Workshop Quantum Computing @ INFN, Bologna, 15/11/2022

Entanglement entropy production in Quantum Neural Networks

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arxiv:2206.02474

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Digital quantum computing

Qubits are lines with time flowing from left to right

CNOT, apply X on crossed qubit (target) if dotted qubit (control) is in $|1\rangle$

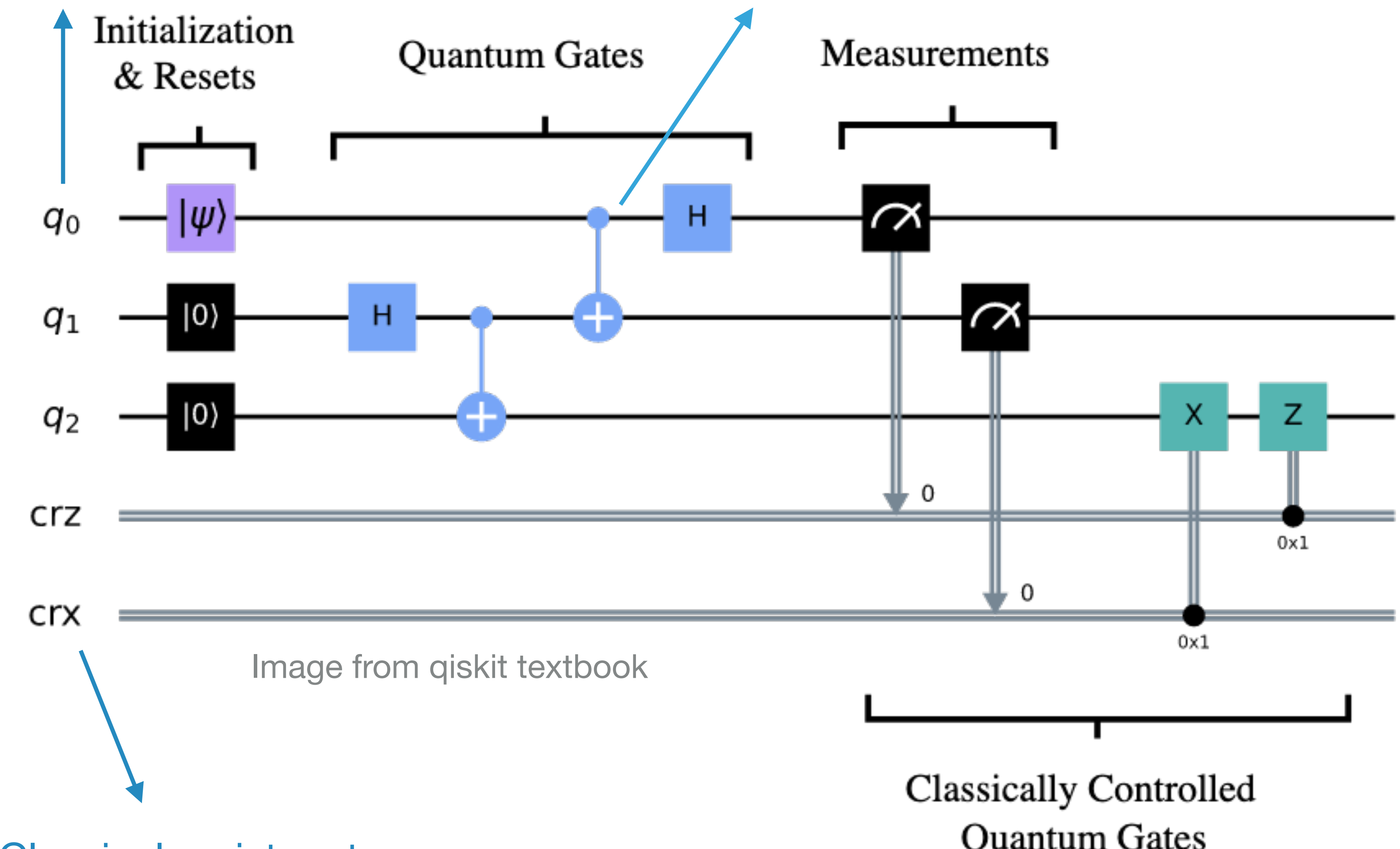


Image from qiskit textbook

Classical registers to store the results of measurements

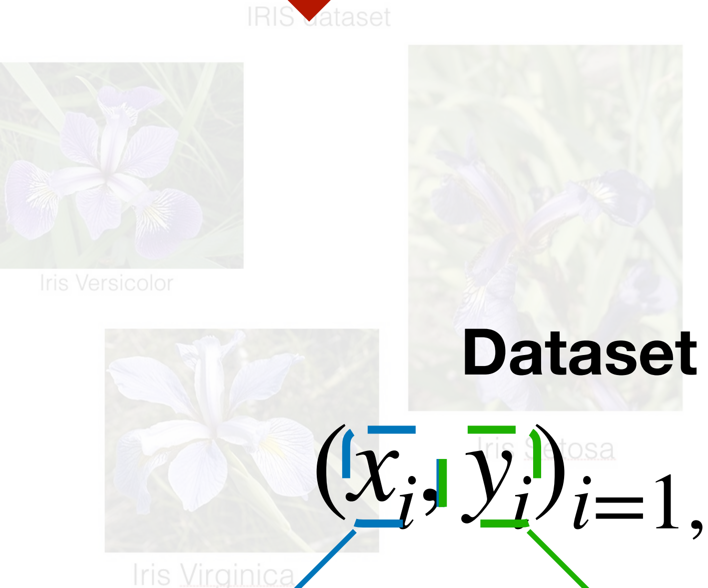
DIGITAL QUANTUM SIMULATIONS

QUANTUM ALGORITHMS

QUANTUM CHEMISTRY

QUANTUM MACHINE LEARNING

Quantum machine learning



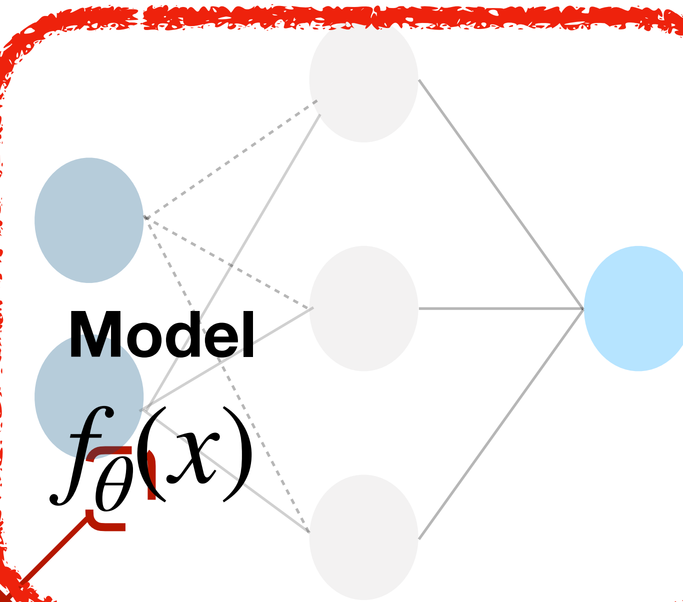
Dataset

$(x_i, y_i)_{i=1,\dots,n}$

Input features

Input class

The model is **QUANTUM**



Model

$f_\theta(x)$

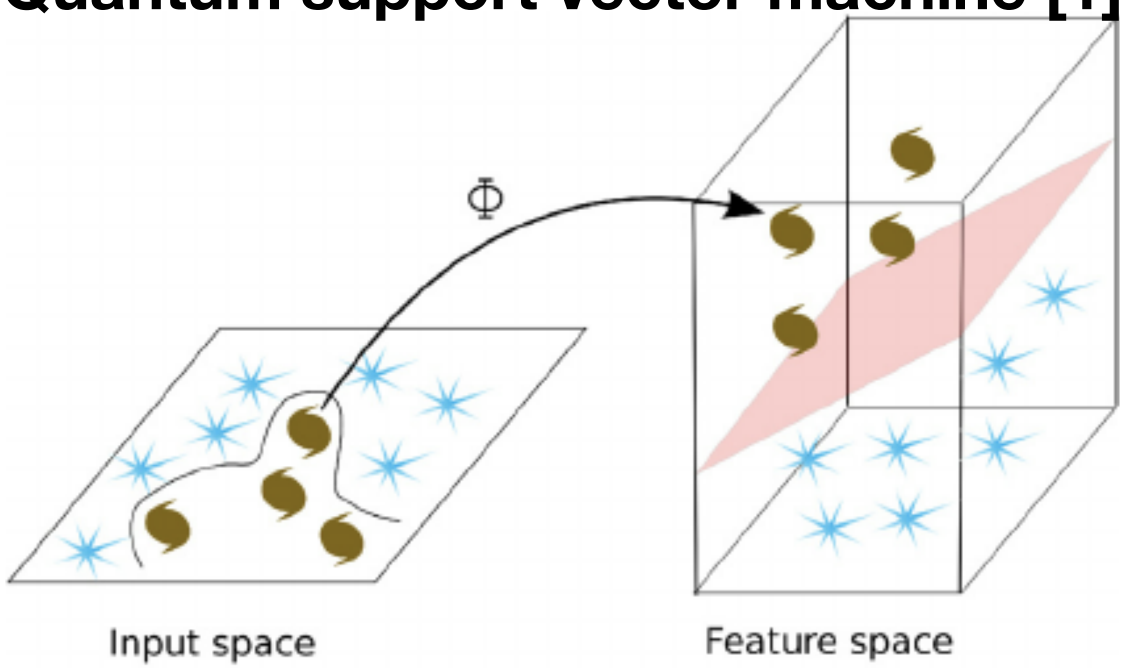
Model parameters

Update θ minimising loss function

Prediction

$f_\theta(x_i) = \tilde{y}_i$

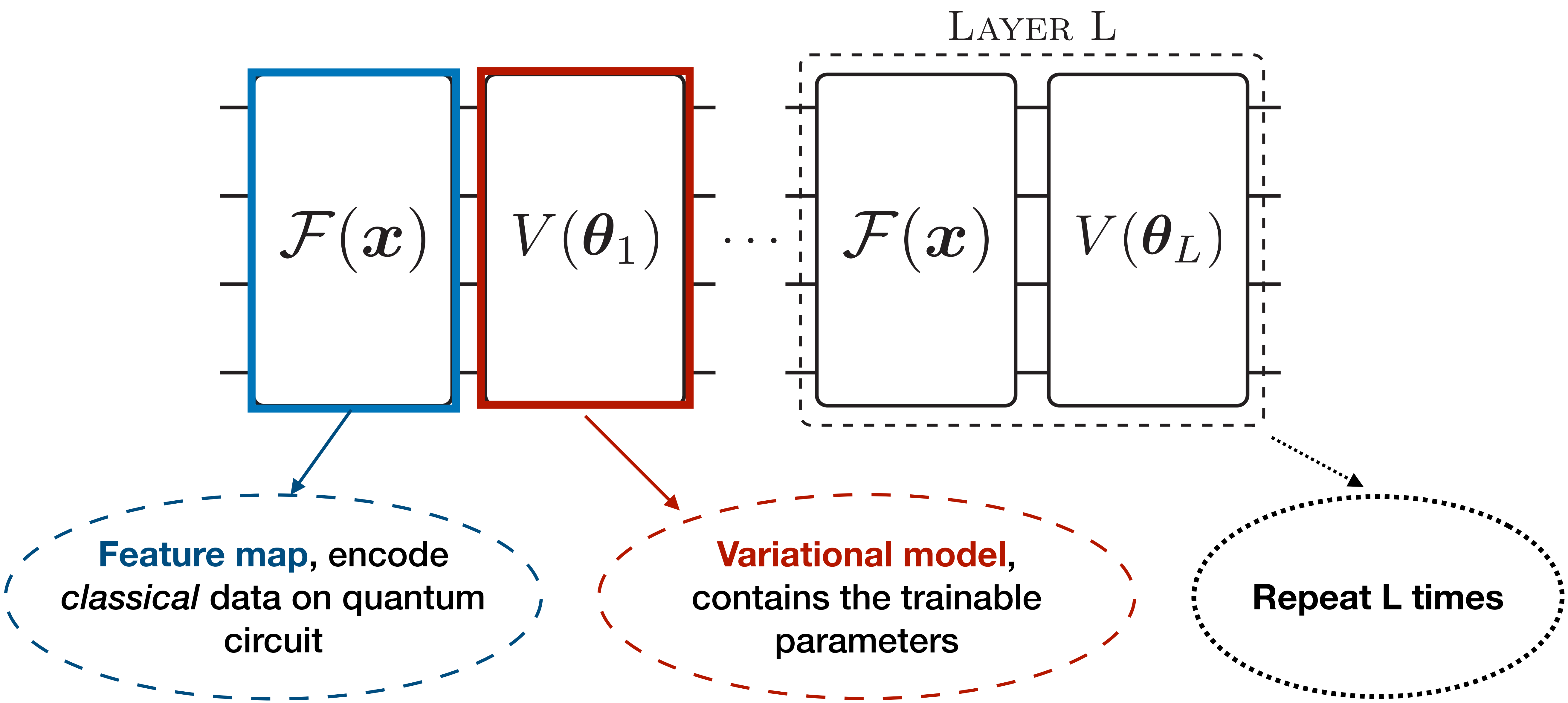
Quantum support vector machine [1]



[1] Havlíček, Vojtěch, et al. "Supervised learning with quantum-enhanced feature spaces." *Nature* 567.7747 (2019): 209-212.

Quantum neural networks

Quantum Neural networks are **variational quantum circuits**.

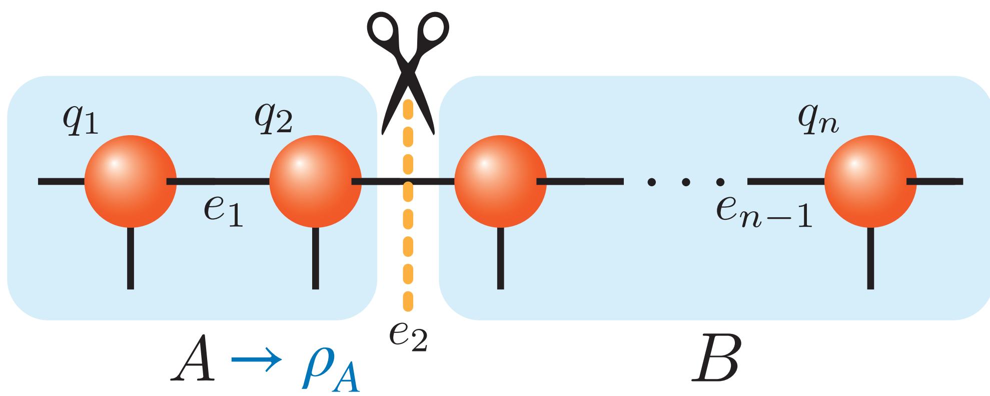


Entanglement: bless or curse?

Random states
⇒ highly entangled!
Haar-random state

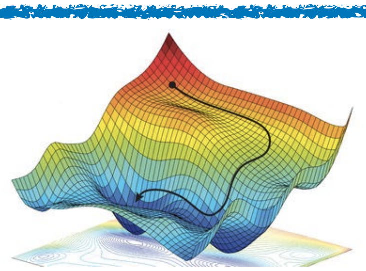
Quantum neural networks promise to be better than classical NN [3]

Entanglement

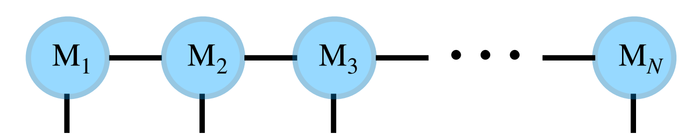


Von Neumann entanglement entropy between bipartitions A and B (across link e_i):

$$S(e_i) = -\,\mathbf{Tr}\left[\rho_A \log \rho_A\right]$$



Highly entangled states ⇒ connected with the emergence of Barren Plateaus [4]



Lowly entangled states ⇒ efficient simulations with tensor networks methods (Quantum matcha tea)

[3] Abbas, Amira, et al. "The power of quantum neural networks." *Nature Computational Science* 1.6 (2021): 403-409.
[4] Marrero, Carlos Ortiz, Mária Kieferová, and Nathan Wiebe. "Entanglement-induced barren plateaus." *PRX Quantum* 2.4 (2021): 040316.

Tensor network emulator

String compression (simple example):

AAABBCDDDDDDDD

Length: 14

Compress

A3B2C1D8

Length: 8

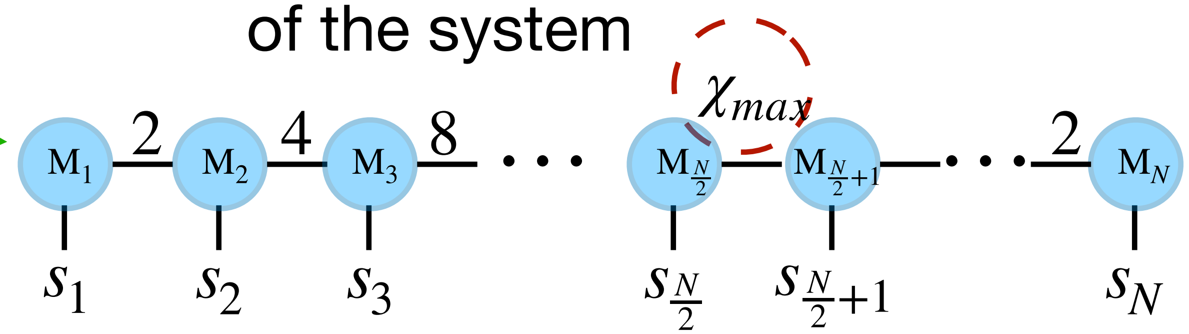
RANDOM

Compress

Tensor networks works in a similar way, but instead of being limited by the Shannon entropy of the string they are limited by the **Entanglement Entropy of the state**

Bond dimension

It controls the entanglement of the system

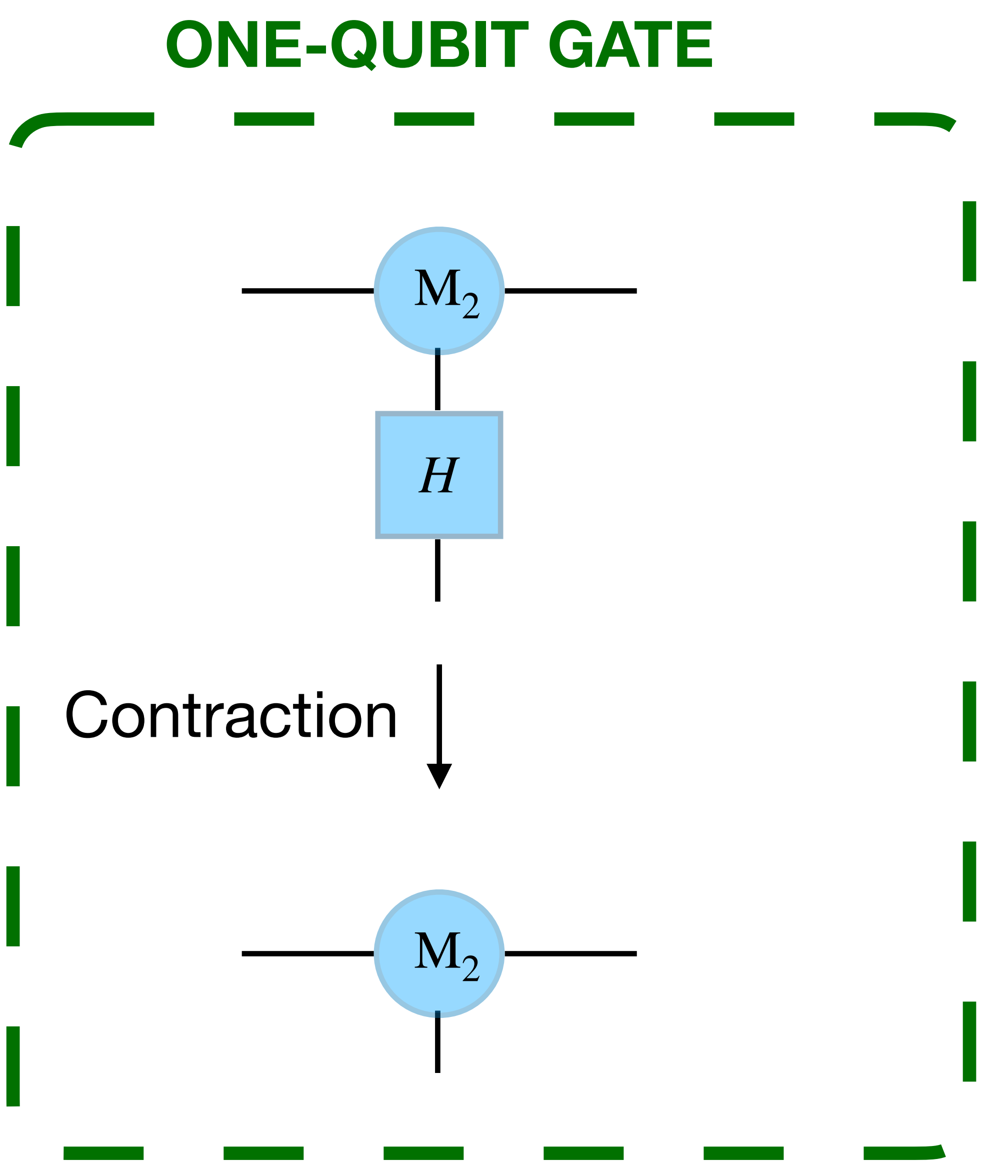


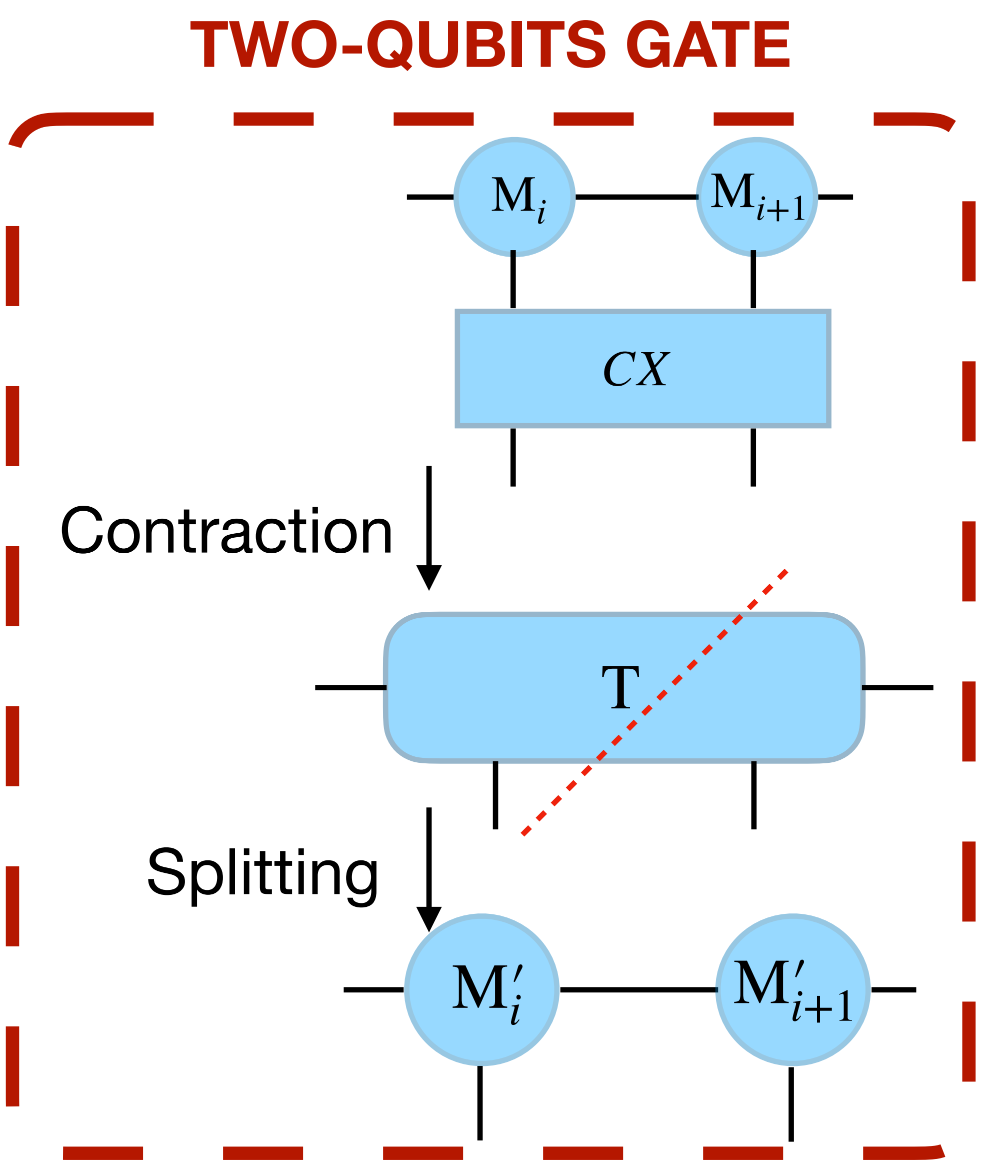
$\chi = 1$ is the Mean Field approximation

Quantum matcha tea: efficient tensor network emulator for Quantum Circuits

State Evolution

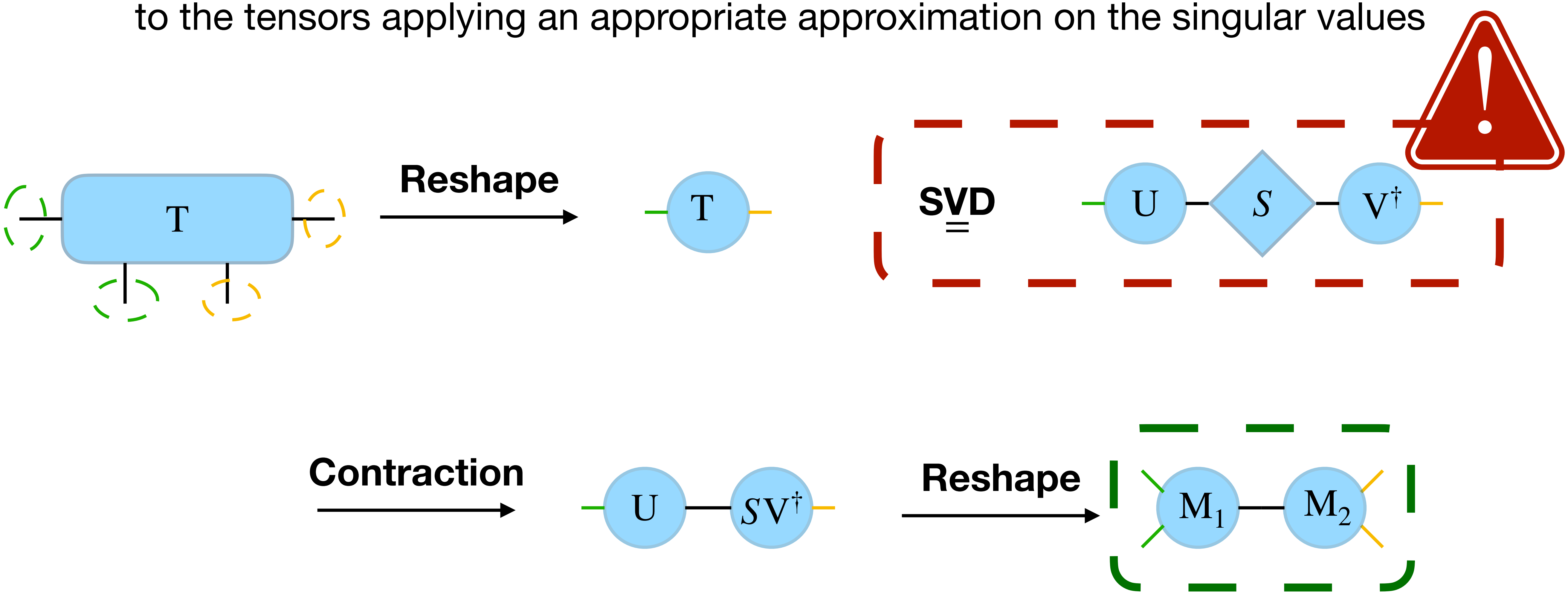
- The initial state can be described by a product state, that can be described exactly by MPS with a bond dimension $\chi = 1$.
- We then apply operators to evolve the state, bringing it into the target state $|\psi\rangle$, as we would do normally with a quantum circuit.





Singular Values Decomposition

The core of tensor networks algorithms lays in the application of SVDs
to the tensors applying an appropriate approximation on the singular values

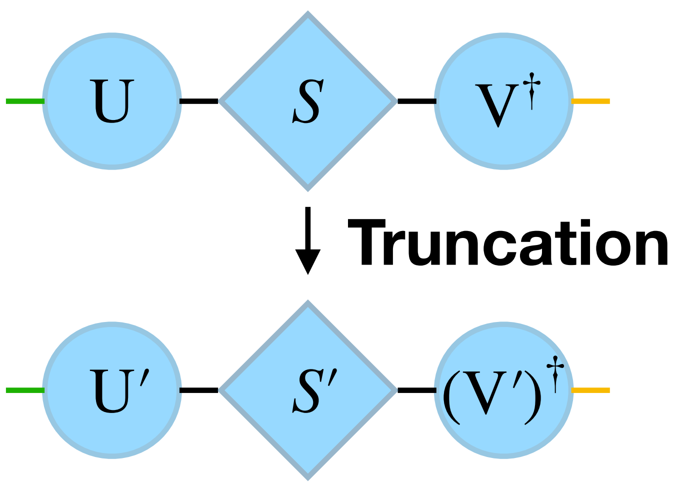


We are back to the MPS form

Truncation

This truncation after the SVD is the core of tensor networks algorithms, and enables the efficient compression of information

- We call χ_{max} **bond dimension** of the system, and denote with s_1 the greatest eigenvalue of S. Then:



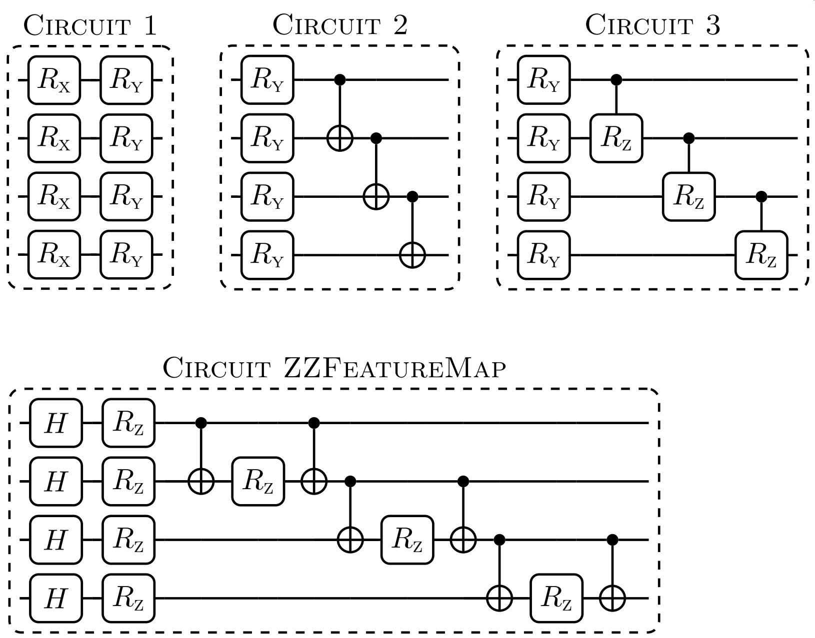
$$S' = \begin{cases} s_i & \textbf{if } \frac{s_i}{s_1} \geq \epsilon \textbf{ and } i \leq \chi_{max} \\ 0 & \textbf{otherwise} \end{cases}$$

We then truncate the 0 term

We keep the eigenvalues only if they are **big enough**. In this way, we are neglecting the sub-leading term for the state description.

We keep only the **first highest** χ_{max} eigenvalues. In this way, we keep the quantum state manageable even for big number of qubits. However, this may be a strong approximation.

Methods

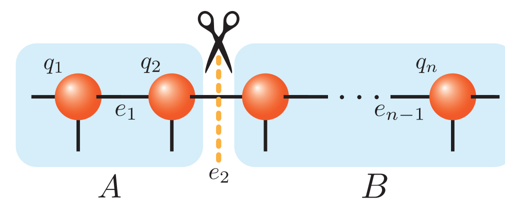


Pick a feature map $\mathscr{F}(x)$
and a variational ansatz $V(\theta)$

Select number of layers L

Sample parameters
$x_i, \theta_i \sim \text{Unif}(0,\pi)$

If L is big enough we create a Haar-random state



Simulate the evolution and compute final state

Compute entanglement on each edge e_i

Repeat M times and take the average over the realisations

Qiskit up to ~ 16 qubits with state vector

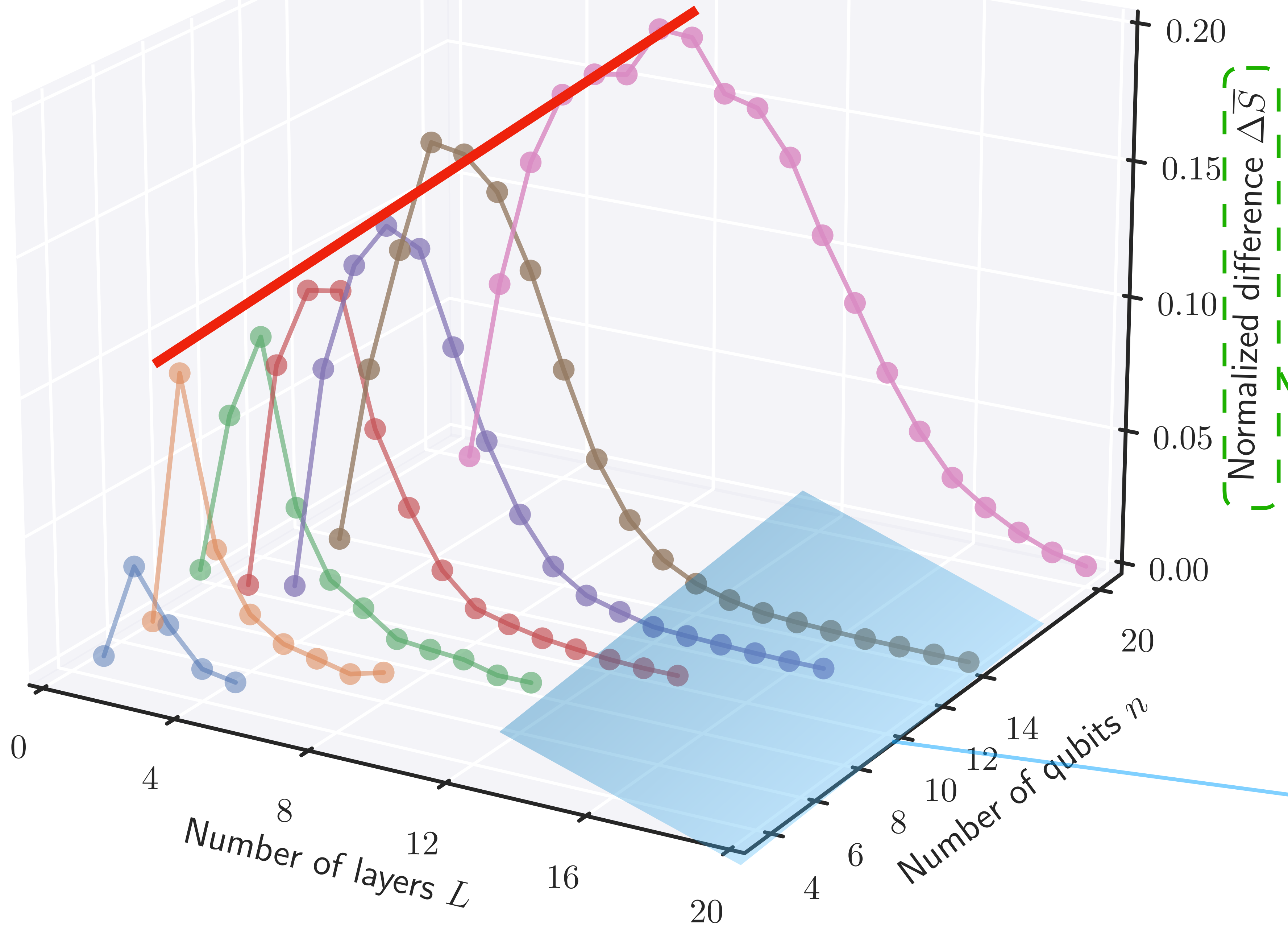
Qiskit

Efficient simulation

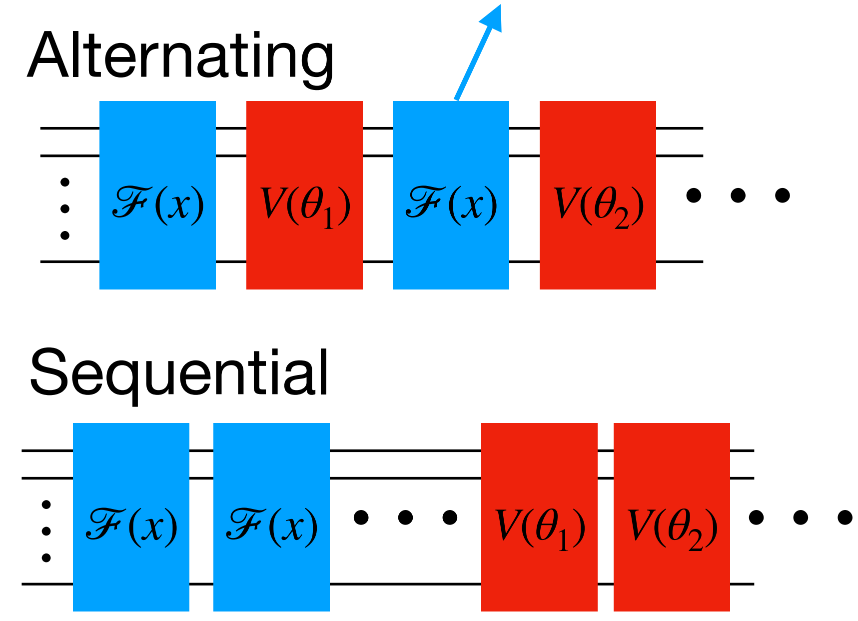
Quantum matcha tea
Tensor network emulator
up to 50 qubits

Alternating VS sequential

Significative difference that increases with the number of qubits n, up to almost $20\ \%$ for $n = 20$



Data re-uploading [5]



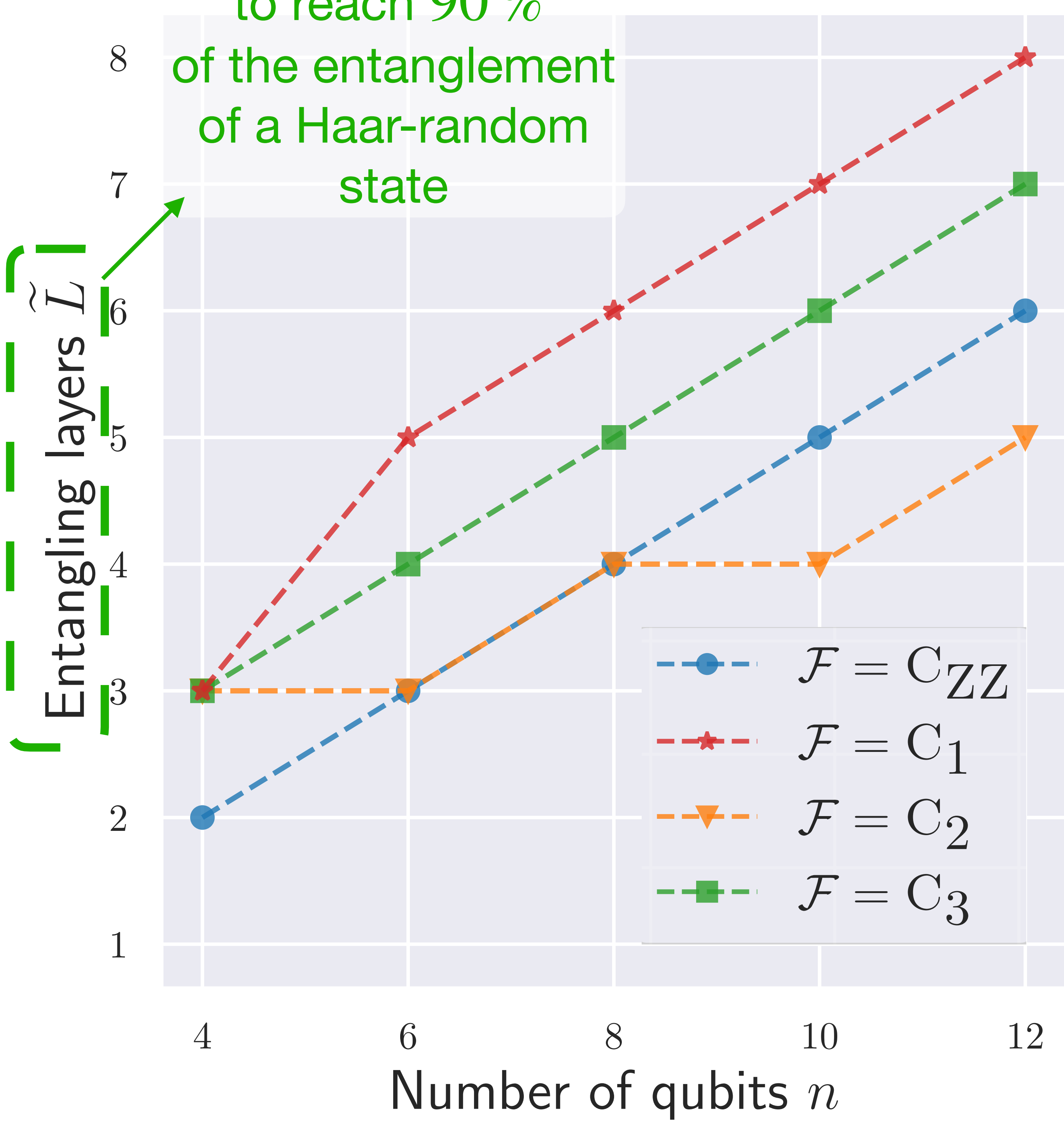
$$\Delta\bar{S} = \frac{S^{alt} - S^{seq}}{(S^{alt} + S^{seq})/2}$$

Both tends towards Haar-random

[5] Pérez-Salinas, Adrián, et al. "Data re-uploading for a universal quantum classifier." *Quantum* 4 (2020): 226.

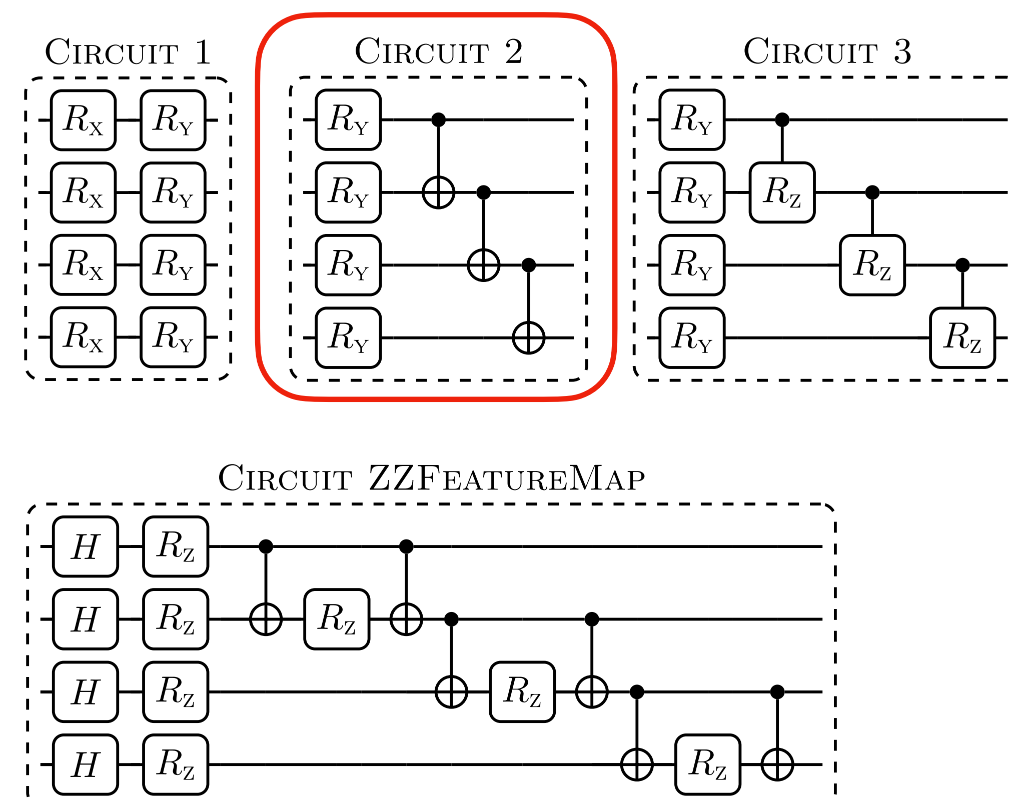
Entanglement scaling with depth

Layers needed
to reach $90\ \%$
of the entanglement
of a Haar-random
state



Number of layers
scales **linearly** with
number of qubits n
to reach Haar-random state

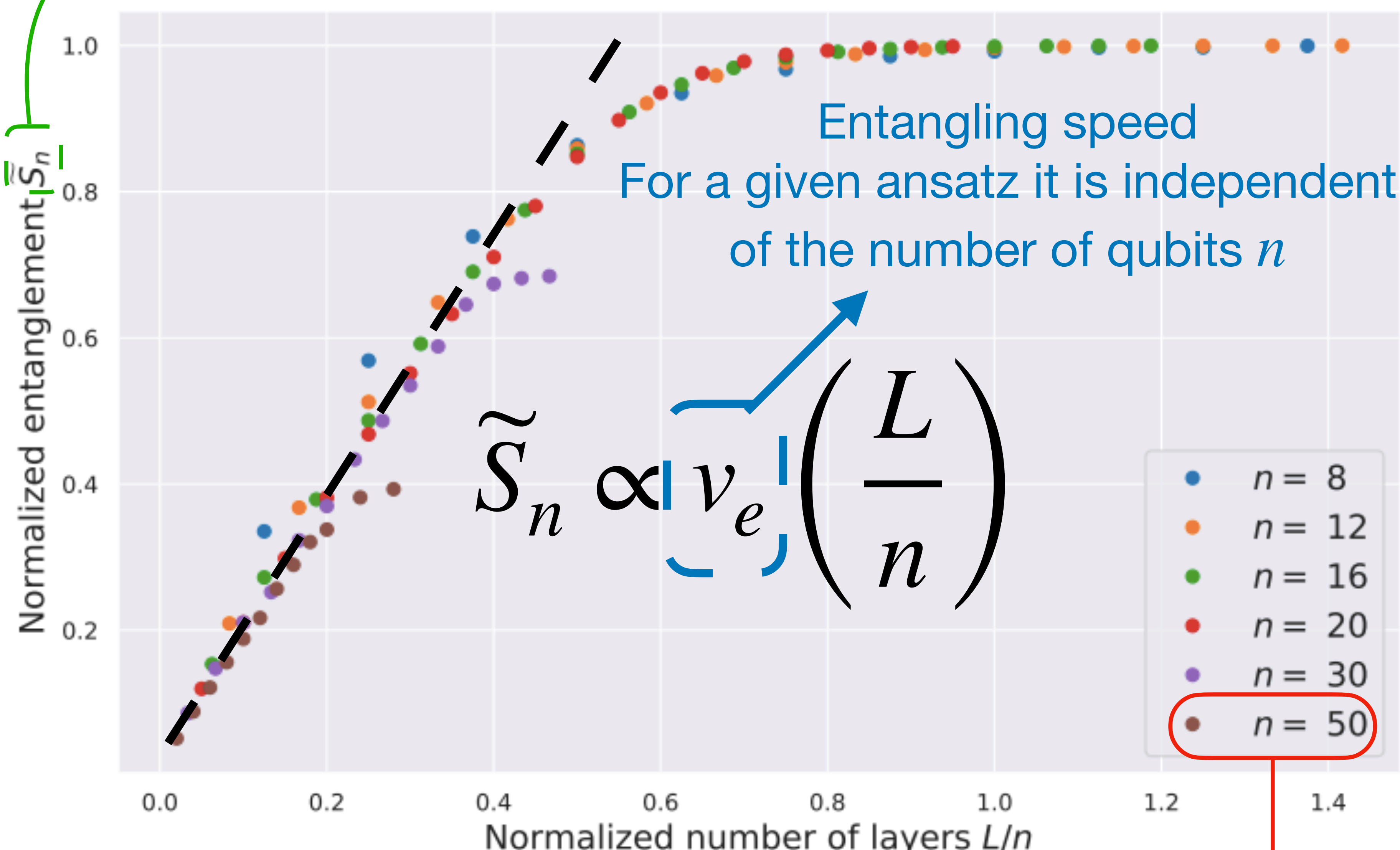
C_2 is always used as
variational ansatz



Entangling speed

$$\widetilde{S}_n = \frac{\mathbf{max}_{e_i}\left[S(e_i)\right]}{S^{Haar}_{n,max}}$$

Maximum entanglement of the chain normalised by the maximum entanglement of a Haar-random state



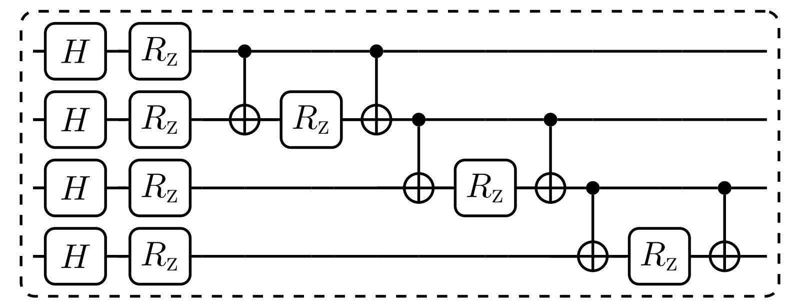
Entangling speed

For a given ansatz it is independent of the number of qubits n

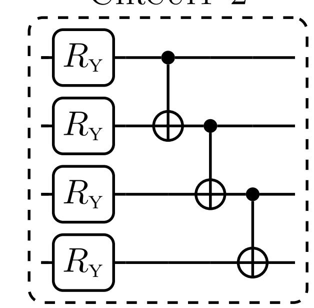
$$\widetilde{S}_n \propto v_e\left(\frac{L}{n}\right)$$

Using Galileo100 HPC from CINECA

Circuit ZZFeatureMap



Circuit 2



Feature map	Variational Ansatz	Entangling speed
C_{zz}	C_2	(1.8 ± 0.1)
C_{zz}	C_3	(0.59 ± 0.02)
C_1	C_3	(0.316 ± 0.006)

Expressibility

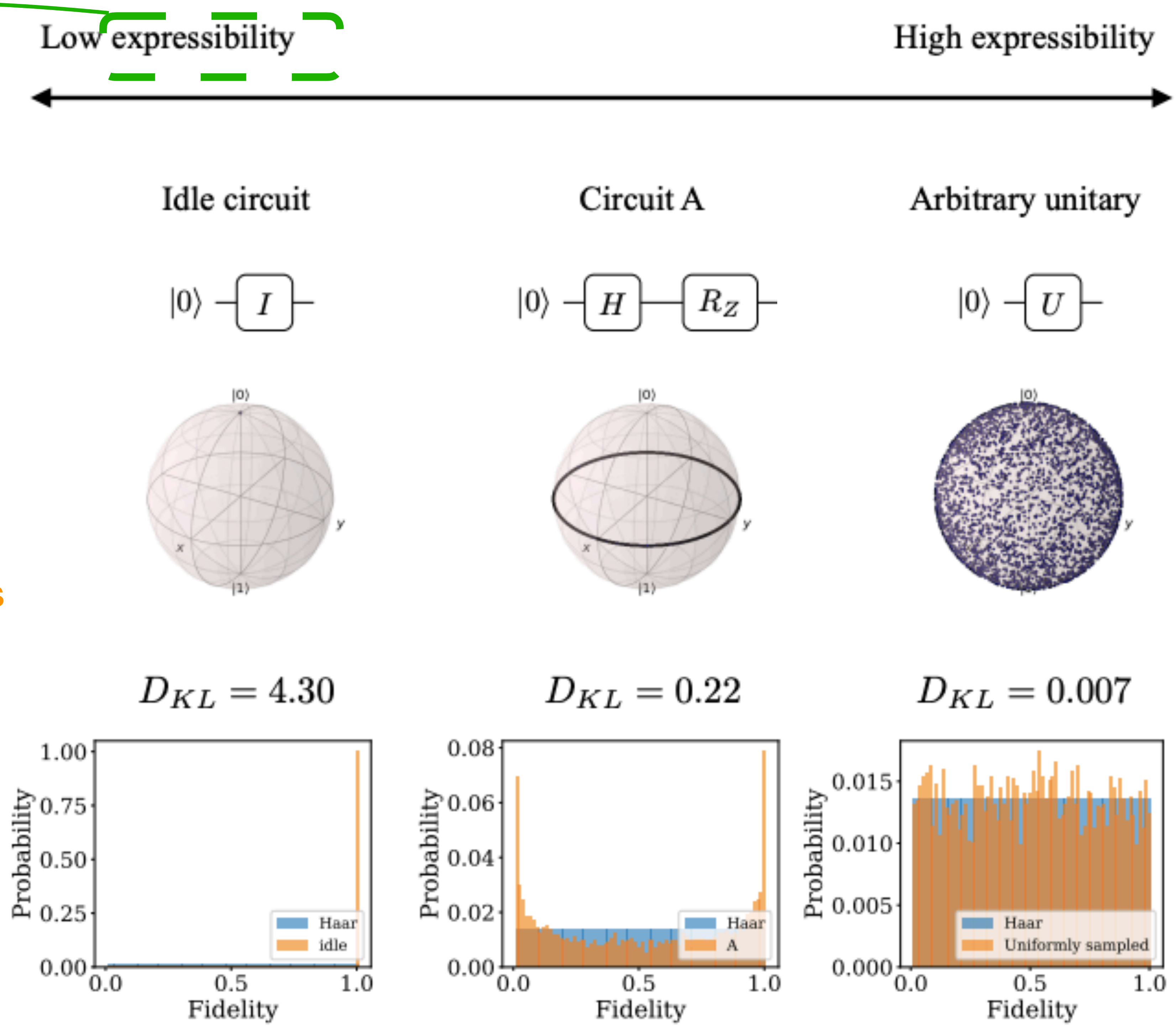
Ability to address the full unitary space

Defined as the distance of the distribution of states generated by a quantum circuit from the distribution of a Haar-random state

$$Expr = D_{KL}\left(\hat{P}_{QNN}(F;\theta)\,||\,P_{Haar}(F)\right)$$

1. Sample $|\psi_\gamma\rangle, |\psi_\phi\rangle$ from the QNN states
2. Compute the overlap $F = |\langle\psi_\gamma|\psi_\phi\rangle|^2$
3. Repeat many times to obtain statistics

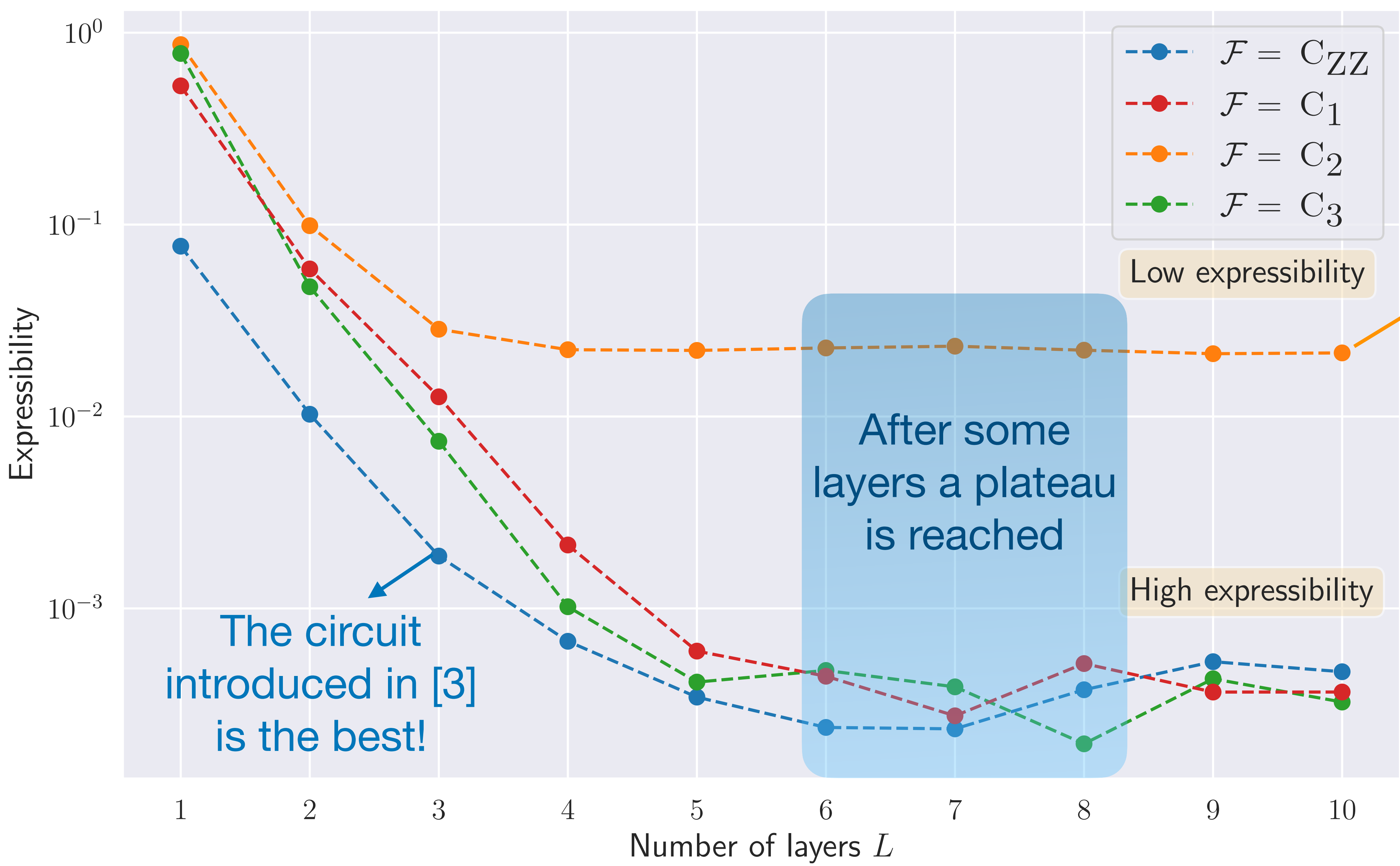
Uniformly distributed fidelity
⇒ address the full space



[6] Sim, Sukin, Peter D. Johnson, and Alán Aspuru-Guzik. "Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms." *Advanced Quantum Technologies* 2.12 (2019): 1900070.

Expressibility

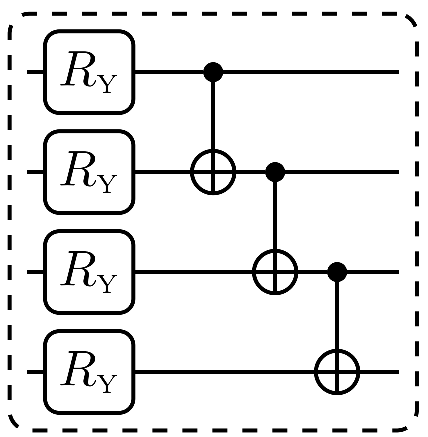
$n = 8$ qubits, linear topology



The circuit that builds entanglement faster has the worst expressibility

Variational ansatz

Circuit 2



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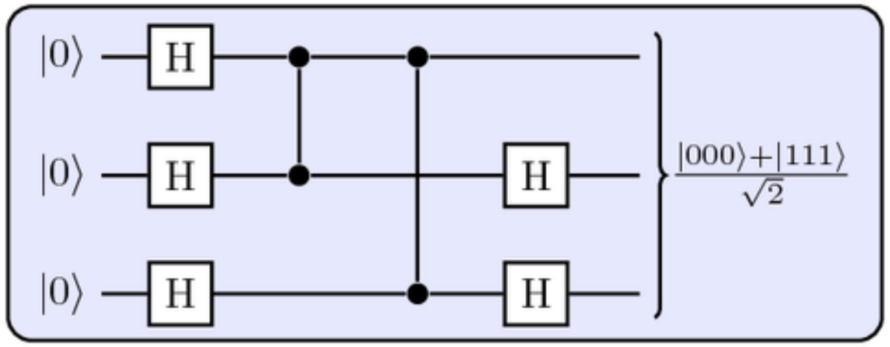
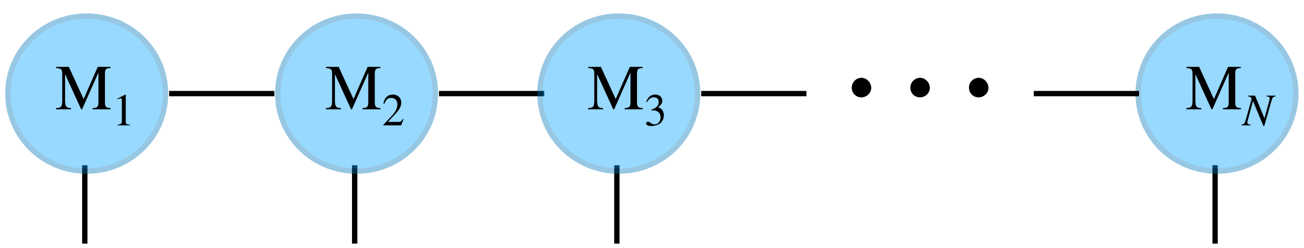
Tensor network emulator



Input:
Quantum circuit



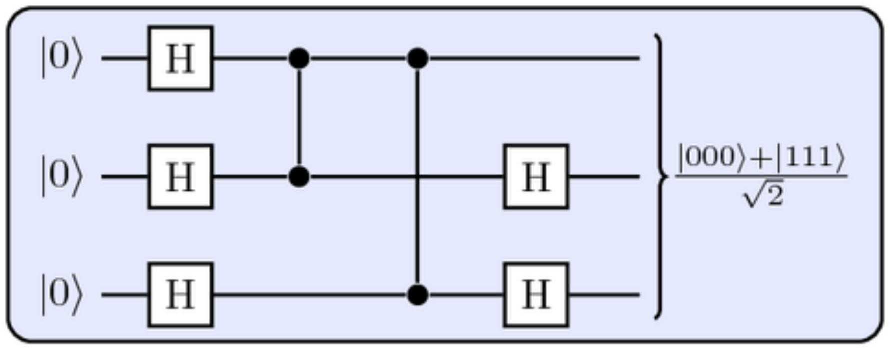
Emulator:
- Python interface
- Fortran and python backend
- MPI enabled for clusters
- GPU backend

$$\langle \psi | A | \psi \rangle$$

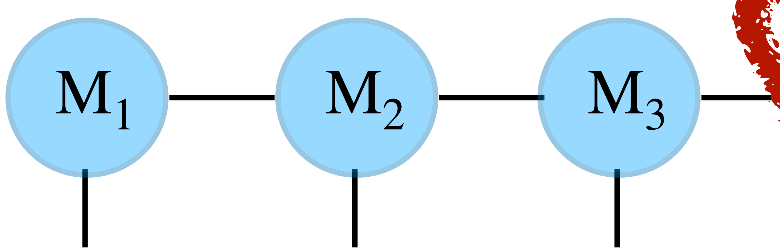
Output:
Expectation values of observables

Quantum Matcha Tea

Tensor network emulator



Input:
Quantum circuit



Soon Public

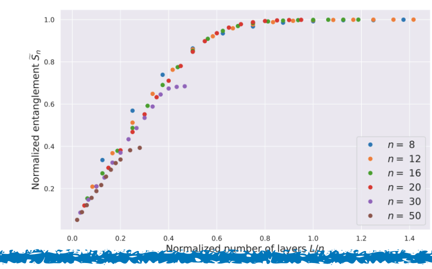
- …terface
- …ran and python backend
- MPI enabled for clusters
- GPU backend

$$\langle \psi | A | \psi \rangle$$

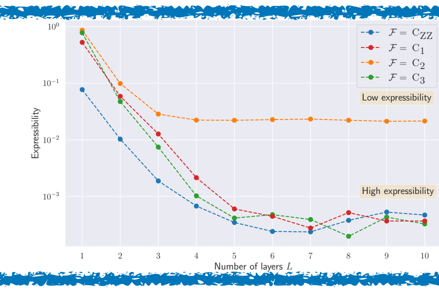
Output:
Expectation values of observables

Conclusions and outlook

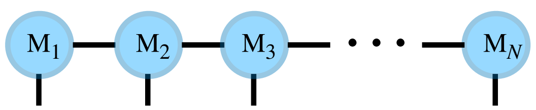
Entangling speed: characterise the entanglement production of a given QNN architecture



Expressibility: necessity of finding a sweet spot between the entanglement production and the expressibility of the QNN



Tensor network methods: use of efficient methods to simulate large system (up to 50 qubits) to investigate the limiting behaviour. **Quantum matcha tea!**



Training: Extend the analysis of the paper to the entanglement produced during the training.
How much entanglement is really needed?

Using different distribution: how is the entanglement changing when we draw the random parameters from a gaussian distribution? Can we observe a "critical" behavior?

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Riccardo Mengoni

Thank you
for your attention

References

(1) Ballarin, Marco, et al. "Entanglement entropy production in Quantum Neural Networks." *arXiv preprint arXiv:2206.02474* (2022).

(2) Havlíček, Vojtěch, et al. "Supervised learning with quantum-enhanced feature spaces." *Nature* 567.7747 (2019): 209-212.

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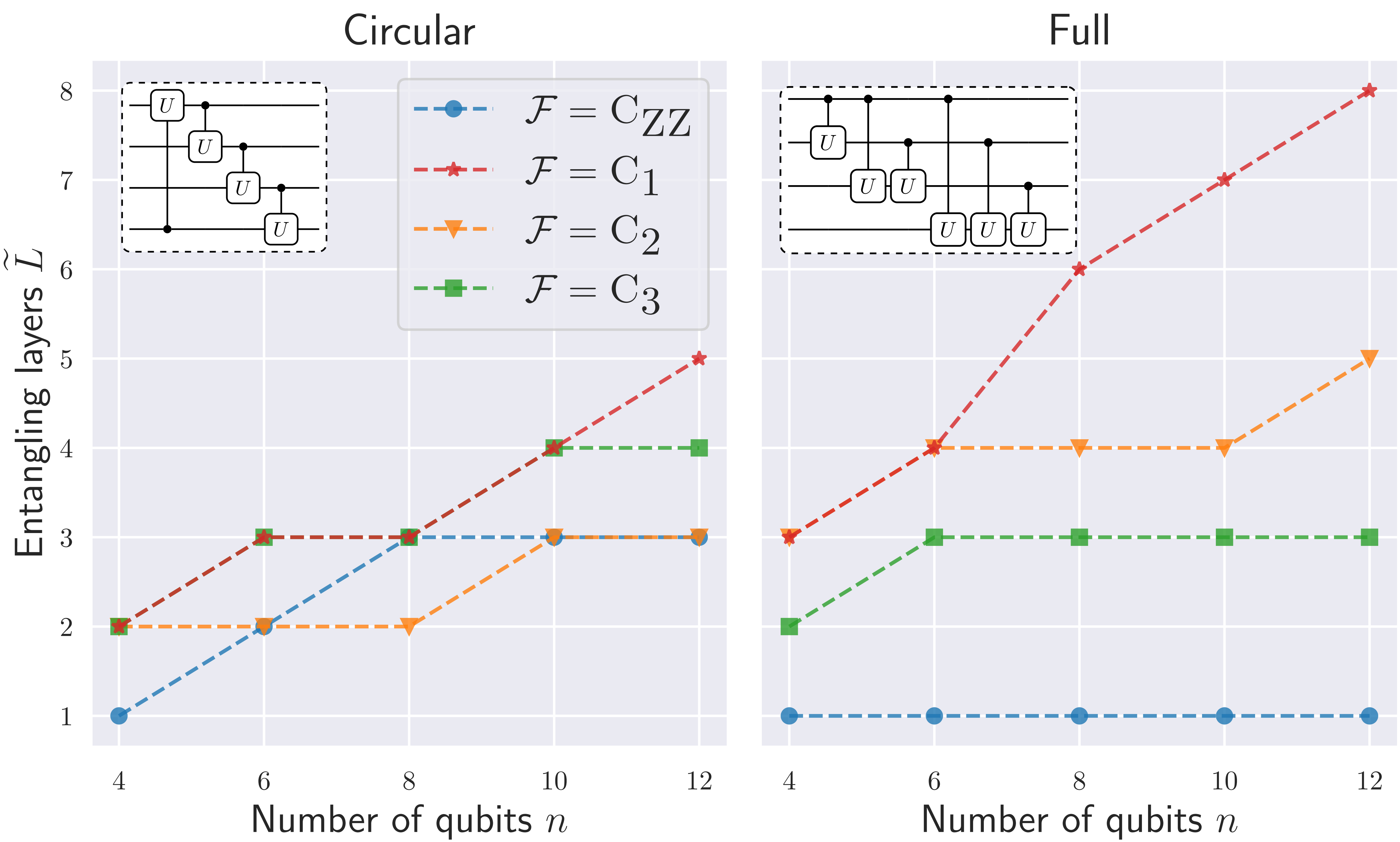
Entanglement scaling with depth



As expected, entanglement increases much faster in these cases!