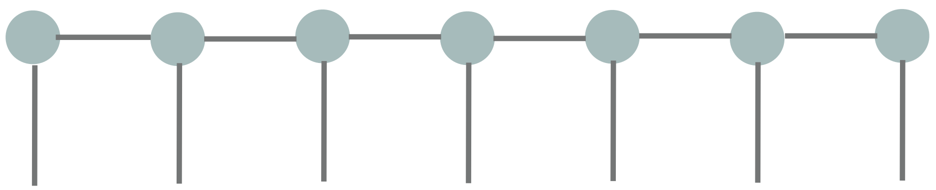
$$|C|^2 = \sum_k C_k C_k^*$$

norm

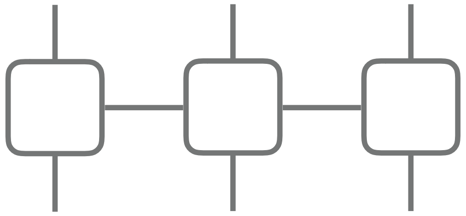
$$\text{Tr } W M = \sum_{k,j} W_{k,j} M_{j,k}$$



Matrix Product States (MPS)



Matrix Product Operators (MPO)



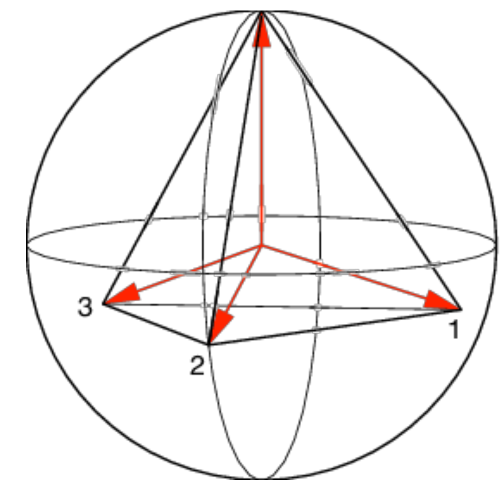
MEASUREMENTS: POSITIVE OPERATOR VALUED MEASURES (POVM)

CONSTRUCTING POVMS: TAKE A SINGLE QUBIT POVM AND MAKE A TENSOR PRODUCT OF MANY

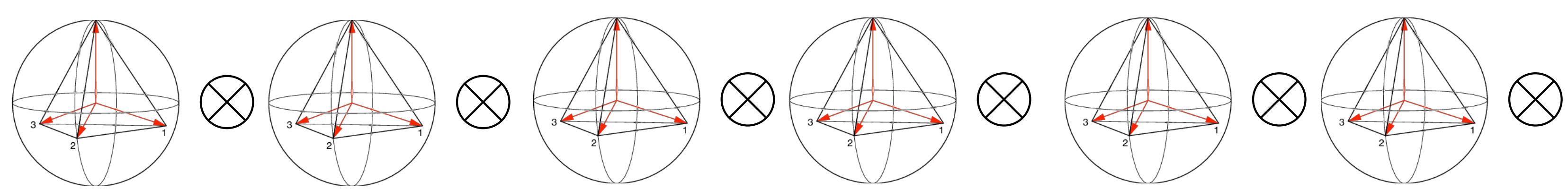
Tetrahedral measurement for one qubit

$$M^{(i)} = \frac{1}{4}\left(\mathbb{1} + \boldsymbol{s}^{(i)} \cdot \boldsymbol{\sigma}\right), \quad i = 1, \ldots, 4$$

$$\mathbf{s}^{(1)} = (0,0,1)\,,\ \mathbf{s}^{(2)} = \left(\frac{2\sqrt{2}}{3}, 0, -\frac{1}{3}\right),\ \mathbf{s}^{(3)} = \left(-\frac{\sqrt{2}}{3}, \sqrt{\frac{2}{3}}, -\frac{1}{3}\right),\ \mathbf{s}^{(4)} = \left(-\frac{\sqrt{2}}{3}, -\sqrt{\frac{2}{3}}, -\frac{1}{3}\right)$$



For multiqubit systems



$$\boldsymbol{M} = \left\{M^{(a_1)} \otimes M^{(a_2)} \otimes \ldots M^{(a_N)}\right\}_{a_1, \ldots a_N}$$

Experimental schemes see: Phys. Rev. A 86, 062107 (2012), Phys. Rev. A 83, 051801(R) (2011), Phys. Rev. A 91, 042101 (2015)

MEASUREMENTS: POSITIVE OPERATOR VALUED MEASURES (POVM)

CONSTRUCTING POVMS: TAKE A SINGLE QUBIT POVM AND MAKE A TENSOR PRODUCT OF MANY

Pauli-4 measurement for one qubit

$$\boldsymbol{M}_{\text{Pauli}-4} = \{ M^{(0)} = \frac{1}{3} \times |0\rangle\langle 0|, M^{(1)} = \frac{1}{3} \times |1\rangle\langle 1|, M^{(2)} = \frac{1}{3} \times |+\rangle\langle +|, M^{(3)} = \frac{1}{3} \times (|-\rangle\langle -| + |r\rangle\langle r| + |l\rangle\langle l|)$$

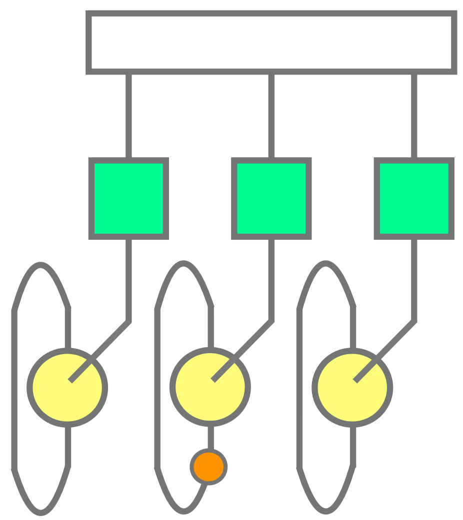
For multiqubit systems $\boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes \boldsymbol{M}_{\text{Pauli}} \otimes$

$$\boldsymbol{M} = \{ M^{(a_1)} \otimes M^{(a_2)} \otimes \ldots M^{(a_N)} \}_{a_1, \ldots a_N}$$

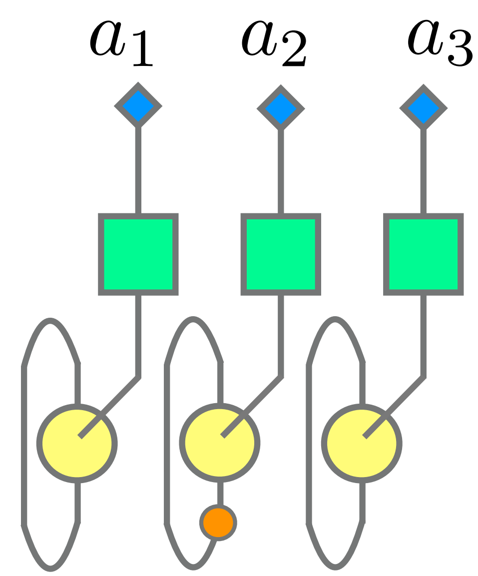
Experimental realization: pick a random direction with probability 1/3, then measure in that direction + postprocess

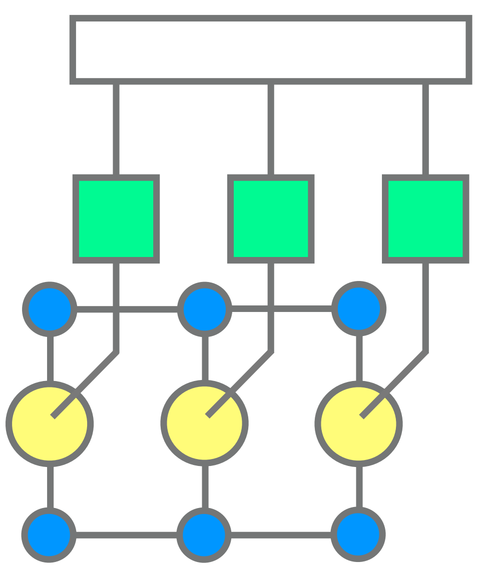
Easy to implement in gate-based QC (Qiskit, Cirq, Rigetti, etc.)

OBSERVABLES AND FIDELITY W.R.T. AN MPS



$$\approx \frac{1}{N_s} \sum_{\boldsymbol{a} \sim \boldsymbol{P}_{\text{model}}}$$





$$\approx \frac{1}{N_s} \sum_{\boldsymbol{a} \sim \boldsymbol{P}_{\text{model}}}$$