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 $|1\rangle$

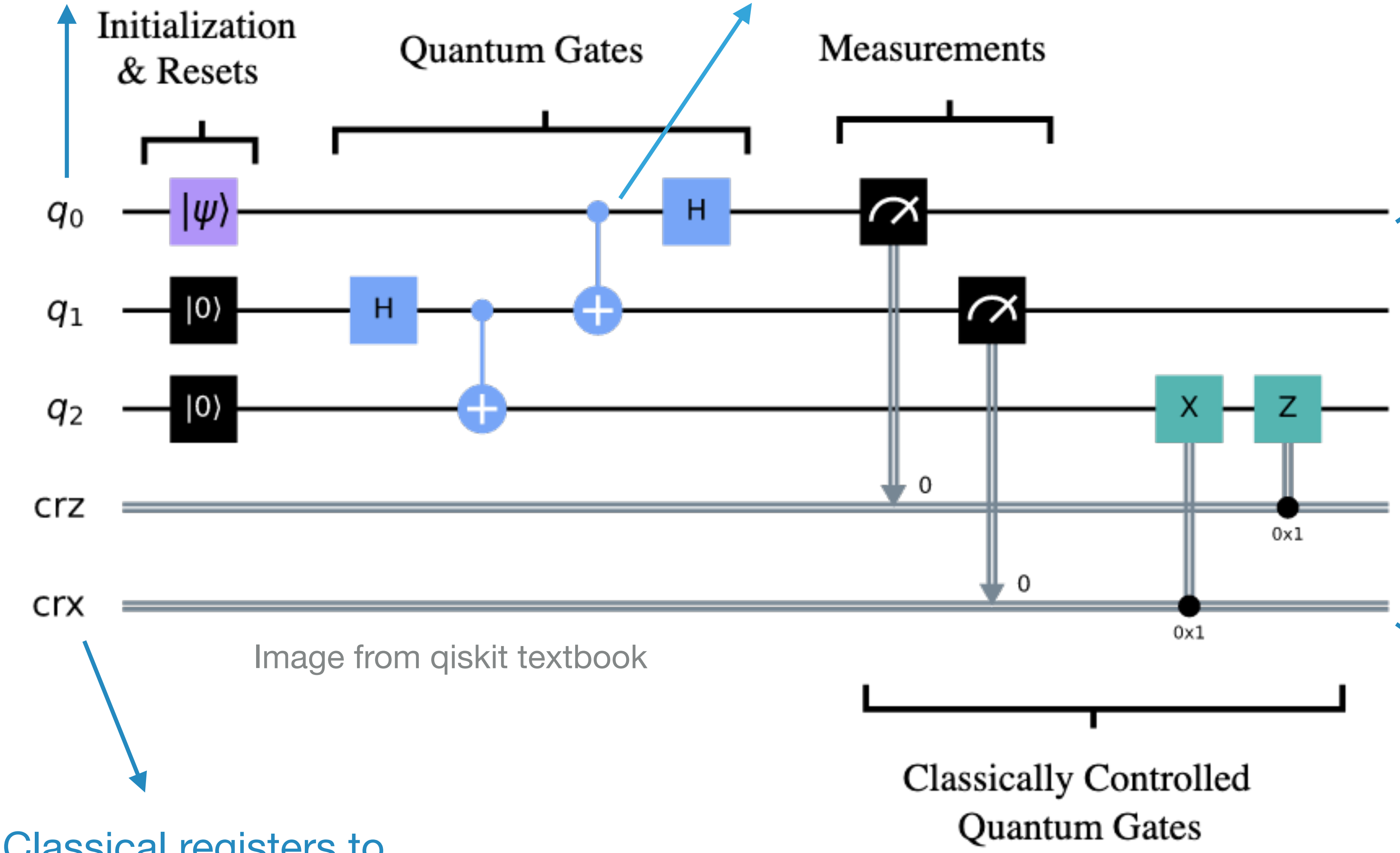

Image from qiskit textbook

Classical registers to store the results of measurements

DIGITAL QUANTUM SIMULATIONS

QUANTUM ALGORITHMS

QUANTUM CHEMISTRY

QUANTUM MACHINE LEARNING

Quantum machine learning

IRIS dataset

Iris Versicolor

Iris Setosa

Iris Virginica

Dataset

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

Quantum machine learning

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Dataset

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

Input features

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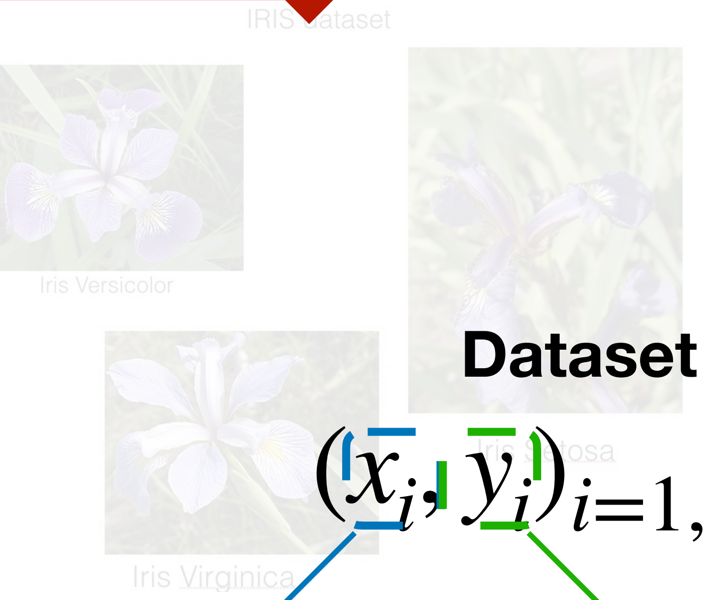

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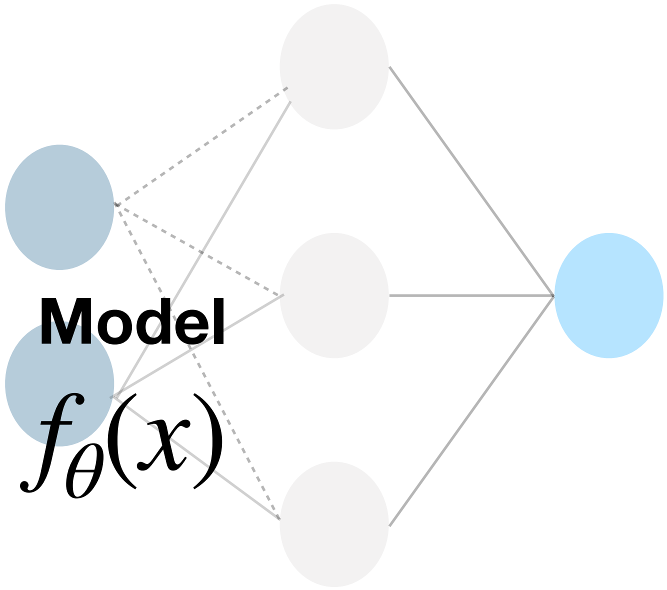
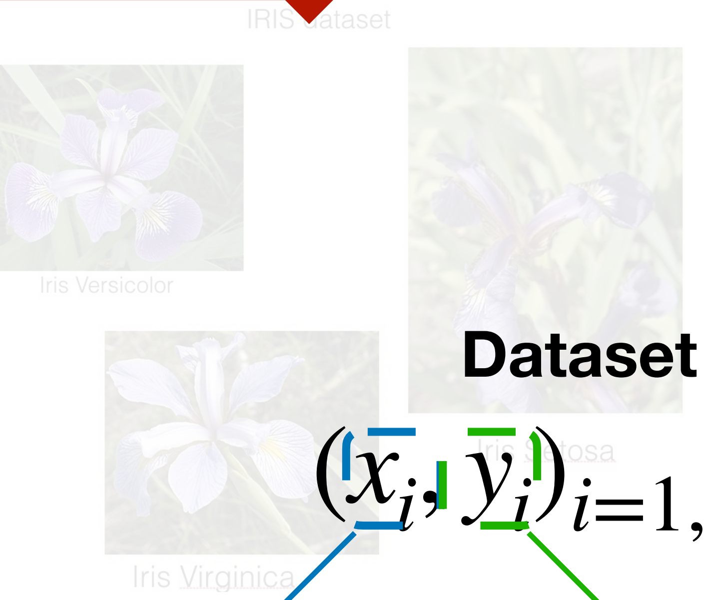


Model

$$f_\theta(x)$$

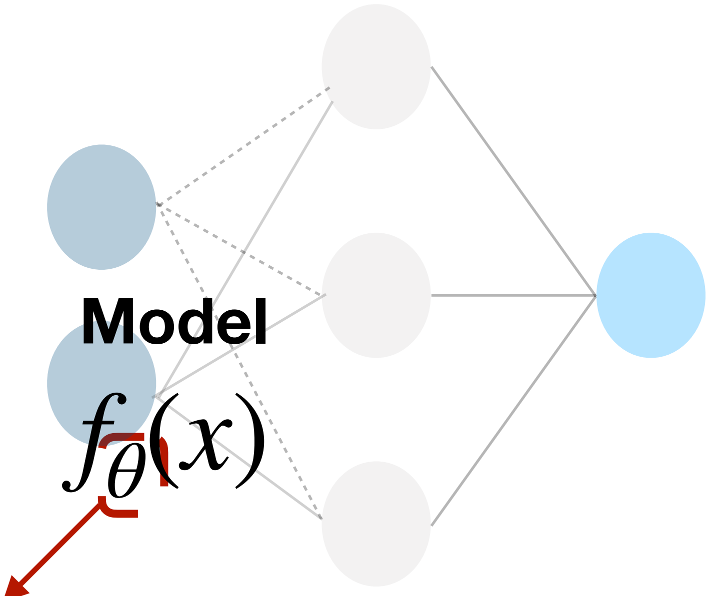
Quantum machine learning



Dataset

$$(\underbrace{x_i}_{\text{Input features}}, \underbrace{y_i}_{\text{Input class}})_{i=1,\ldots,n} \longrightarrow f_{\underbrace{\theta}_{\text{Model parameters}}}(x)$$

Model



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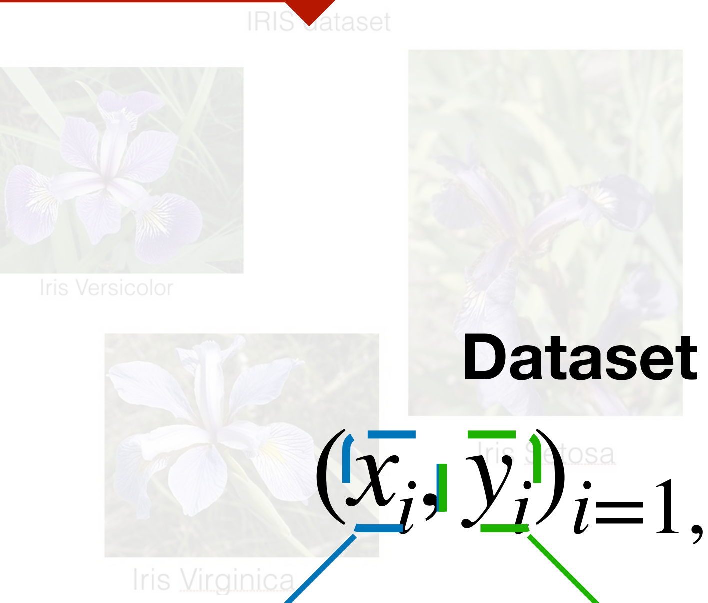

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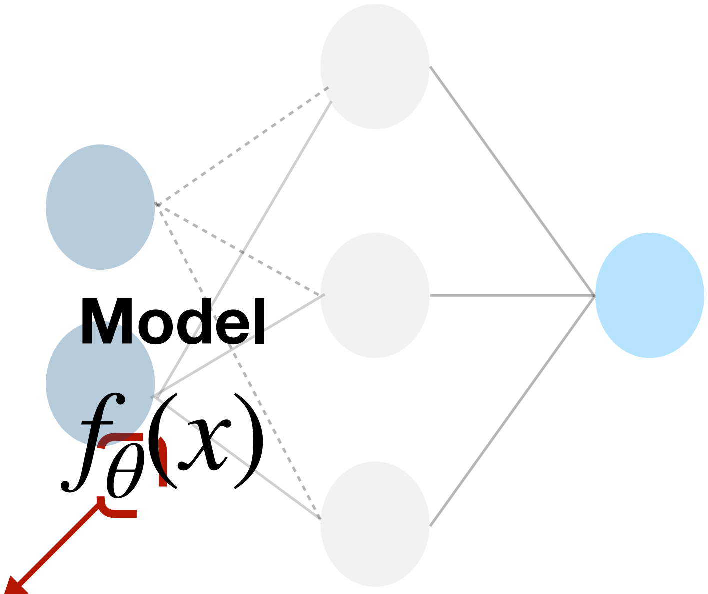


Model

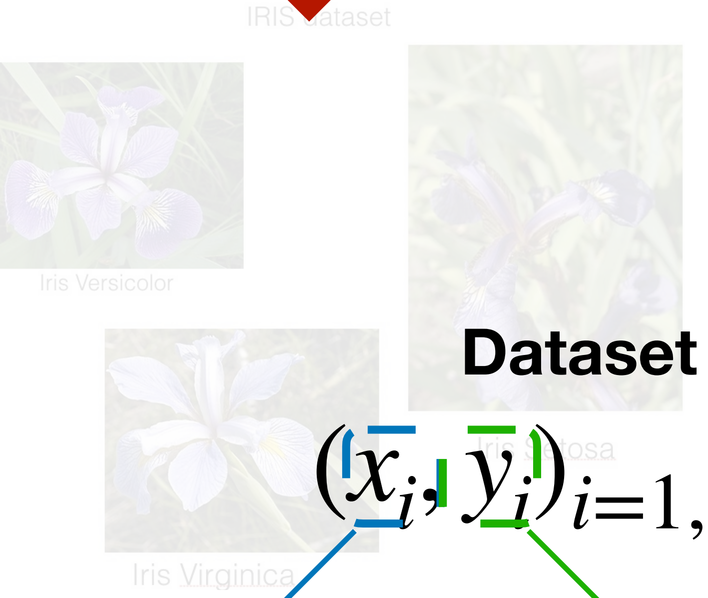
$$f_\theta(x)$$

Model parameters

Prediction

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

Quantum machine learning



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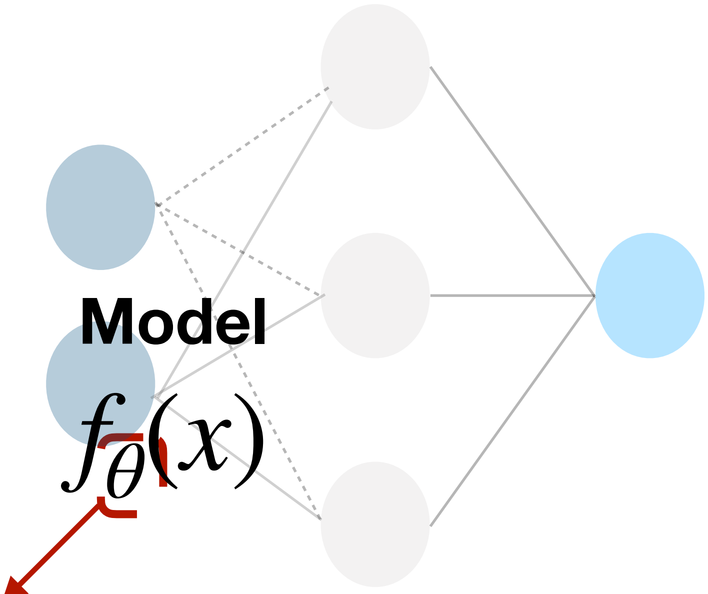

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Update θ minimising loss function

Prediction

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

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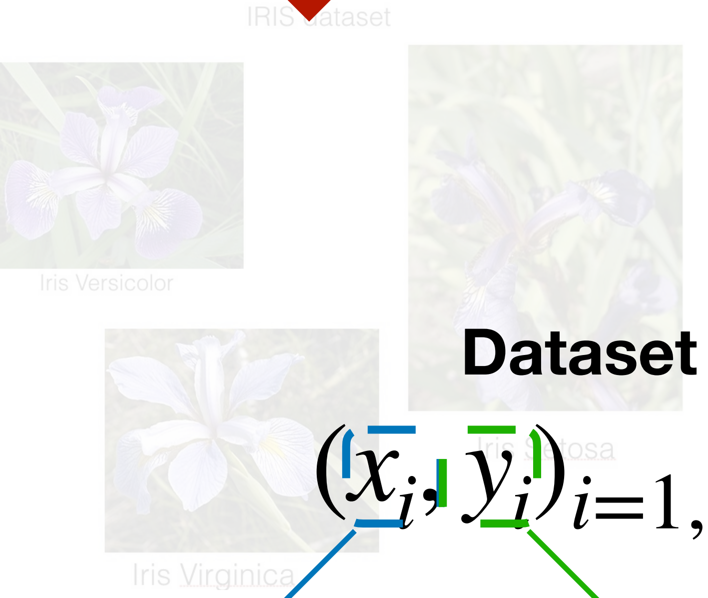

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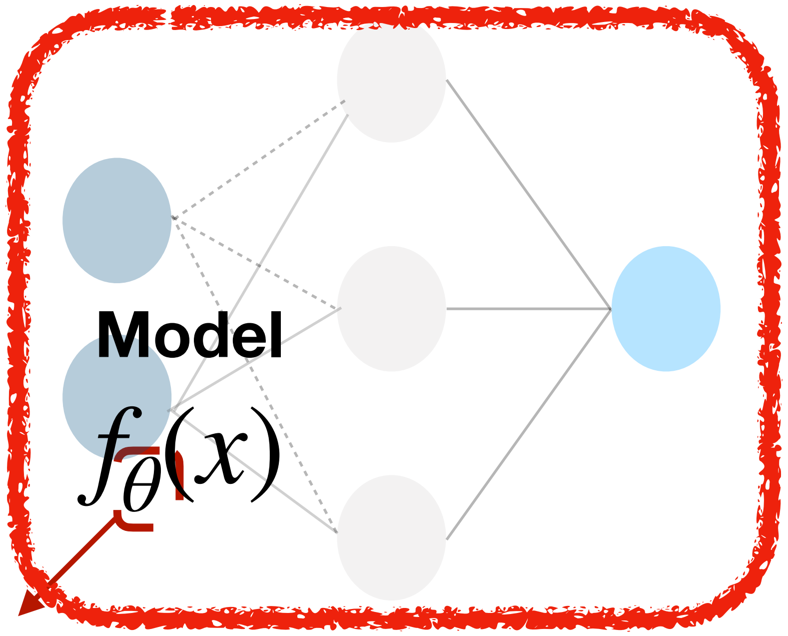

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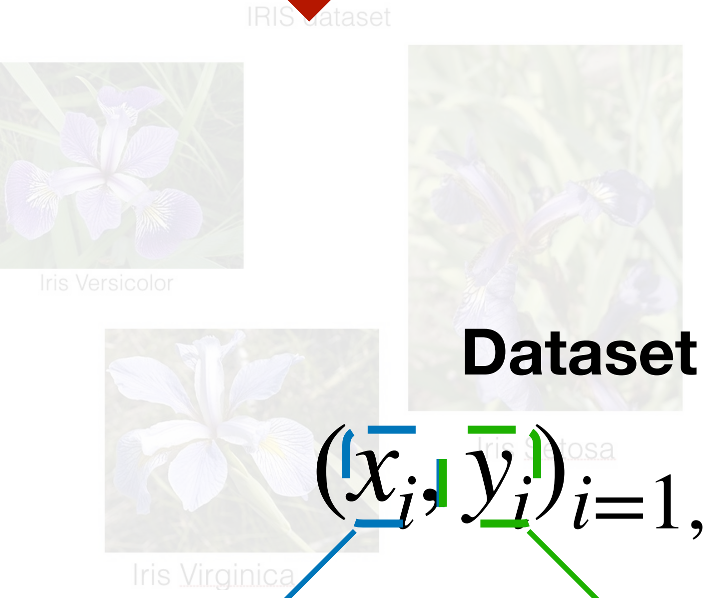

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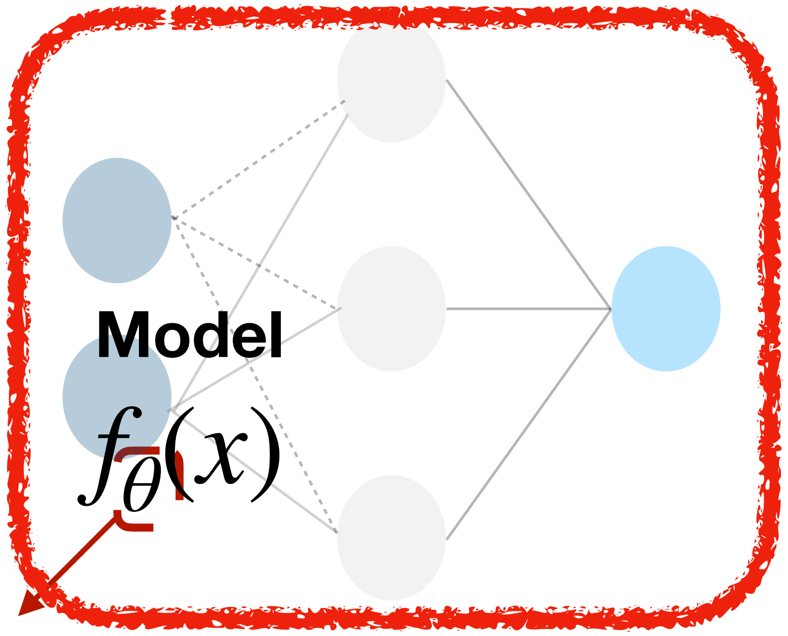

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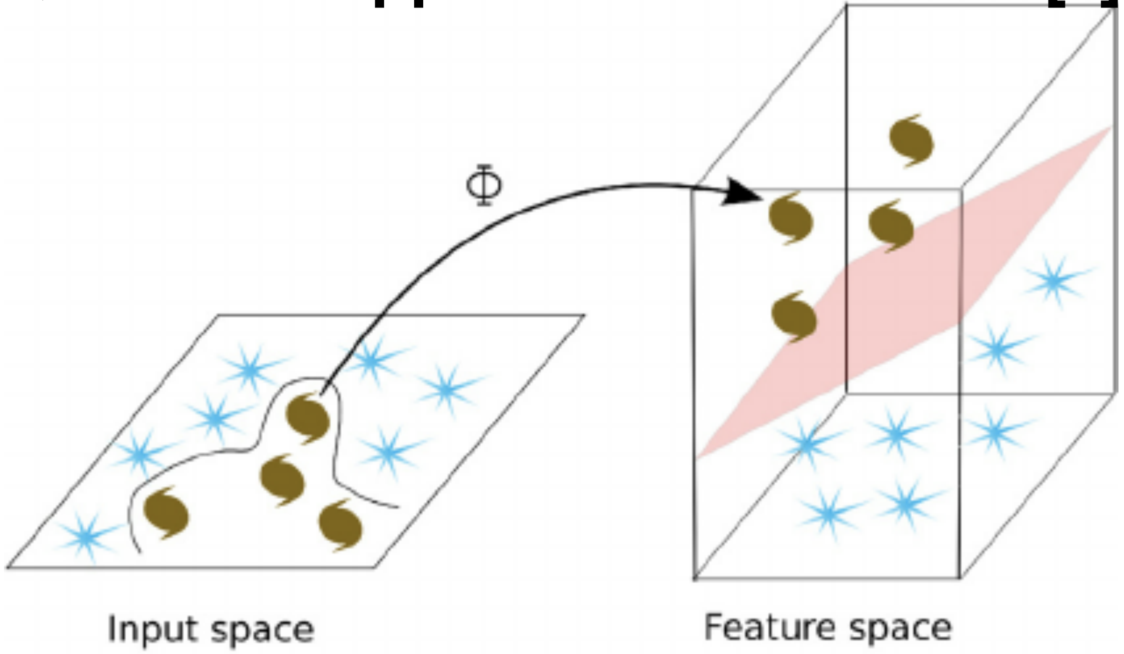
Quantum support vector machine [1]



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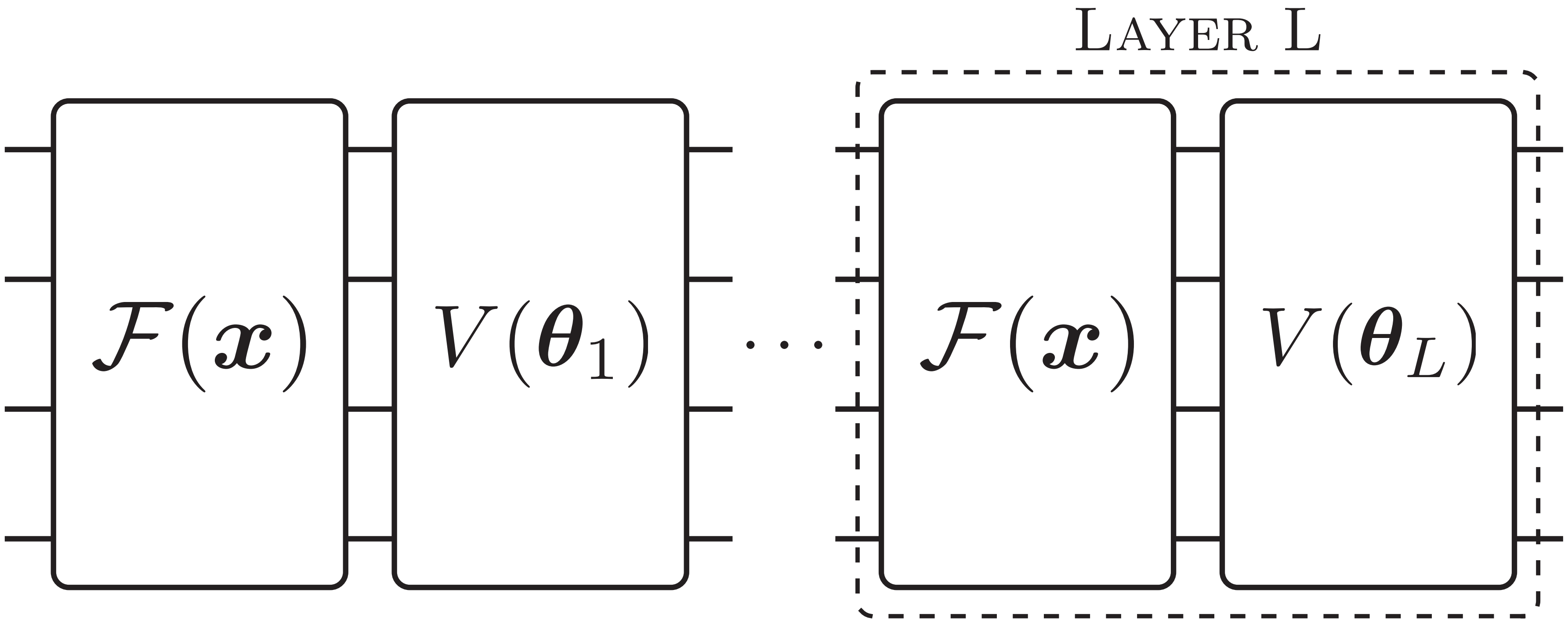
[1] Havlíček, Vojtěch, et al. "Supervised learning with quantum-enhanced feature spaces." *Nature* 567.7747 (2019): 209-212.

Quantum neural networks

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



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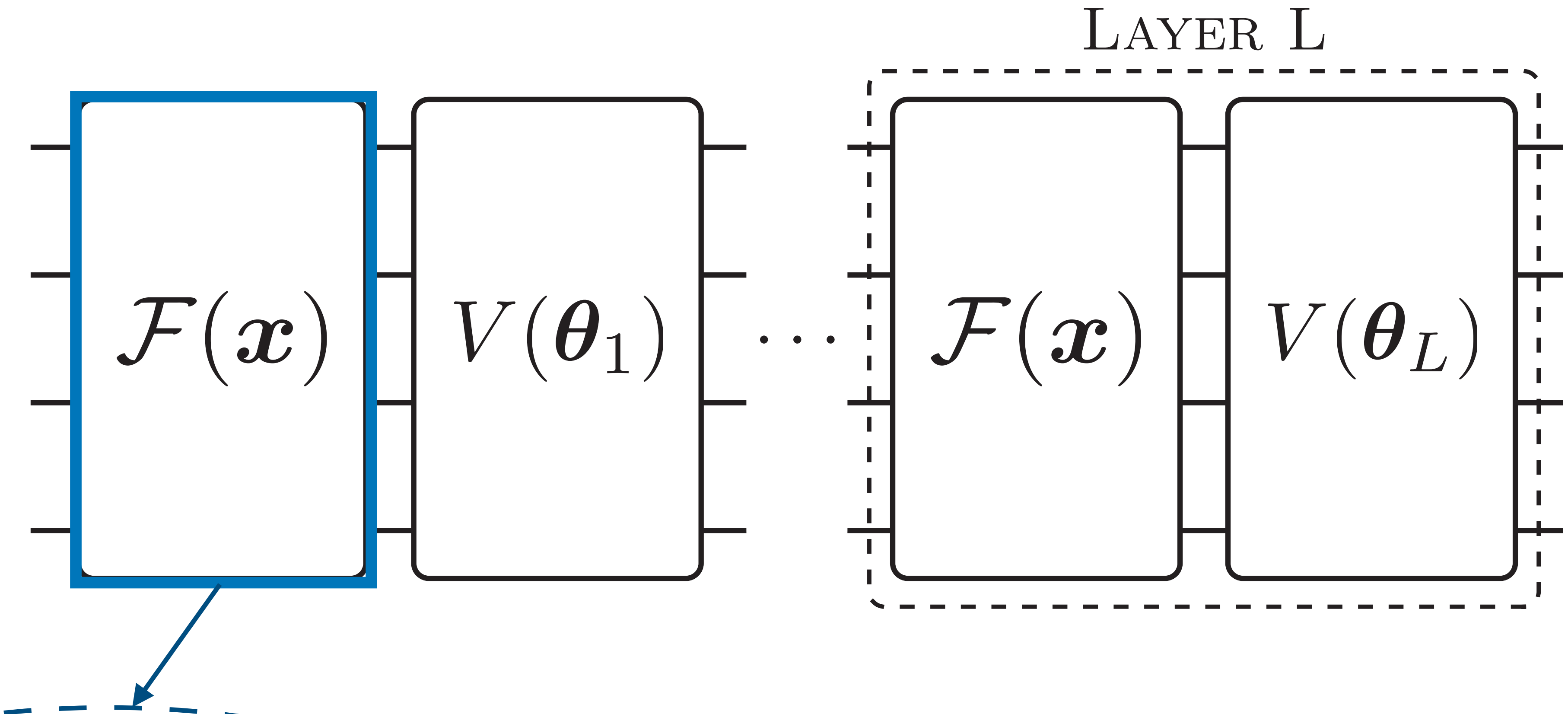

Feature map, encode *classical* data on quantum circuit

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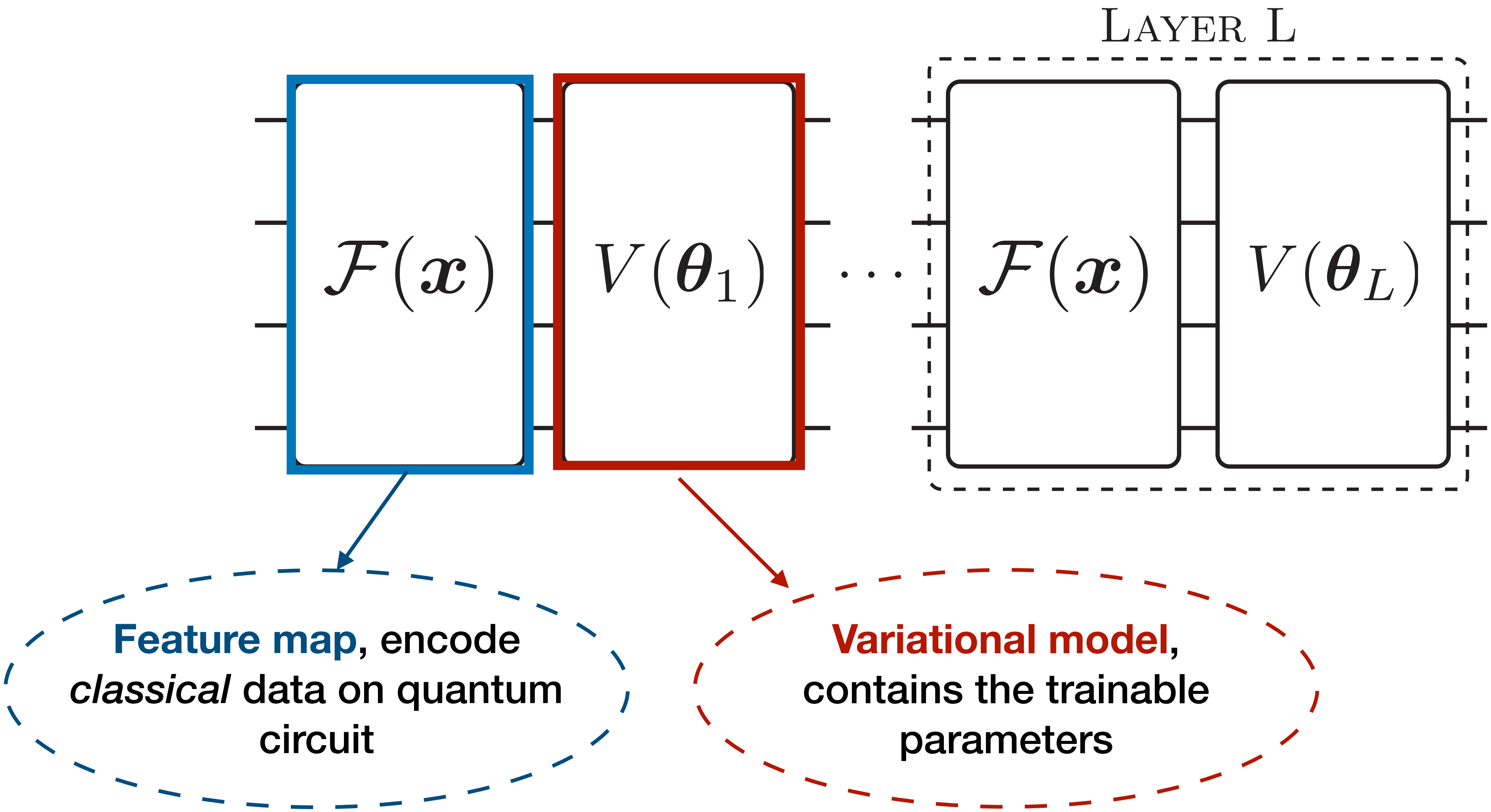

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Variational model, contains the trainable parameters

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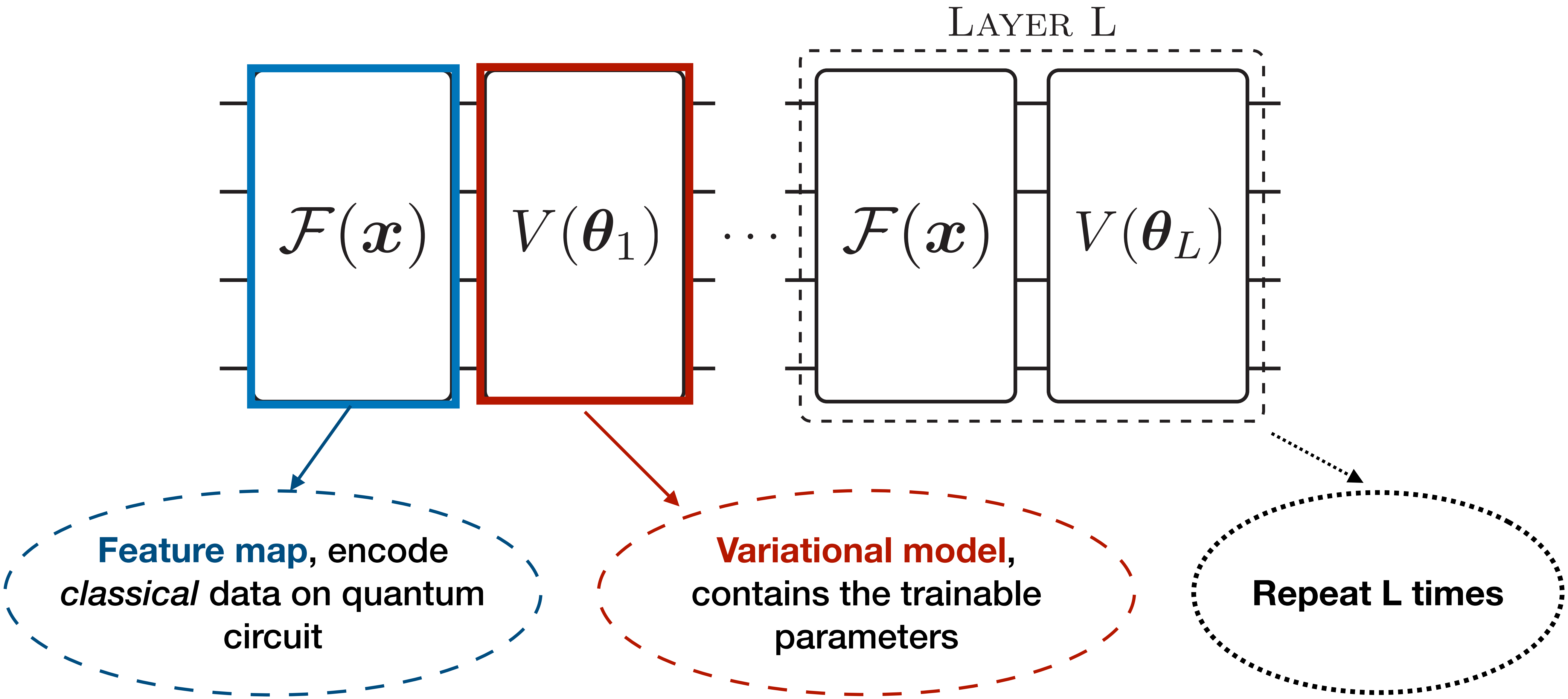

Feature map, encode *classical* data on quantum circuit

Variational model, contains the trainable parameters

Repeat L times

Entanglement: bless or curse?

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

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[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.

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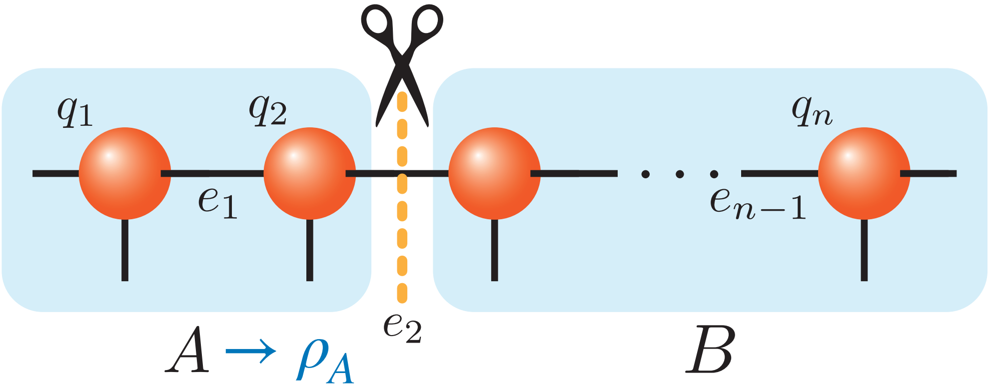

Von Neumann entanglement entropy between bipartitions A and B (across link e_i):

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

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Random states
⇒ highly entangled!
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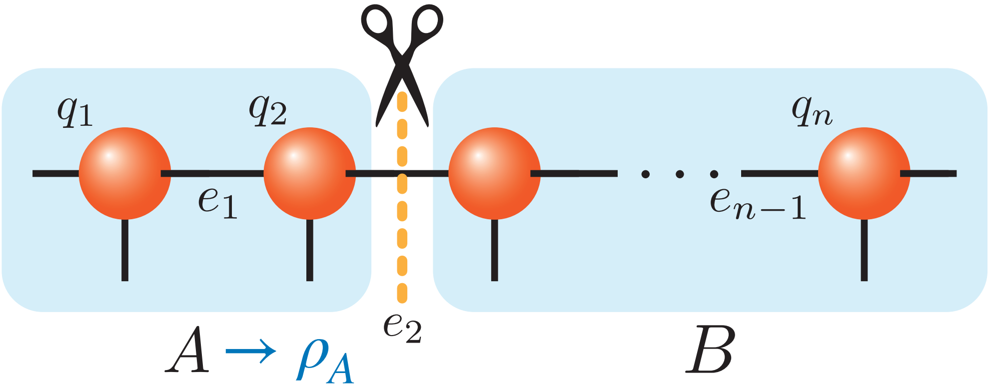

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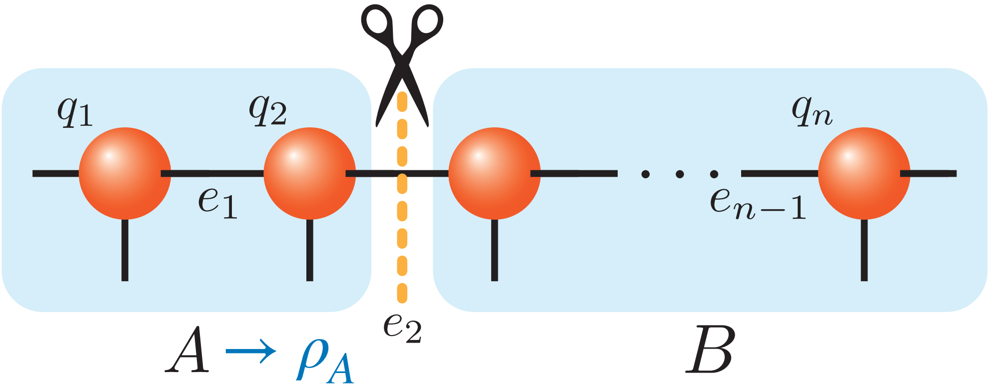

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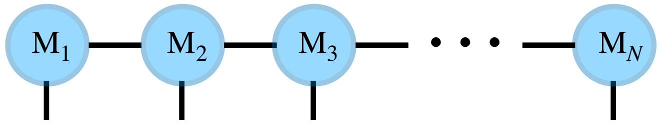

Lowly entangled states ⇒ efficient simulations with tensor networks methods (Quantum matcha tea)

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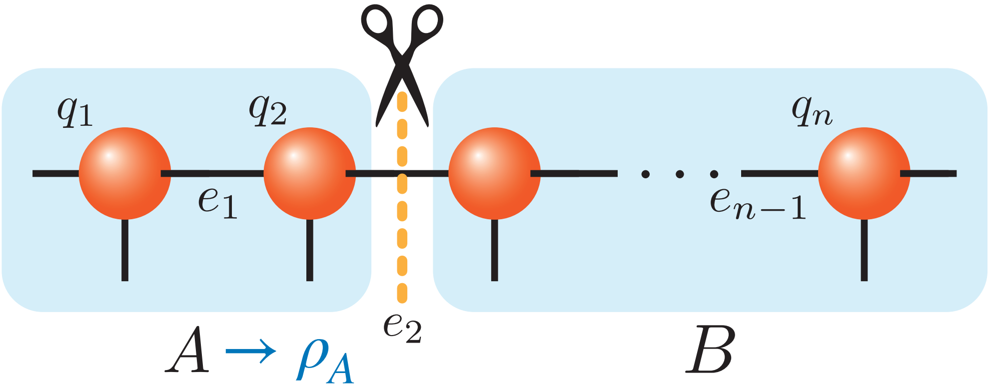

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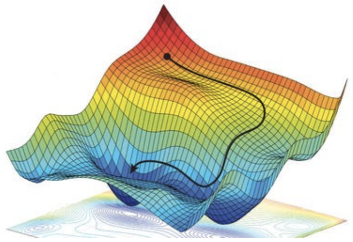
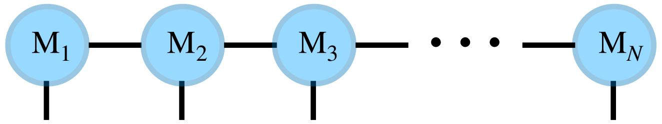


Highly entangled states ⇒ connected with the emergence of Barren Plateaus [4]



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Tensor network emulator

String compression (simple example):

AAABBCDDDDDDDD **Length: 14**

↓ Compress

A3B2C1D8 **Length: 8**

Tensor network emulator

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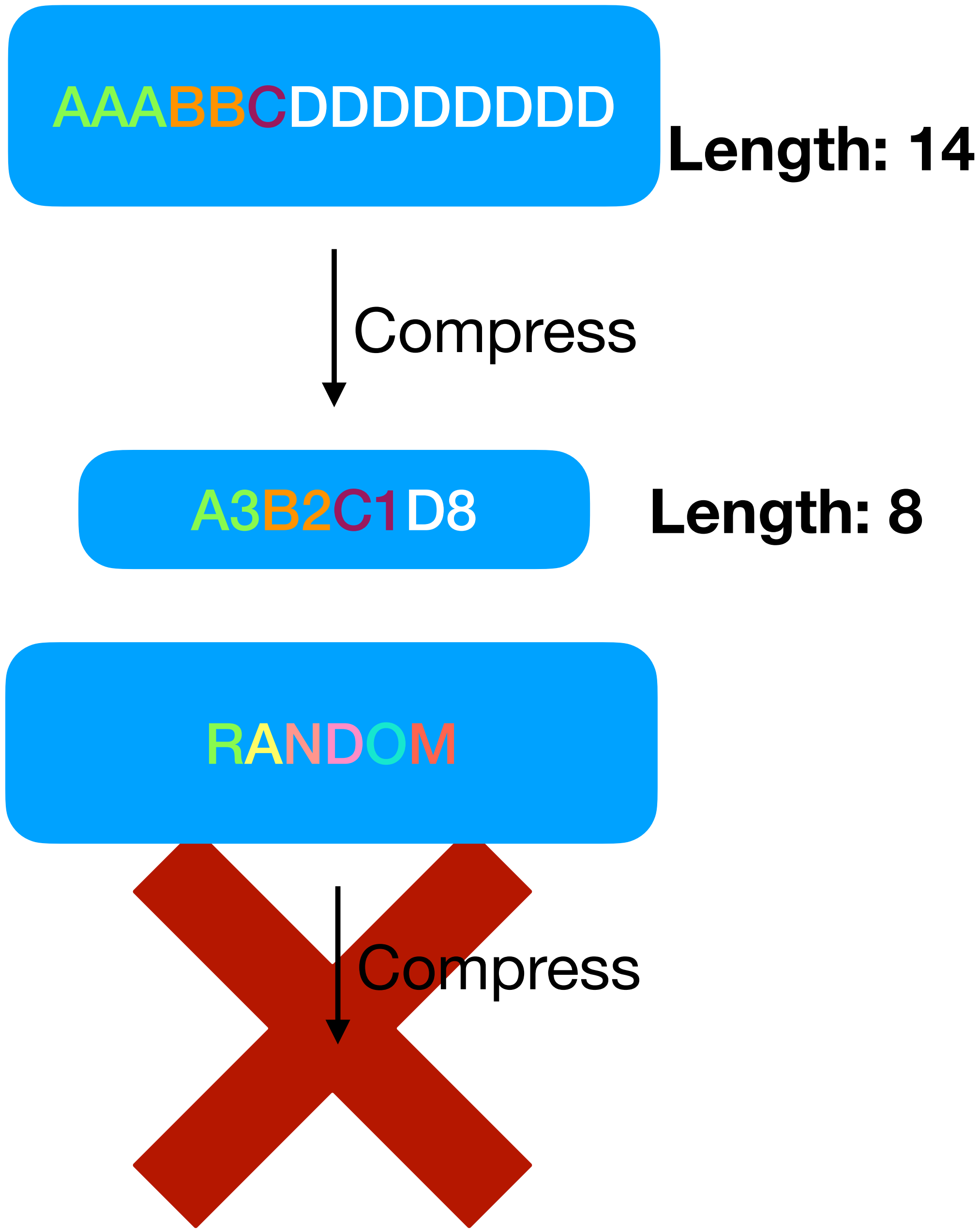

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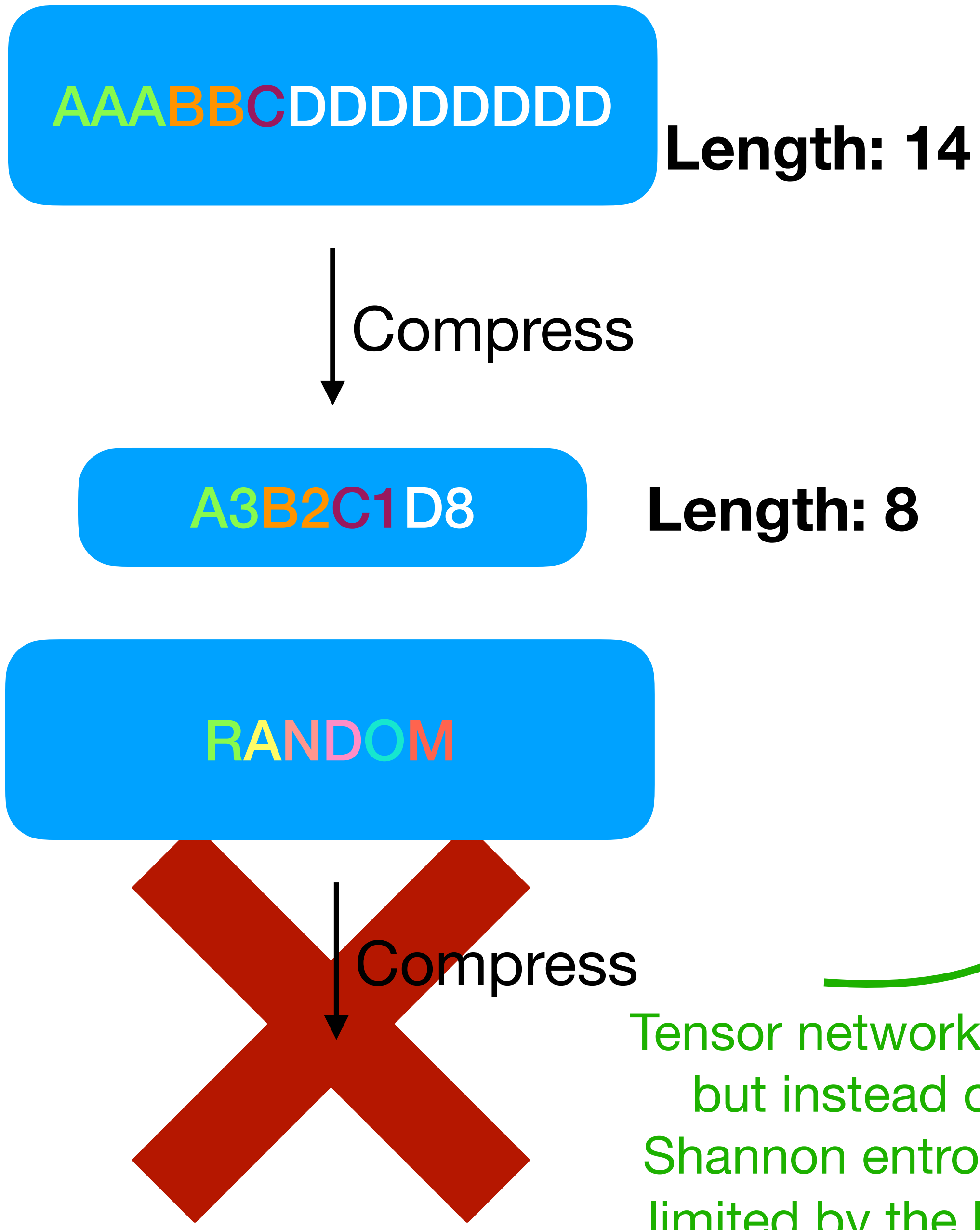

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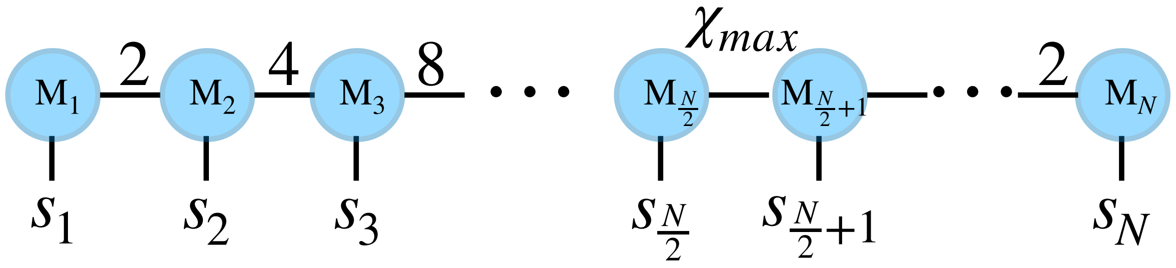

Tensor networks works in a similar way, but instead of being limited by the Shannon entropy of the string they are limited by the **Entanglement Entropy of the state**

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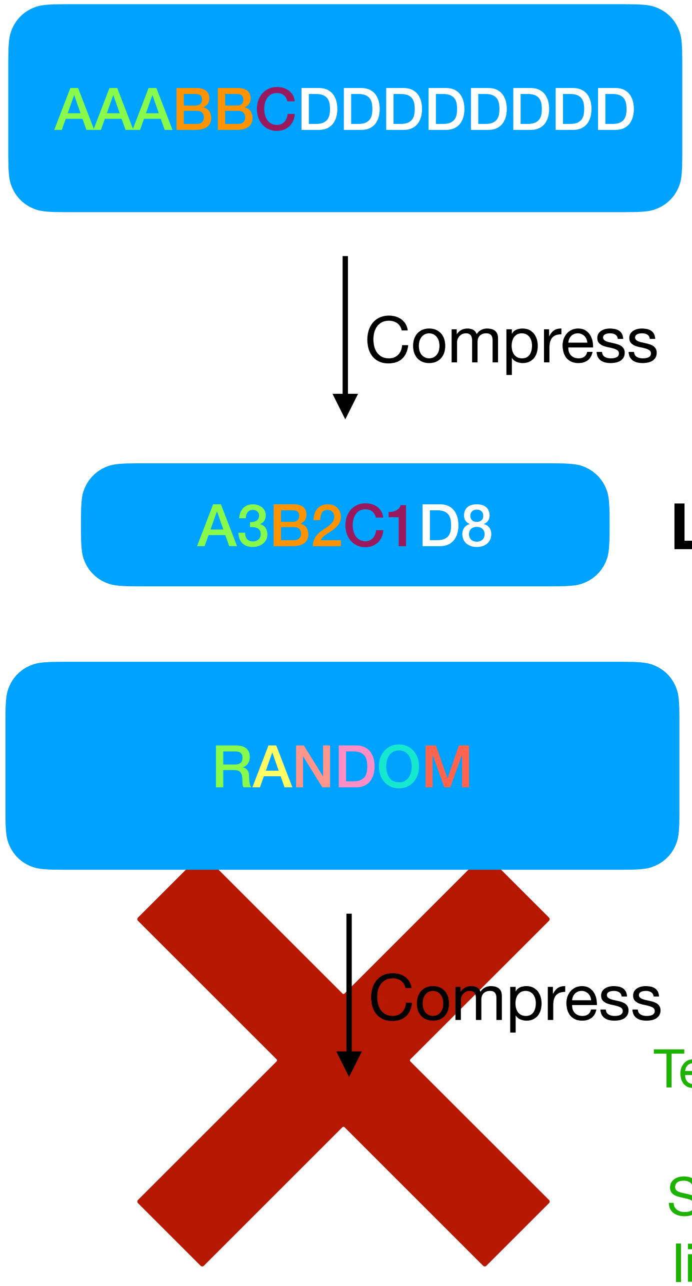
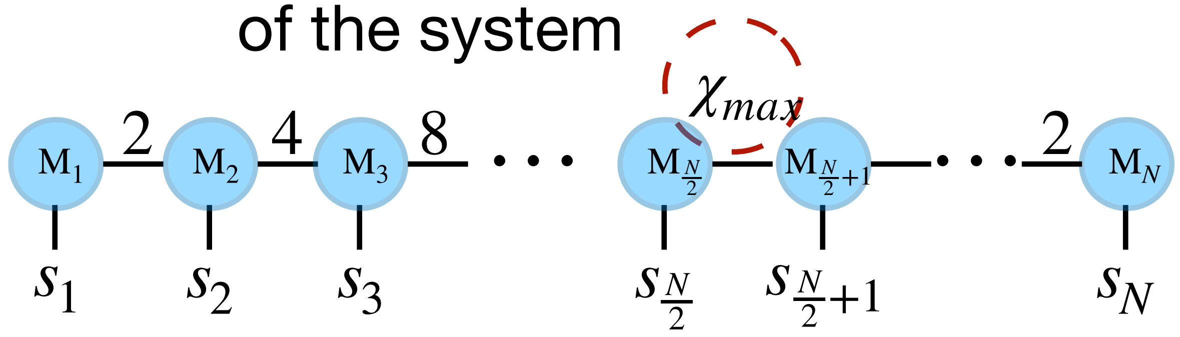


Length: 14

Length: 8

Bond dimension

It controls the entanglement of the system



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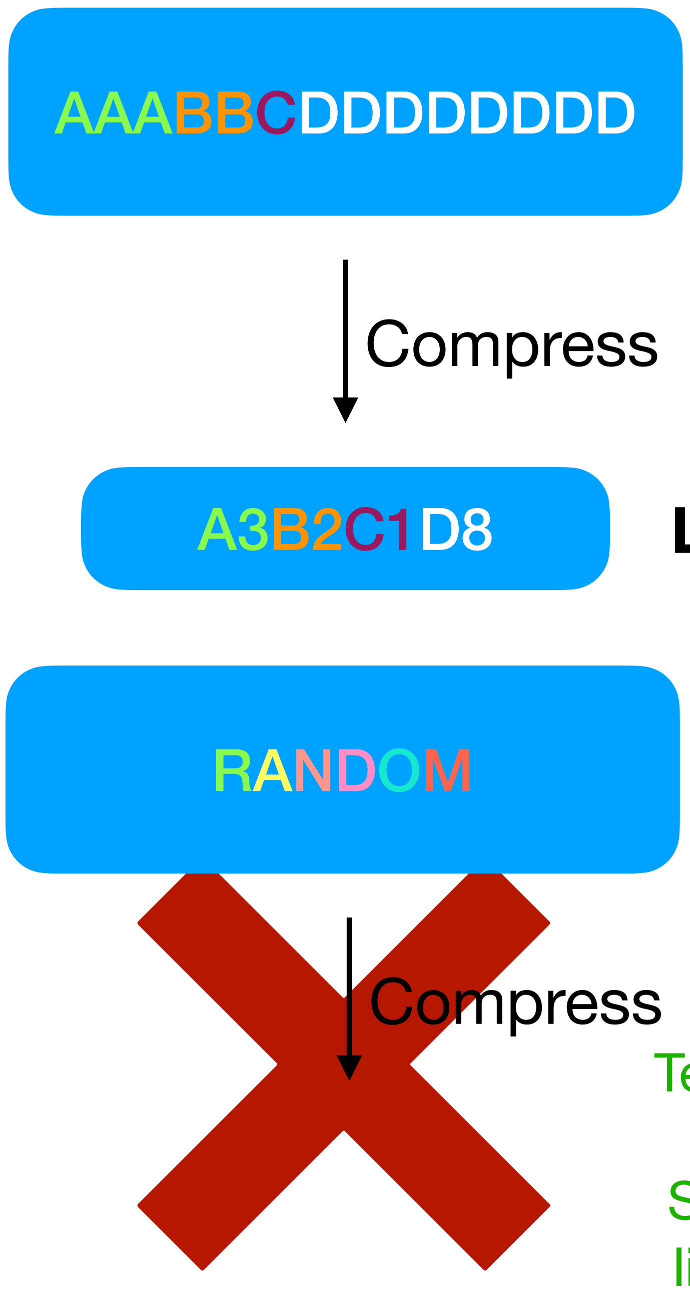

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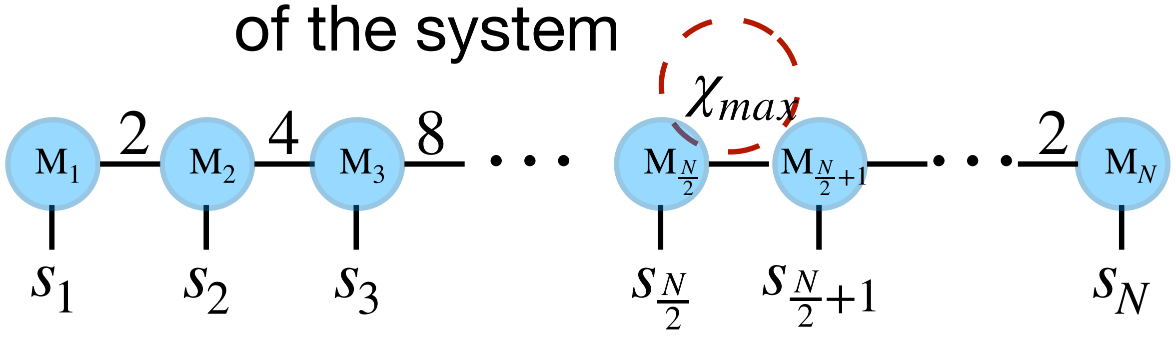

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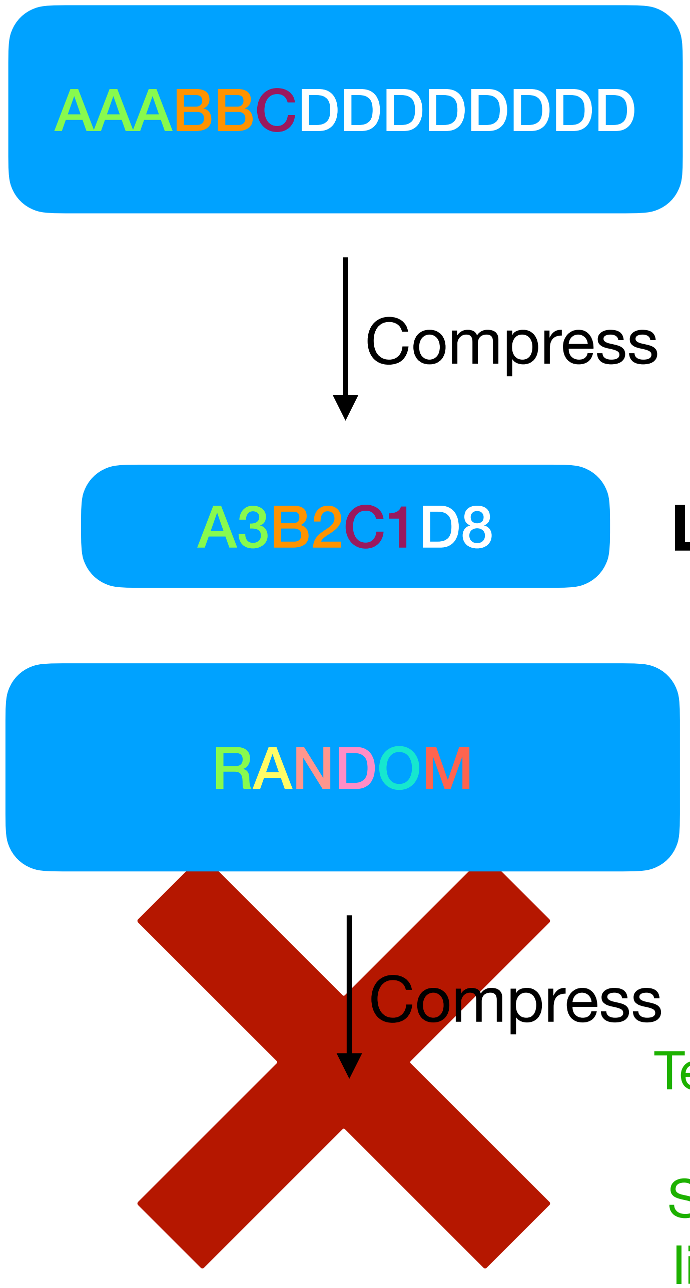

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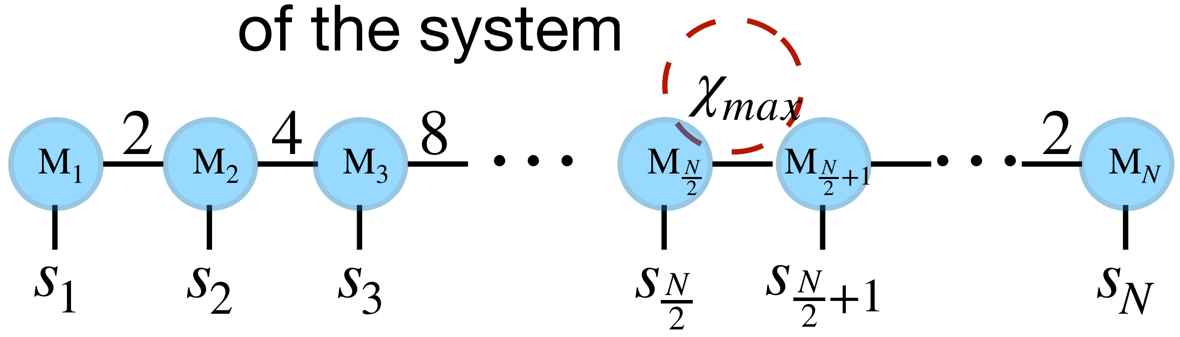

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Quantum matcha tea: efficient tensor network emulator for Quantum Circuits

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**

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.

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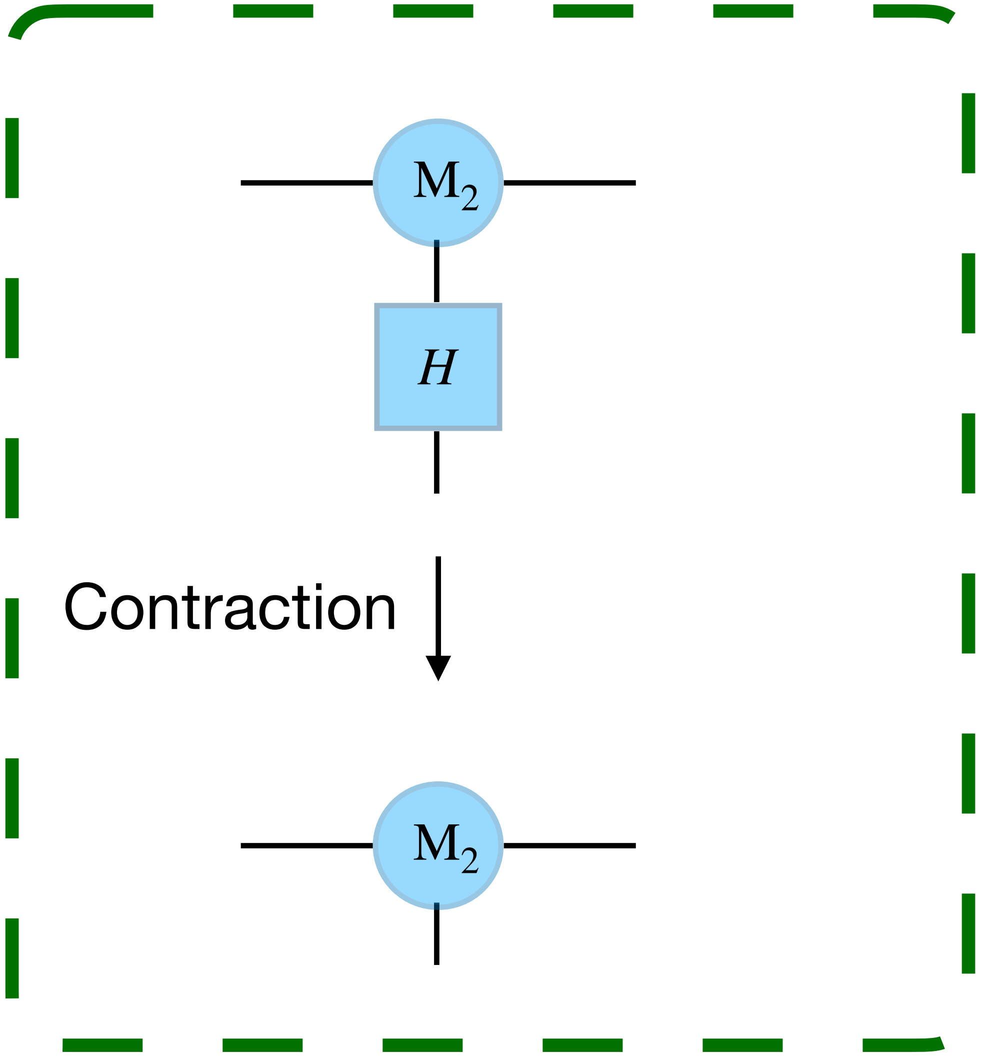

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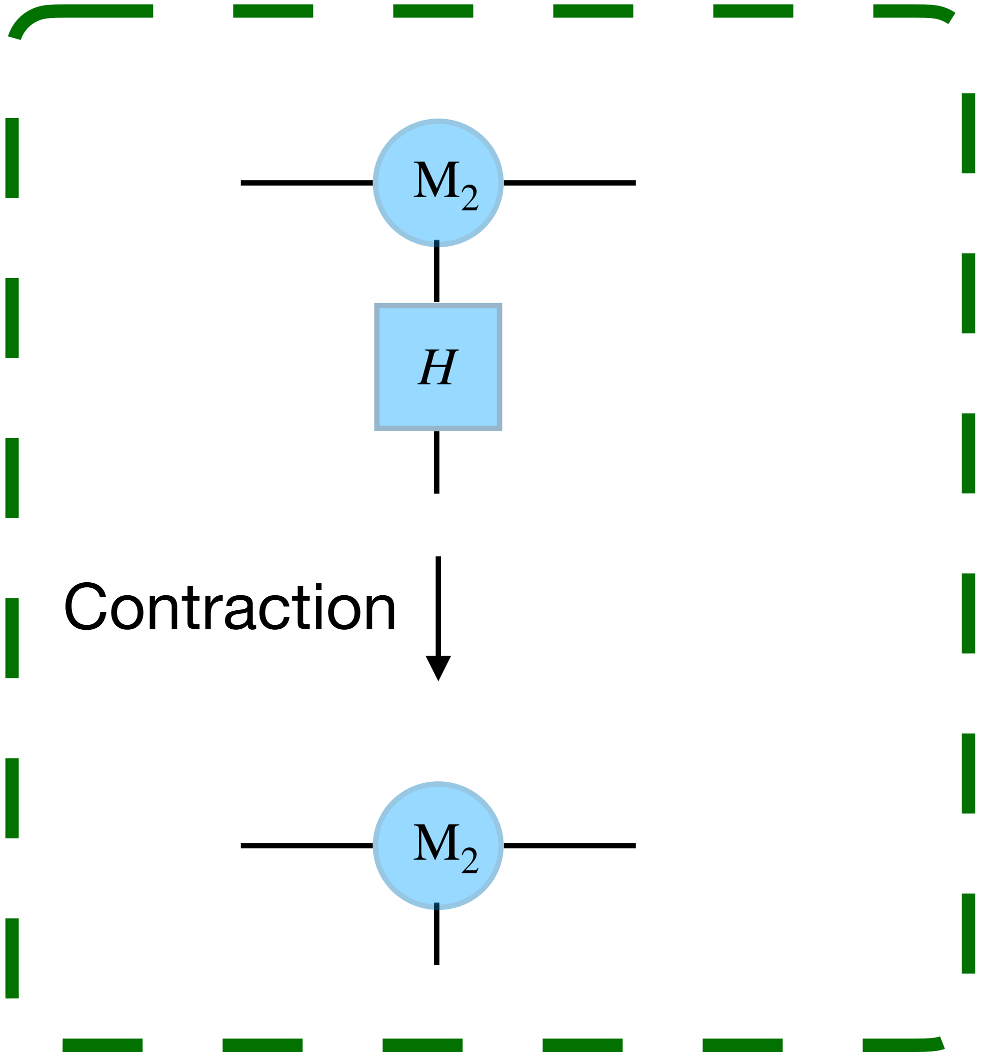
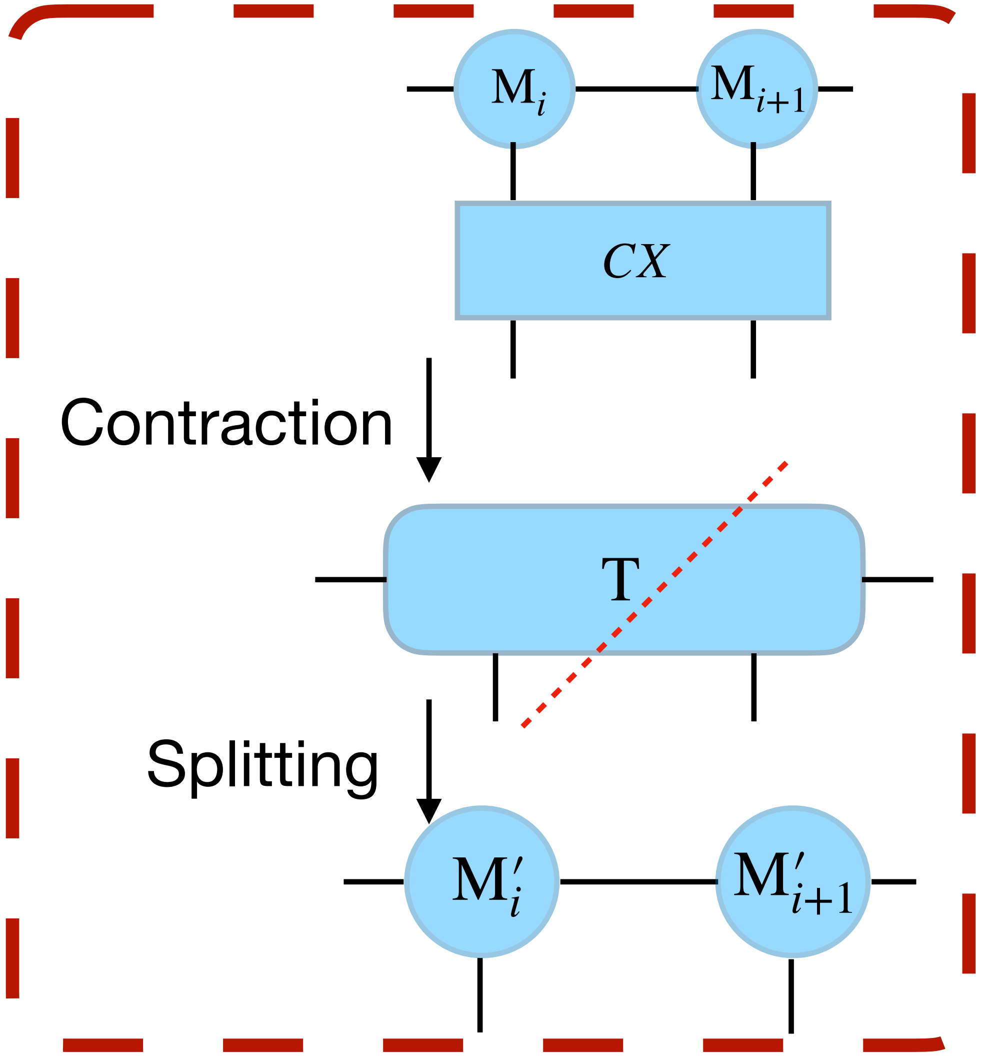
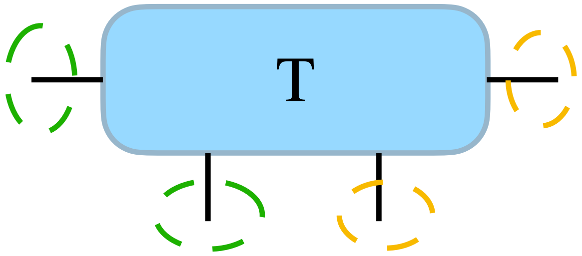


TWO-QUBITS GATE



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



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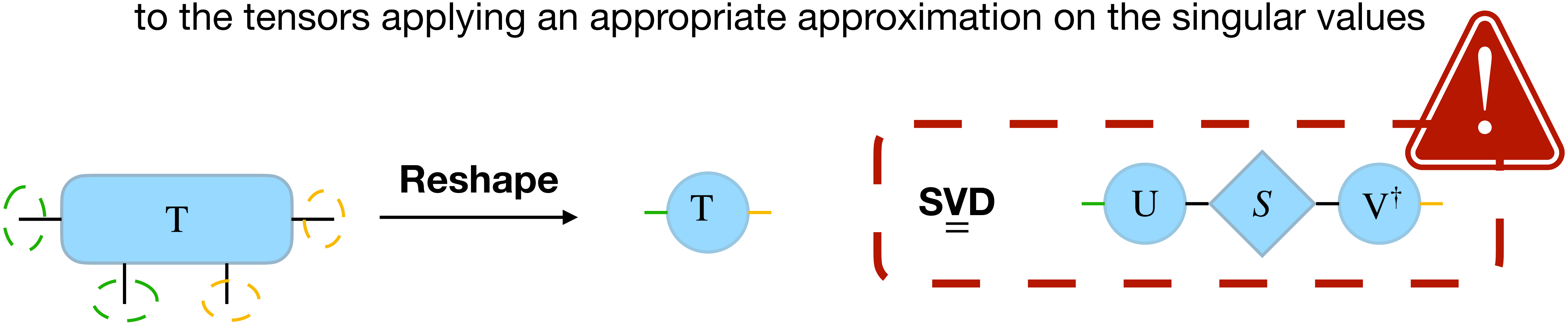

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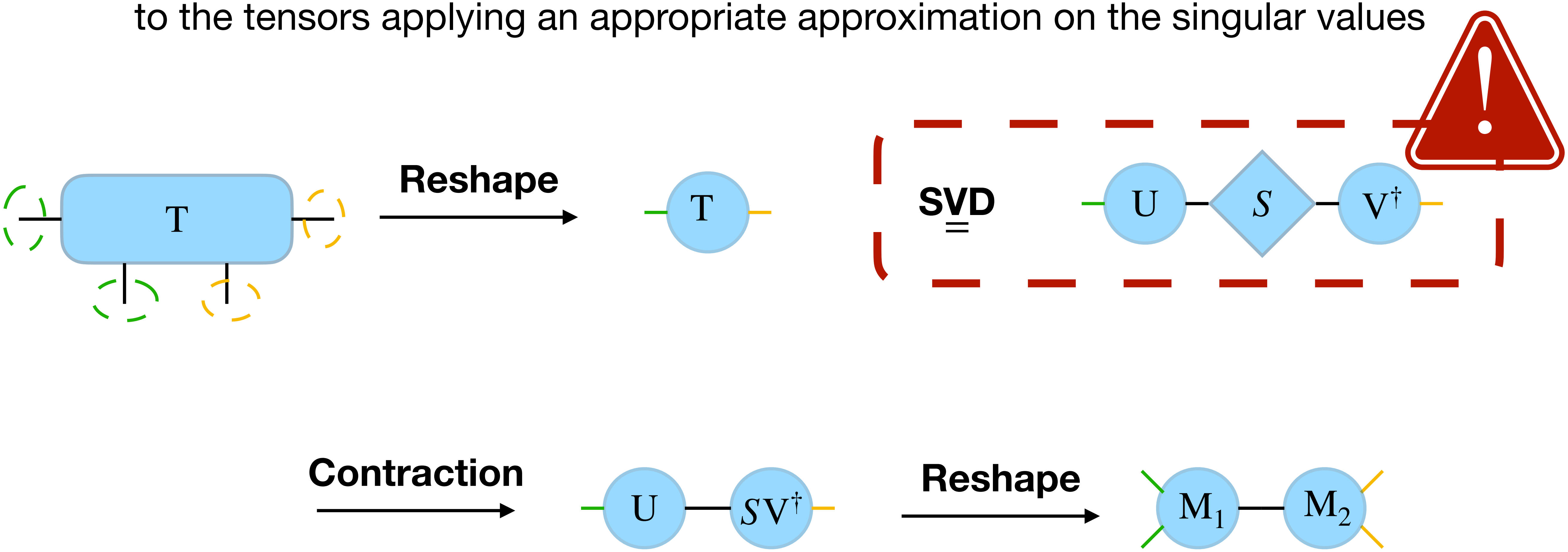

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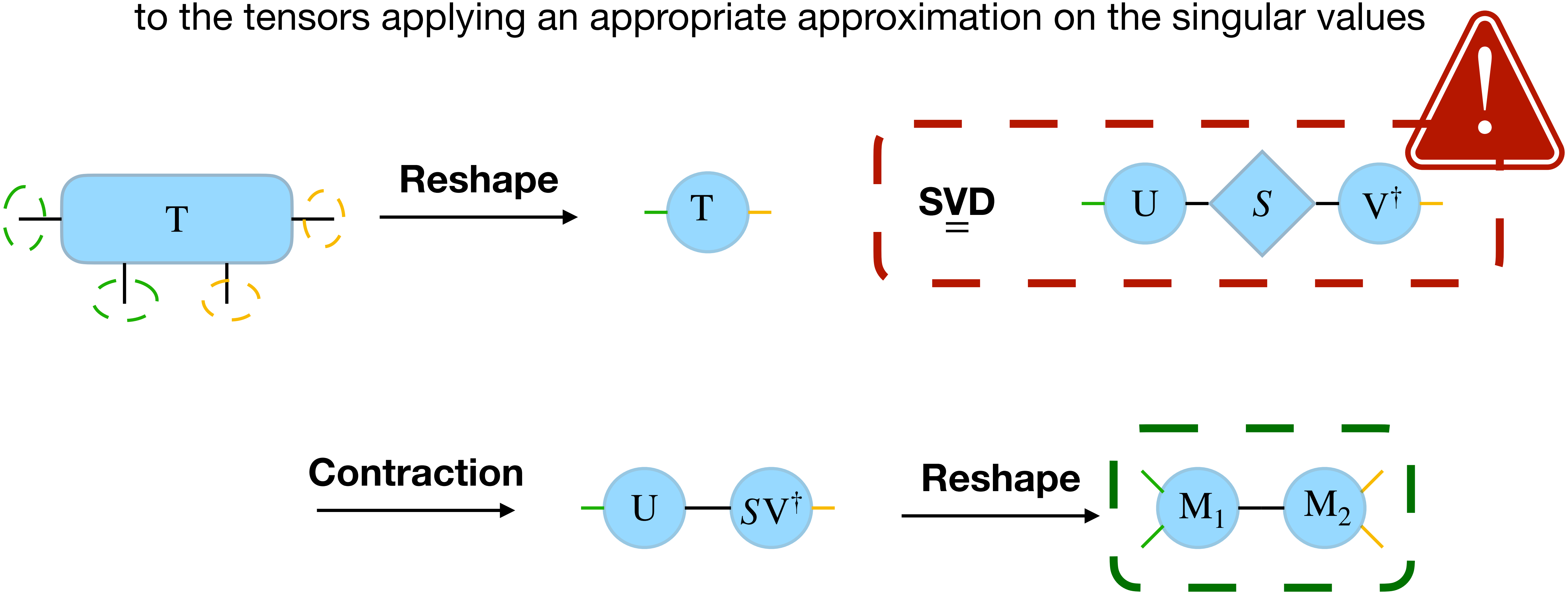

We are back to the MPS form

Truncation

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

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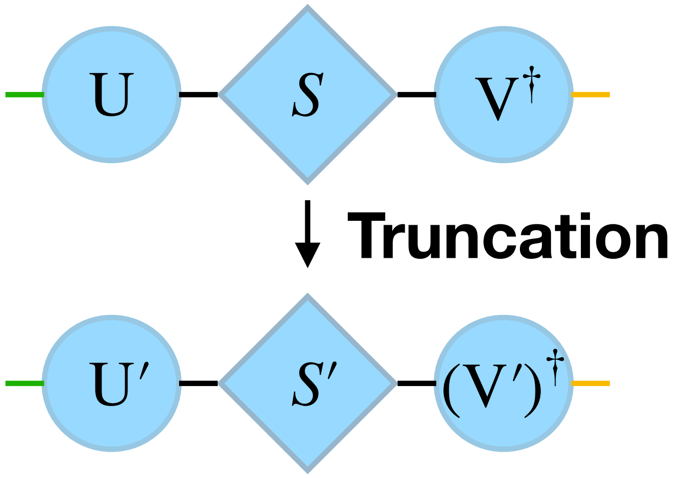
- We call χ_{max} **bond dimension** of the system, and denote with s_1 the greatest eigenvalue of S. Then:



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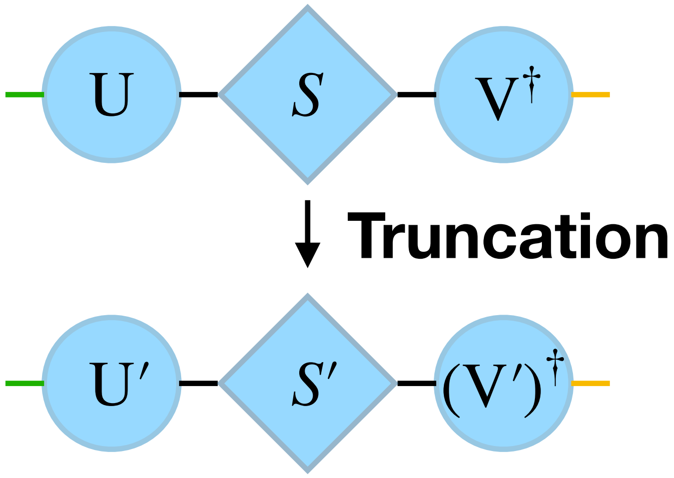

$$S' = \begin{cases} s_i & \textbf{if } \frac{s_i}{s_1} \geq \epsilon \textbf{ and } i \leq \chi_{max} \\ 0 & \textbf{otherwise} \end{cases}$$

We then truncate the 0 term

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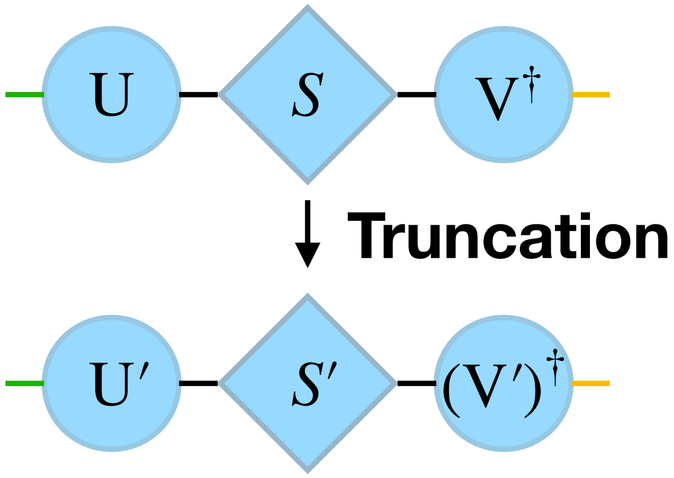

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We keep the eigenvalues only if they are **big enough**. In this way, we are neglecting the sub-leading term for the state description.

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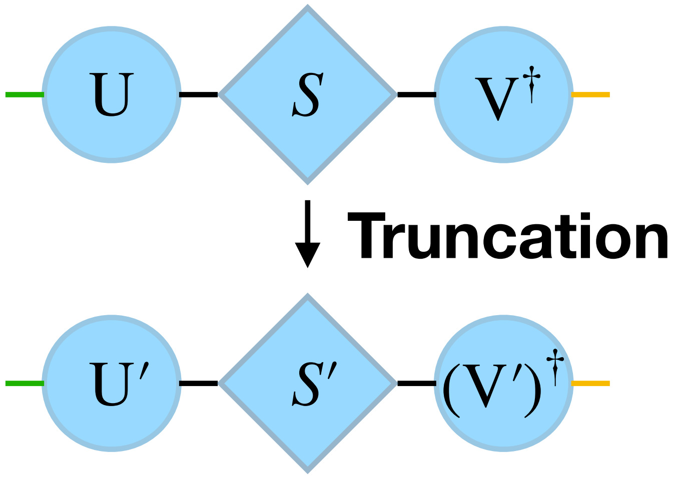


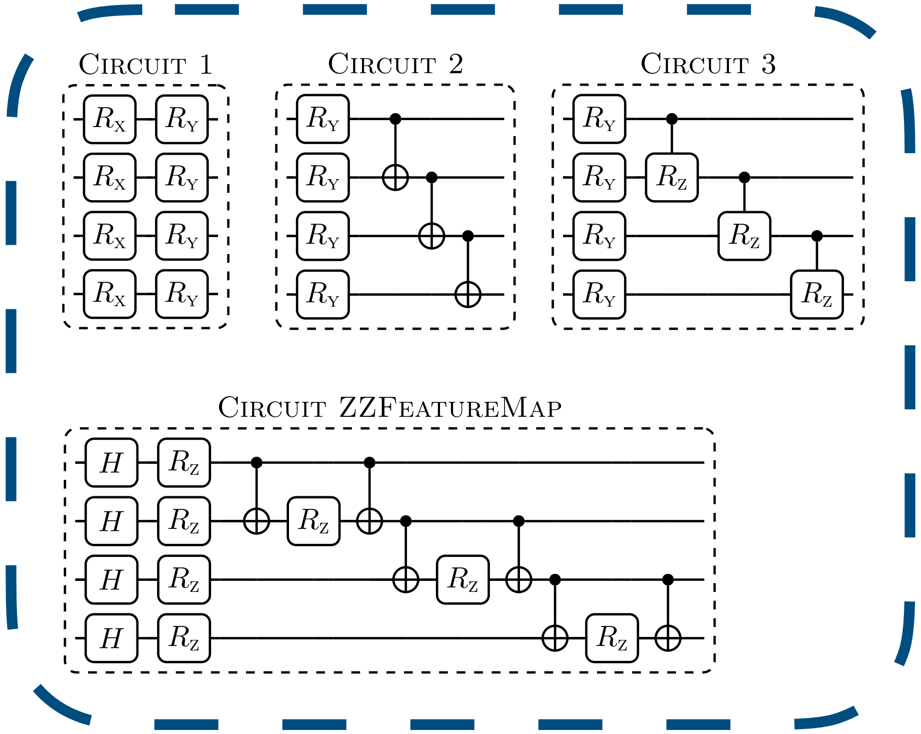
$$S' = \begin{cases} s_i & \textbf{if } \frac{s_i}{s_1} \geq \epsilon \textbf{ and } i \leq \chi_{max} \\ 0 & \textbf{otherwise} \end{cases}$$

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.

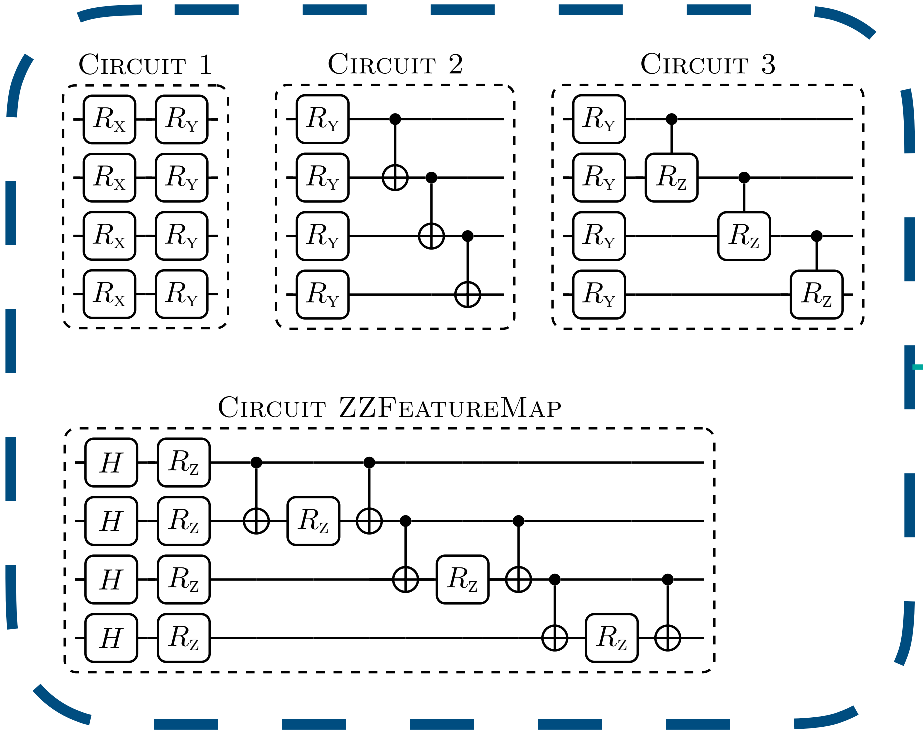
We keep only the **first highest** χ_{max} eigenvalues. In this way, we keep the quantum state manageable even for big number of qubits. However, this may be a strong approximation.

Methods



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

Methods



Select number of layers L

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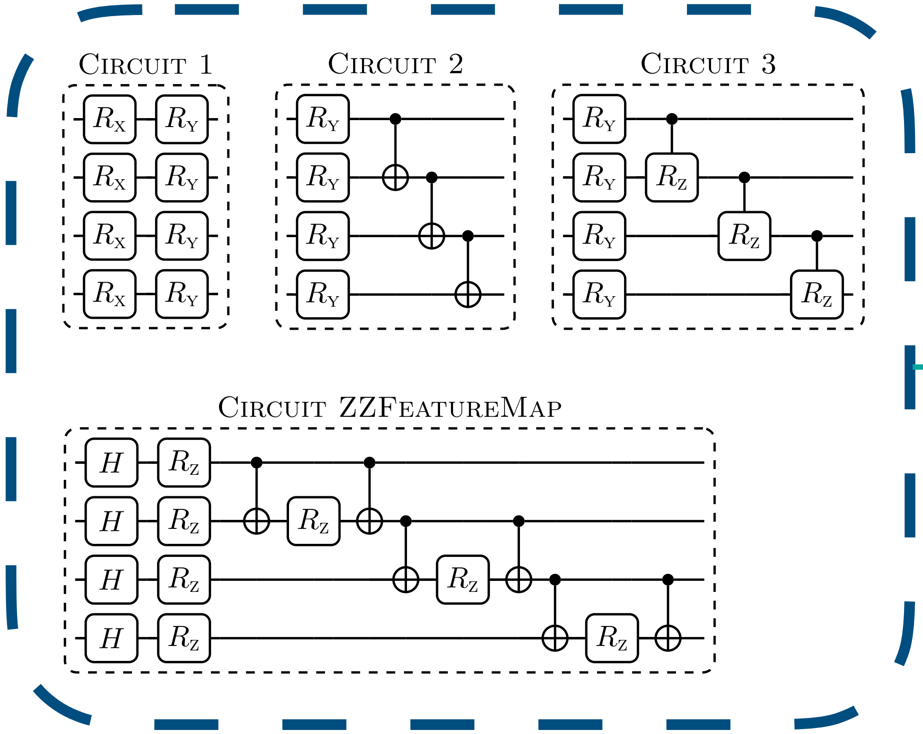

Pick a feature map $\mathscr{F}(x)$
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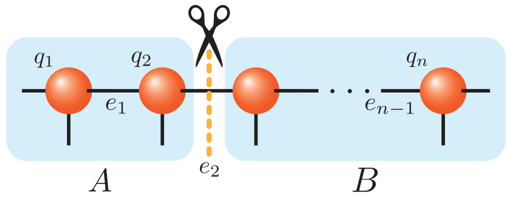
Select number
of layers L

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

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

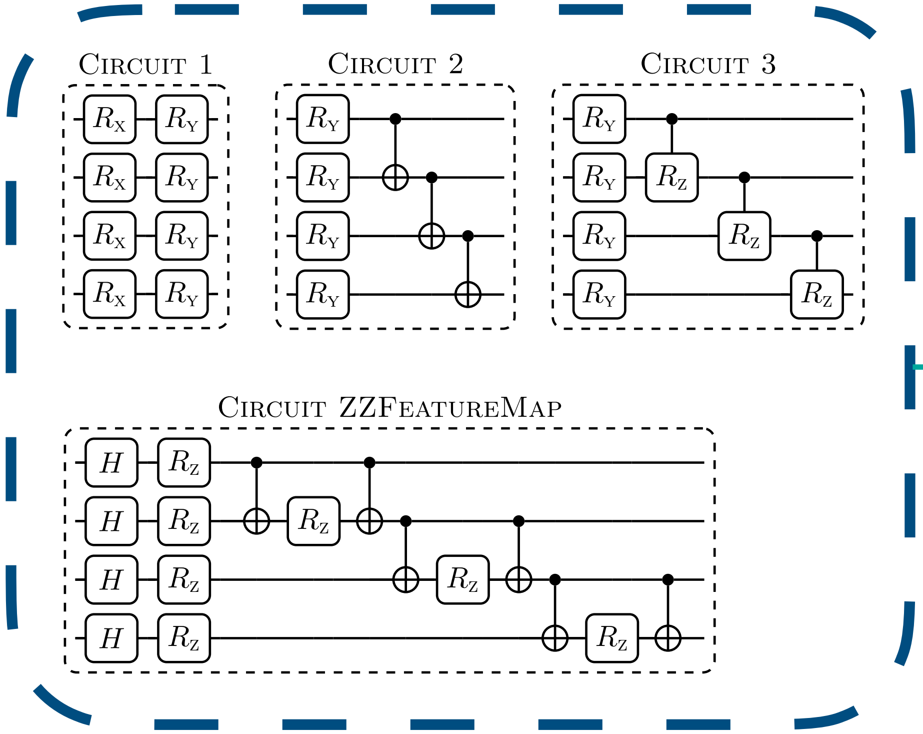


Simulate the evolution
and compute final state

Compute entanglement
on each edge e_i

Repeat M times and take the
average over the realisations

Methods



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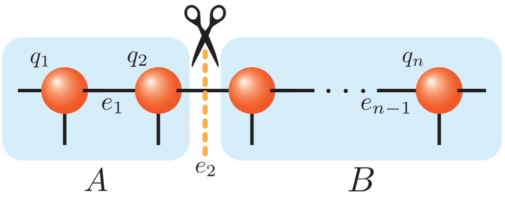

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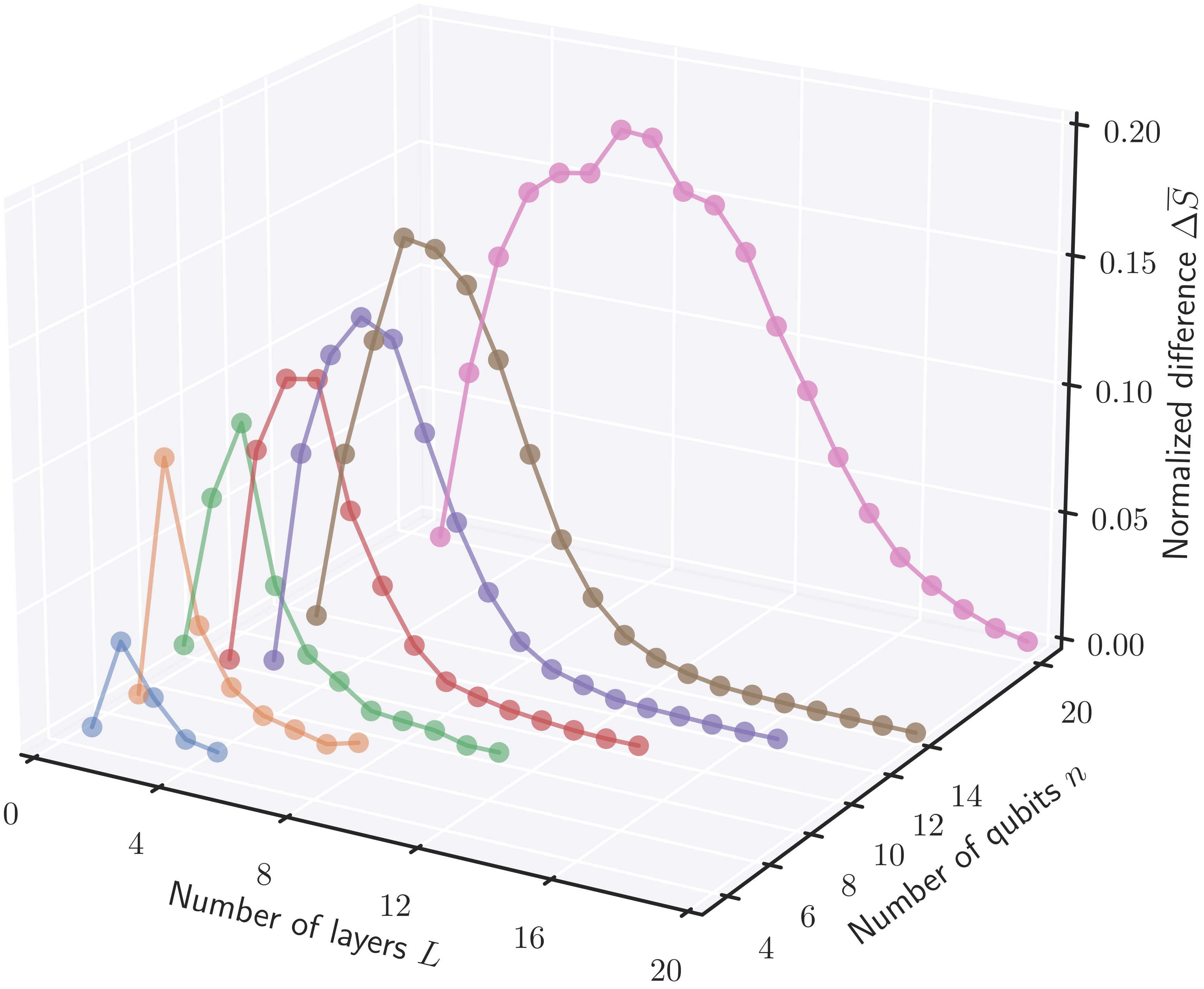
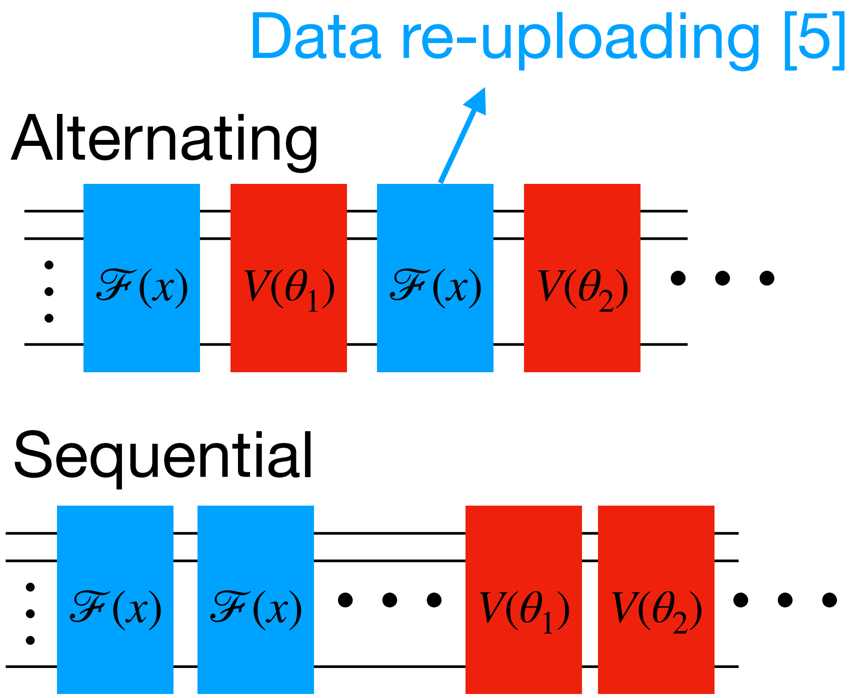
Qiskit up to ~ 16 qubits
with state vector

Efficient simulation

Quantum matcha tea
Tensor network emulator
up to 50 qubits

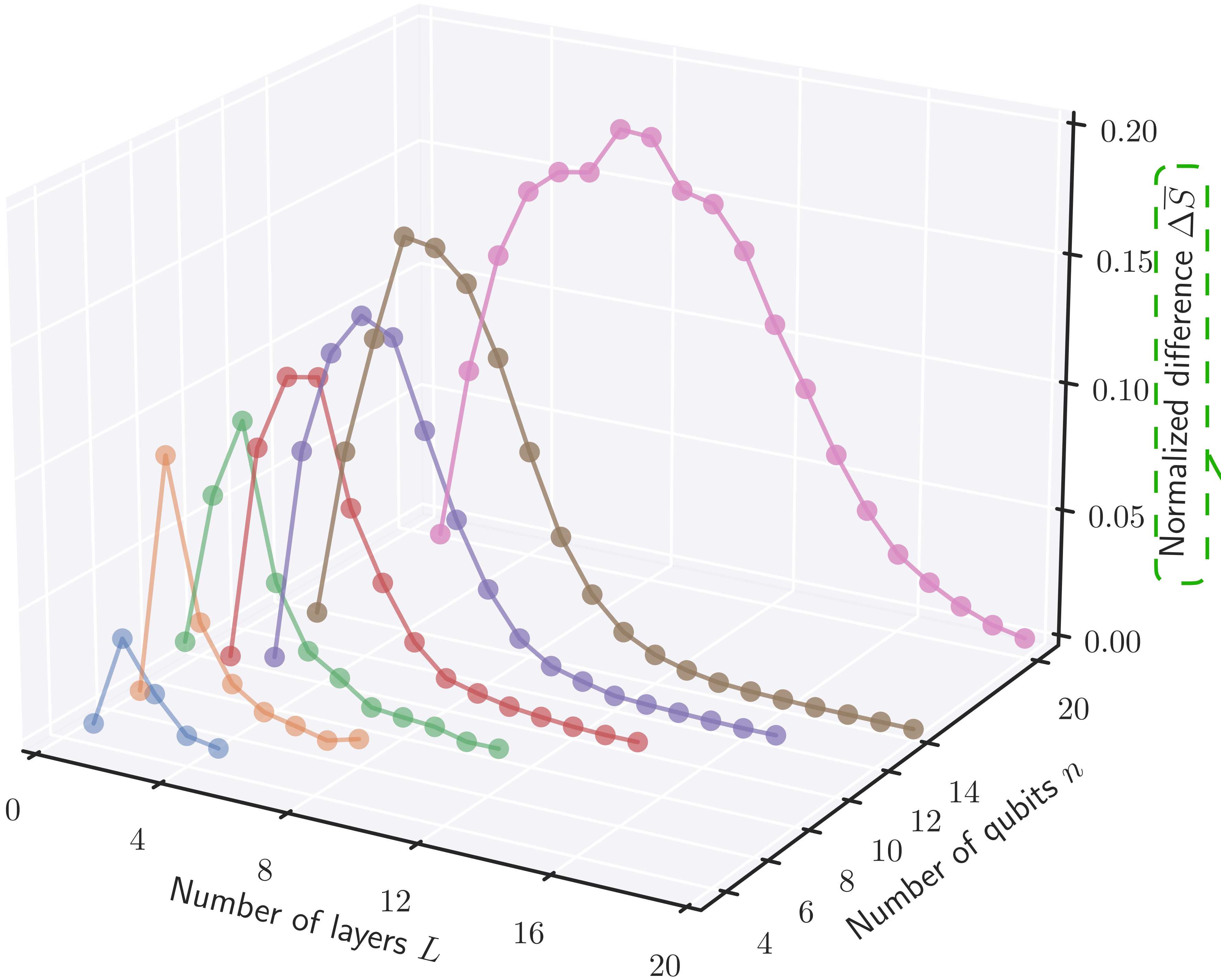
Alternating VS sequential



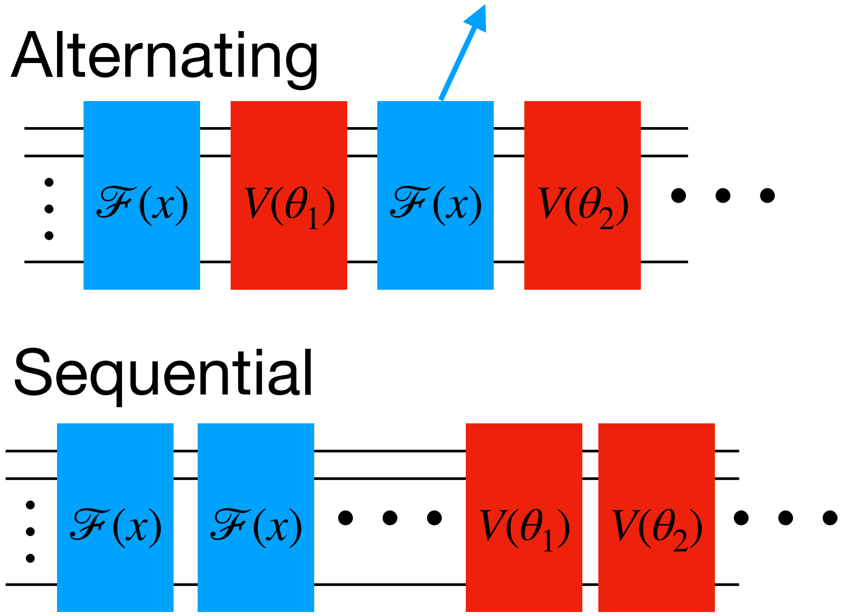


[5] Pérez-Salinas, Adrián, et al. "Data re-uploading for a universal quantum classifier." *Quantum* 4 (2020): 226.

Alternating VS sequential



Data re-uploading [5]



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

---

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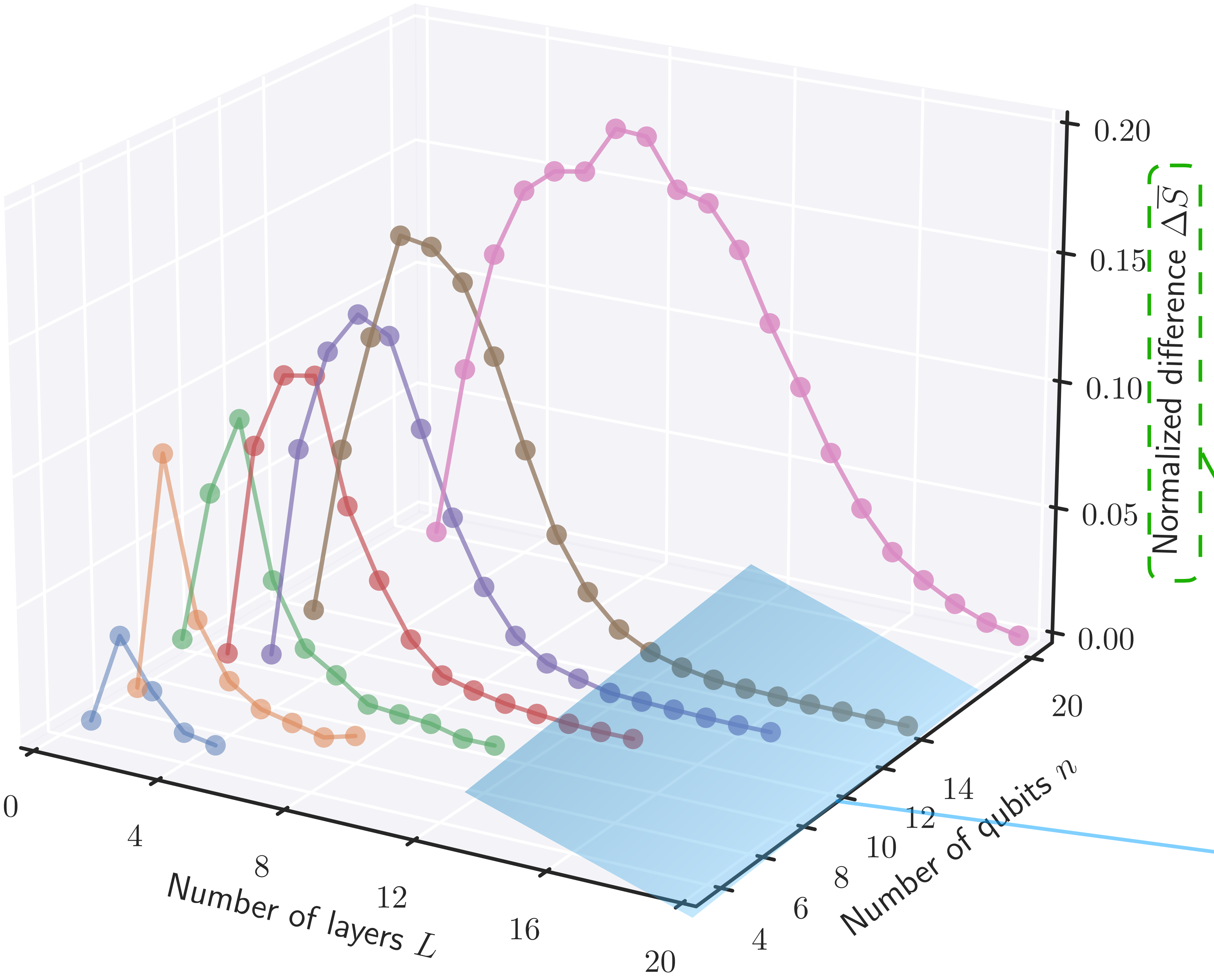

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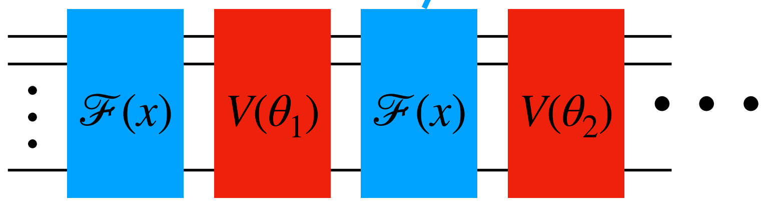
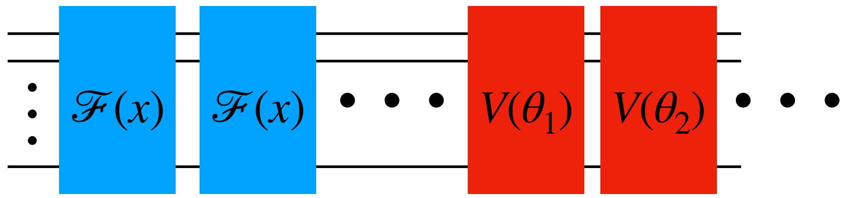


Sequential



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Both tends towards Haar-random

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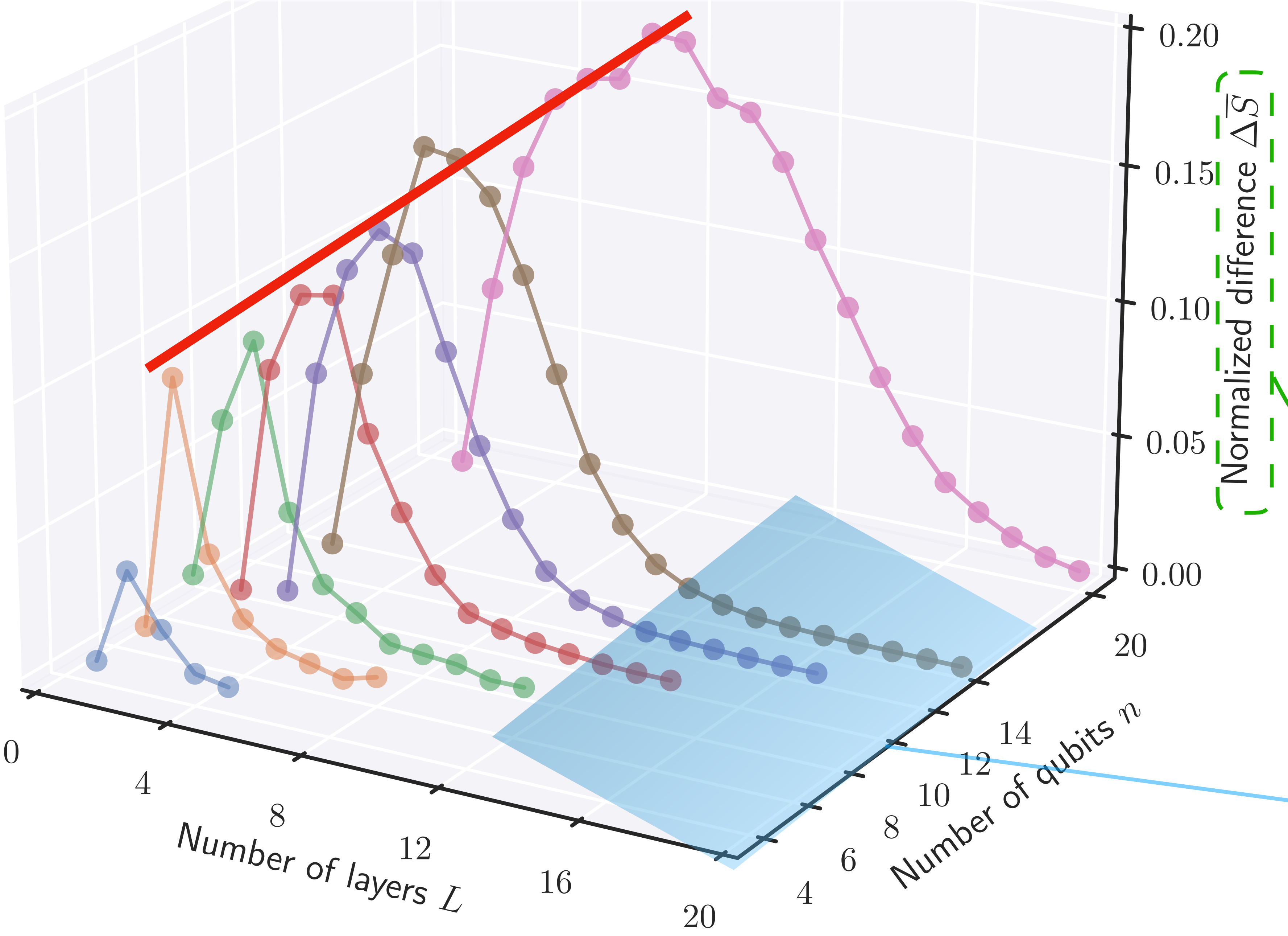
Alternating VS sequential

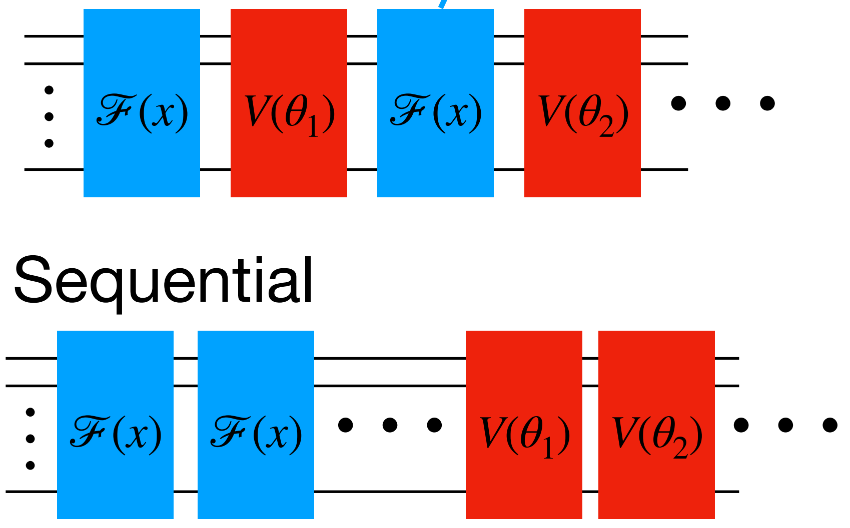
Significative difference that increases with the number of qubits n, up to almost $20\ \%$ for $n = 20$



Data re-uploading [5]

Alternating

Sequential



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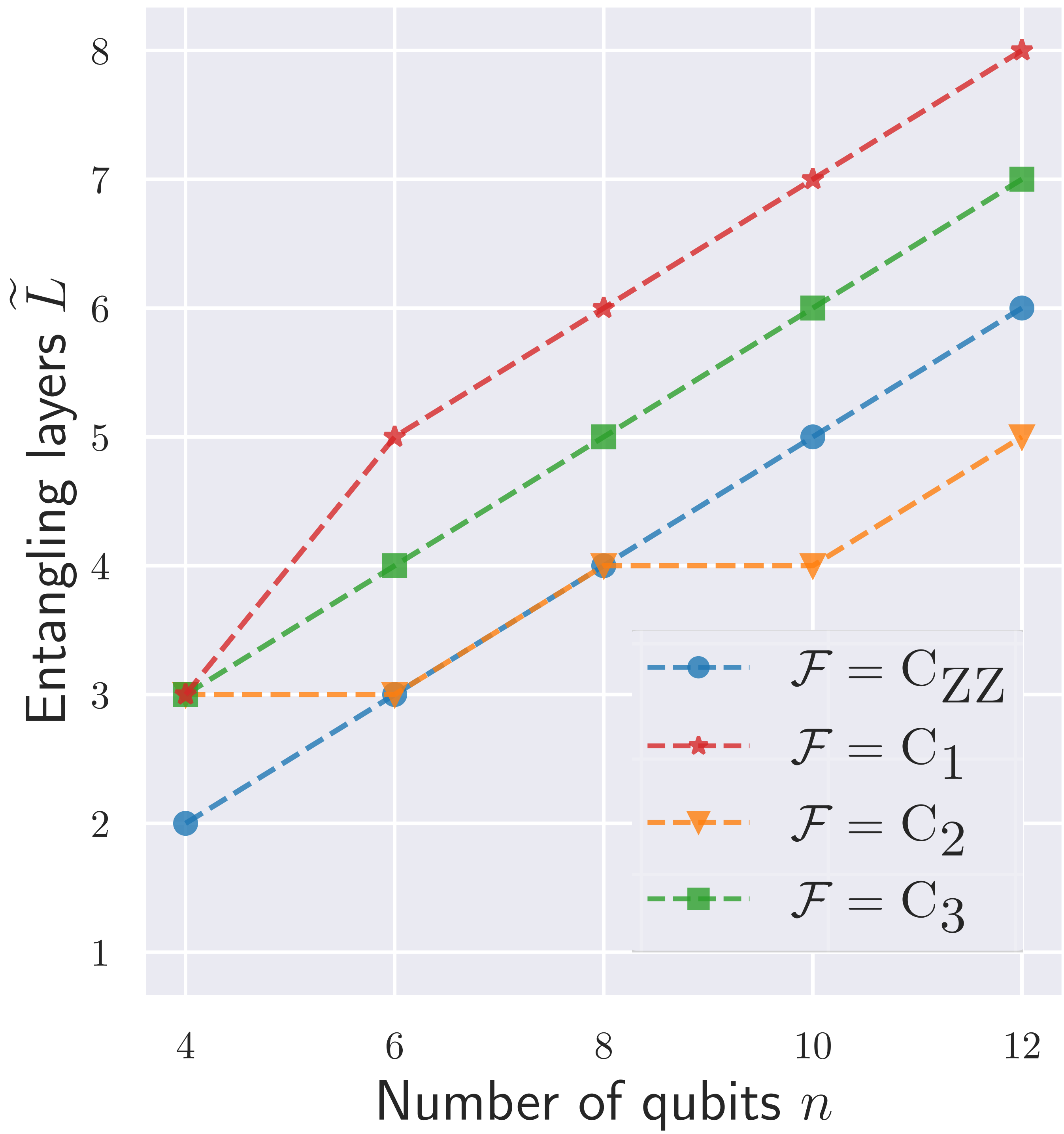
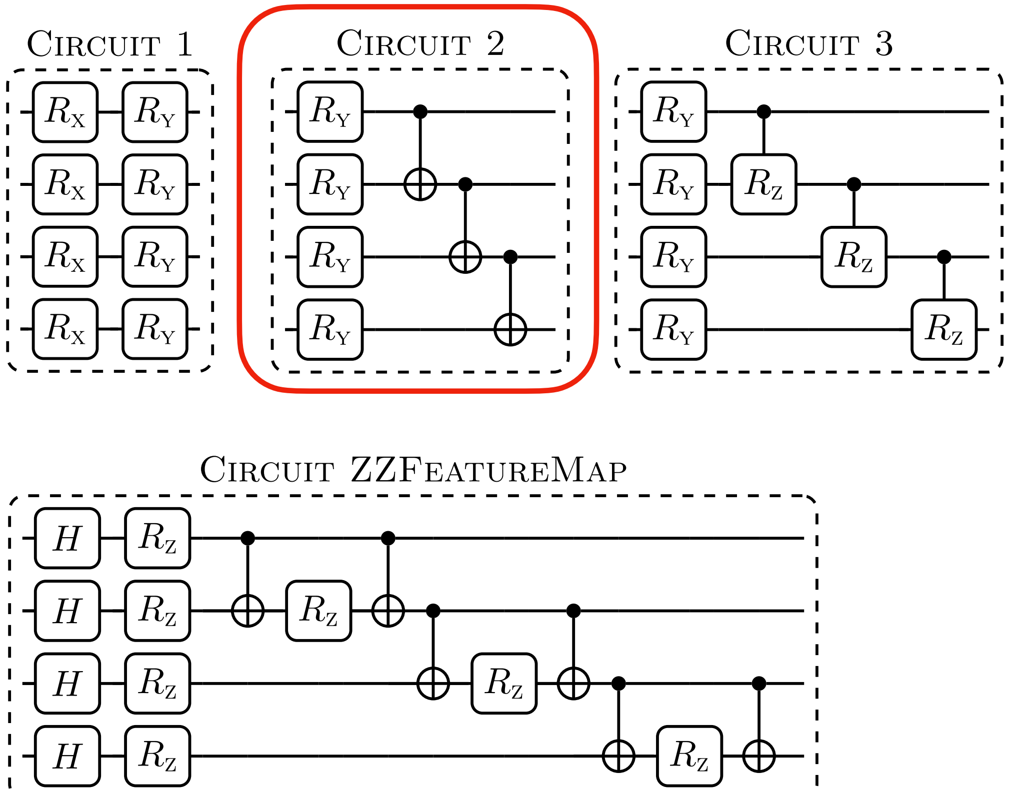
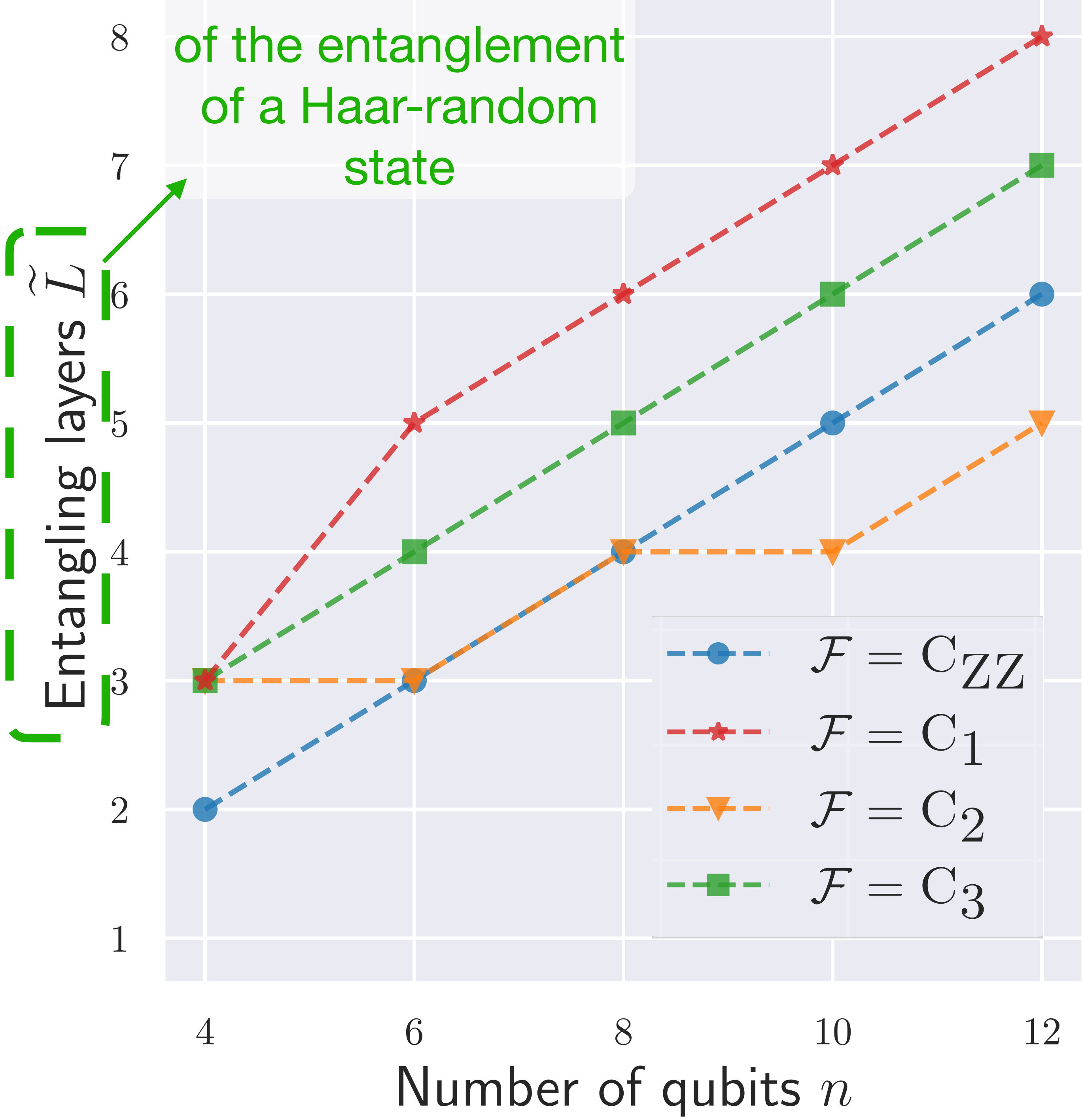
Entanglement scaling with depth





C_2 is always used as variational ansatz

Entanglement scaling with depth



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

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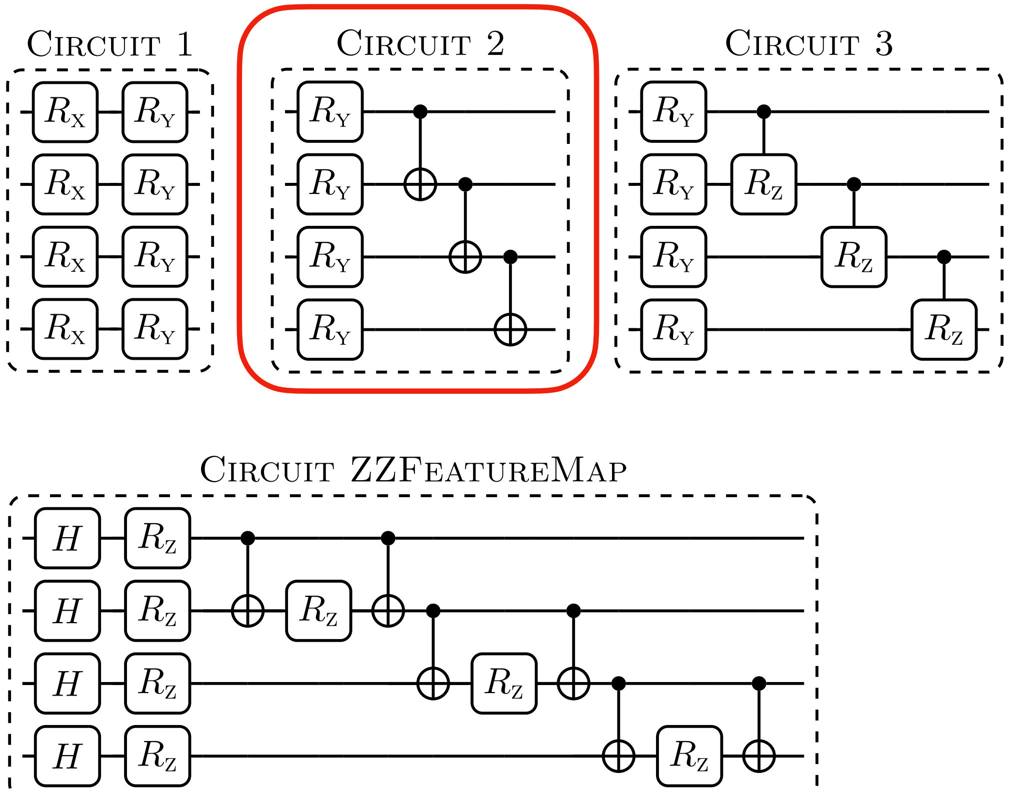

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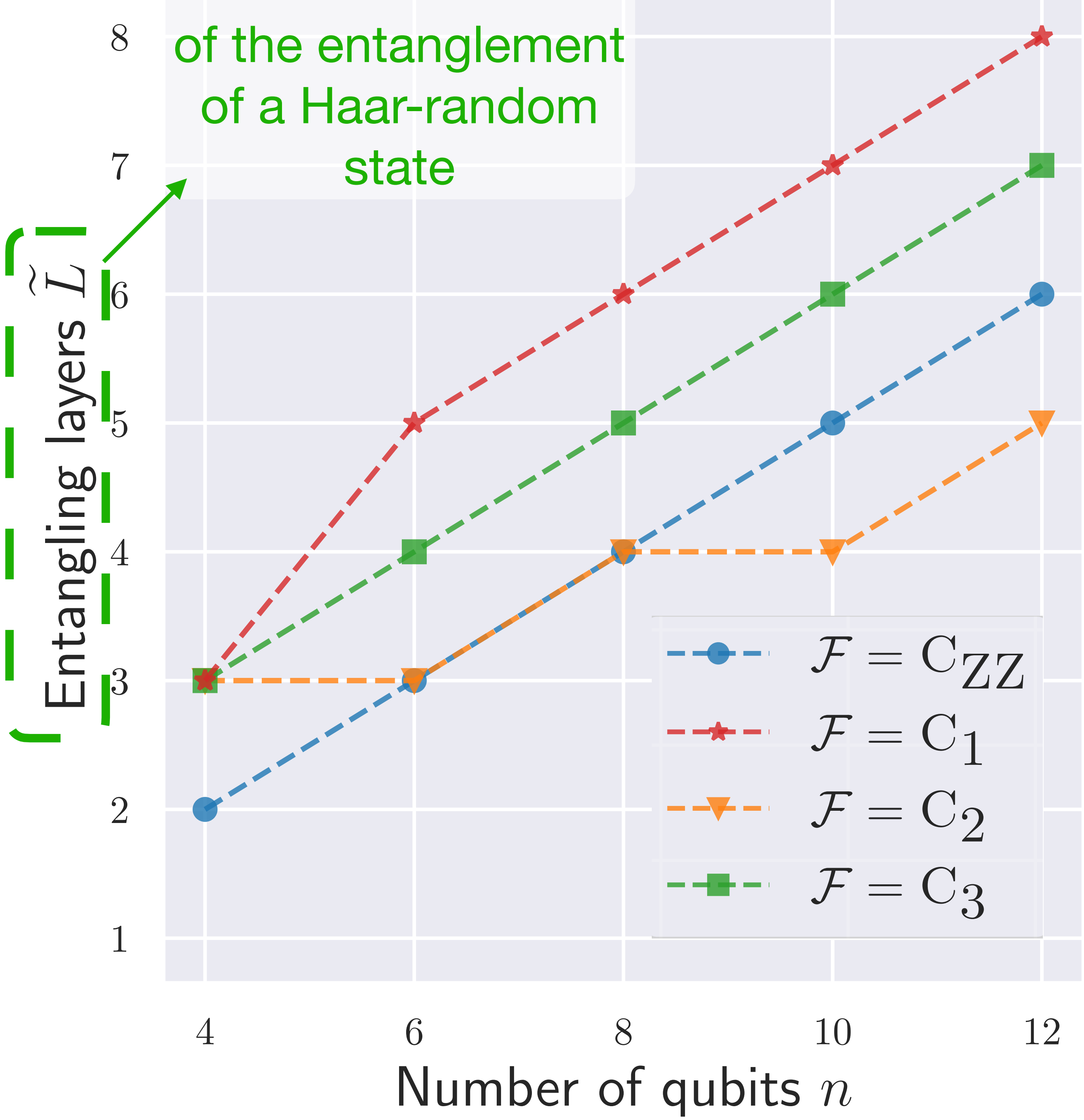
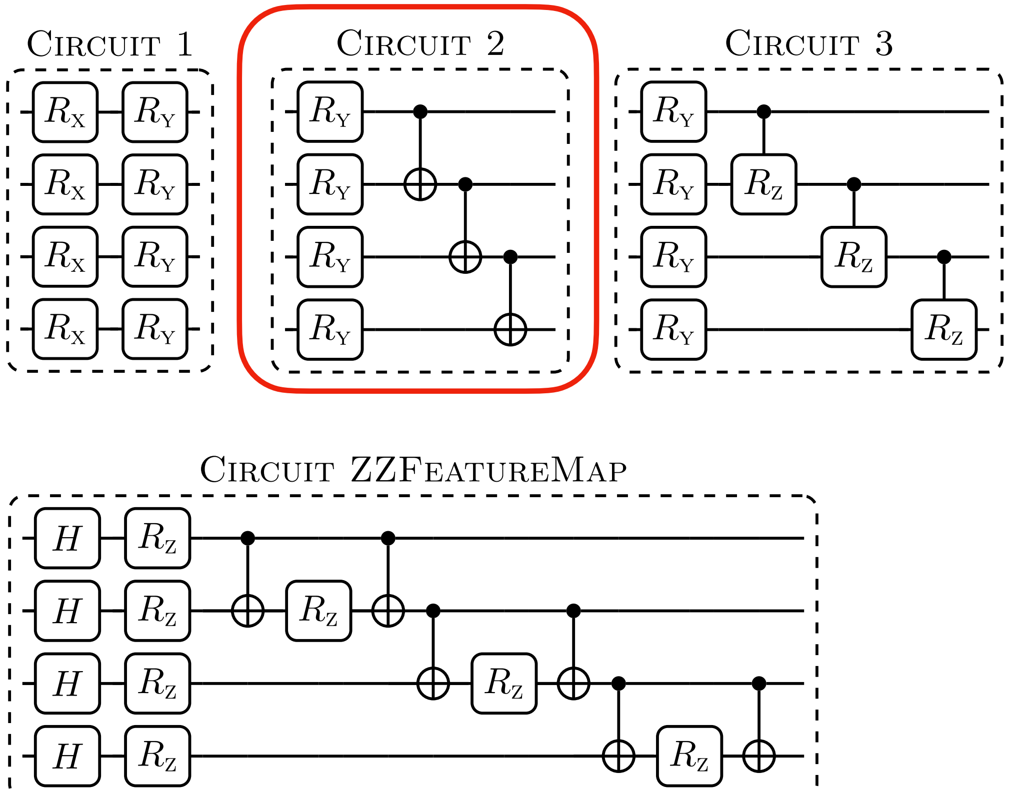


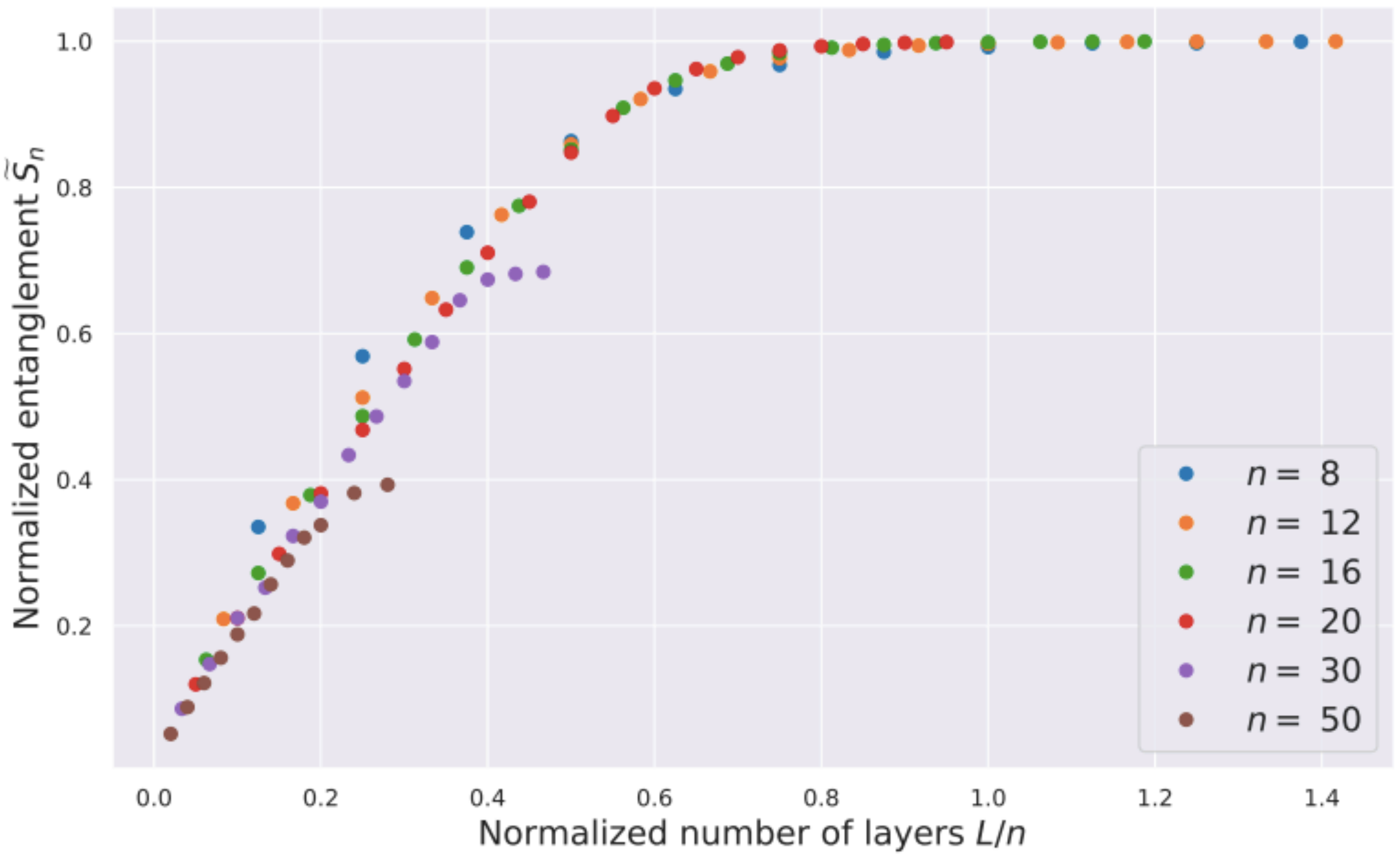
Layers needed
to reach $90\,\%$
of the entanglement
of a Haar-random
state

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

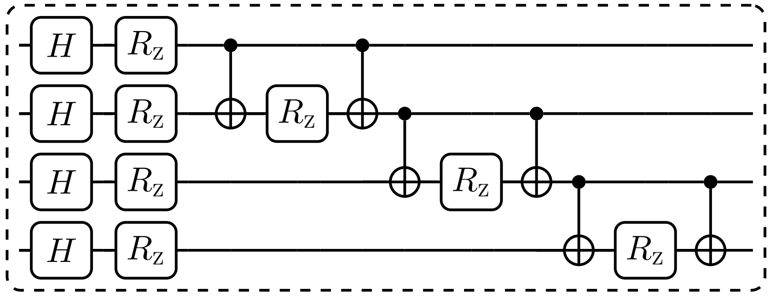
C_2 is always used as
variational ansatz



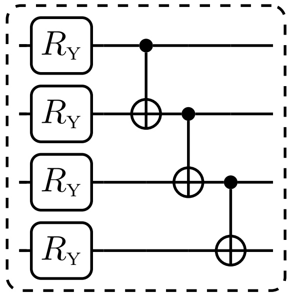
Entangling speed



Circuit ZZFeatureMap



Circuit 2

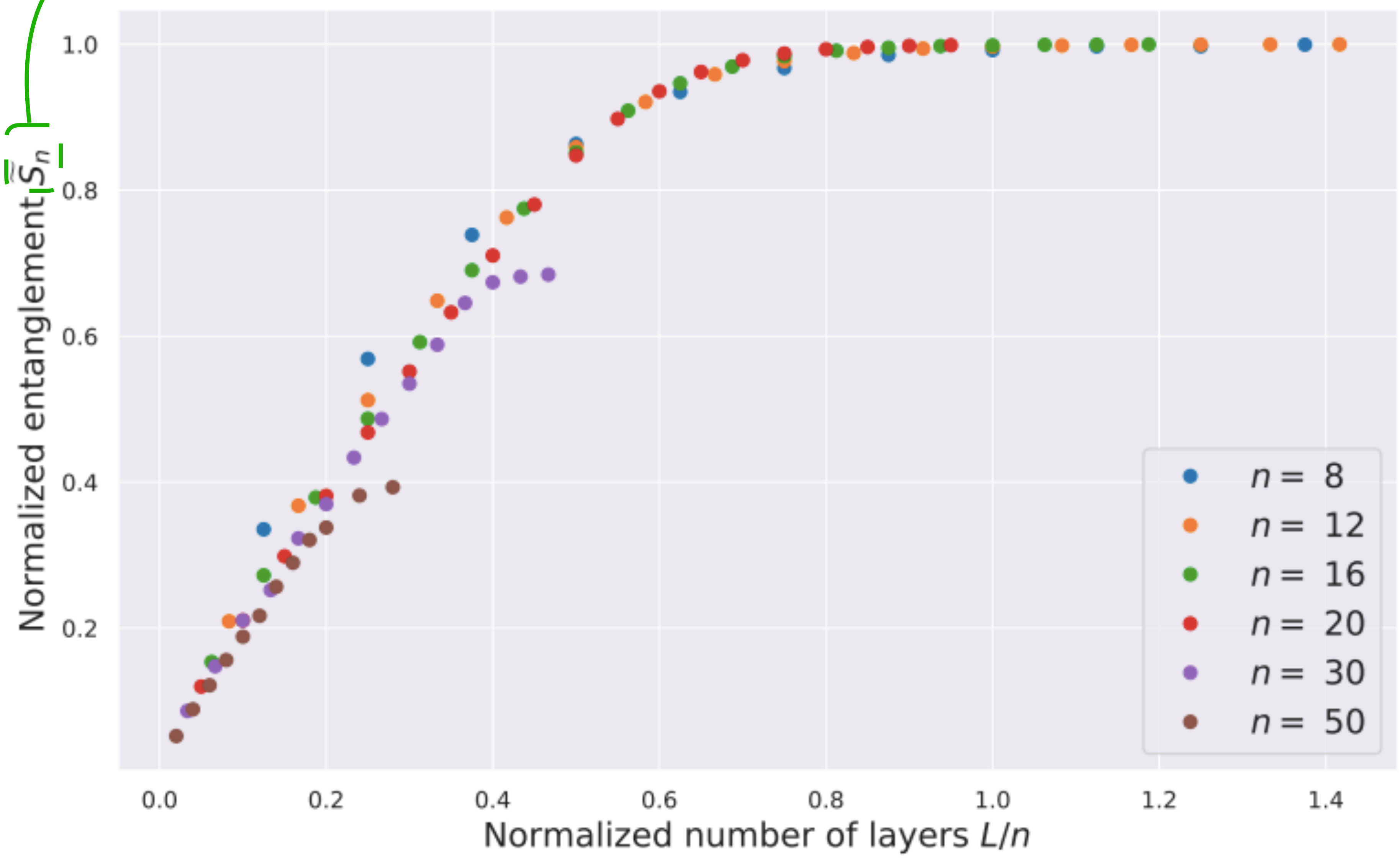


Feature map	Variational Ansatz	Entangling speed
C_{zz}	C_2	(1.8 ± 0.1)
C_{zz}	C_3	(0.59 ± 0.02)
C_1	C_3	(0.316 ± 0.006)

Entangling speed

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

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



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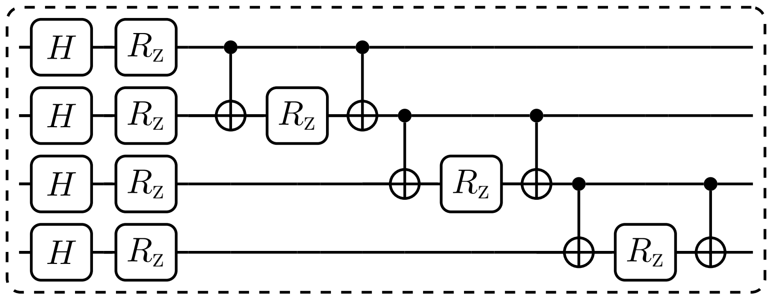

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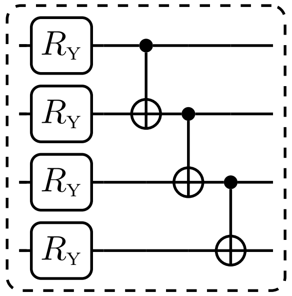

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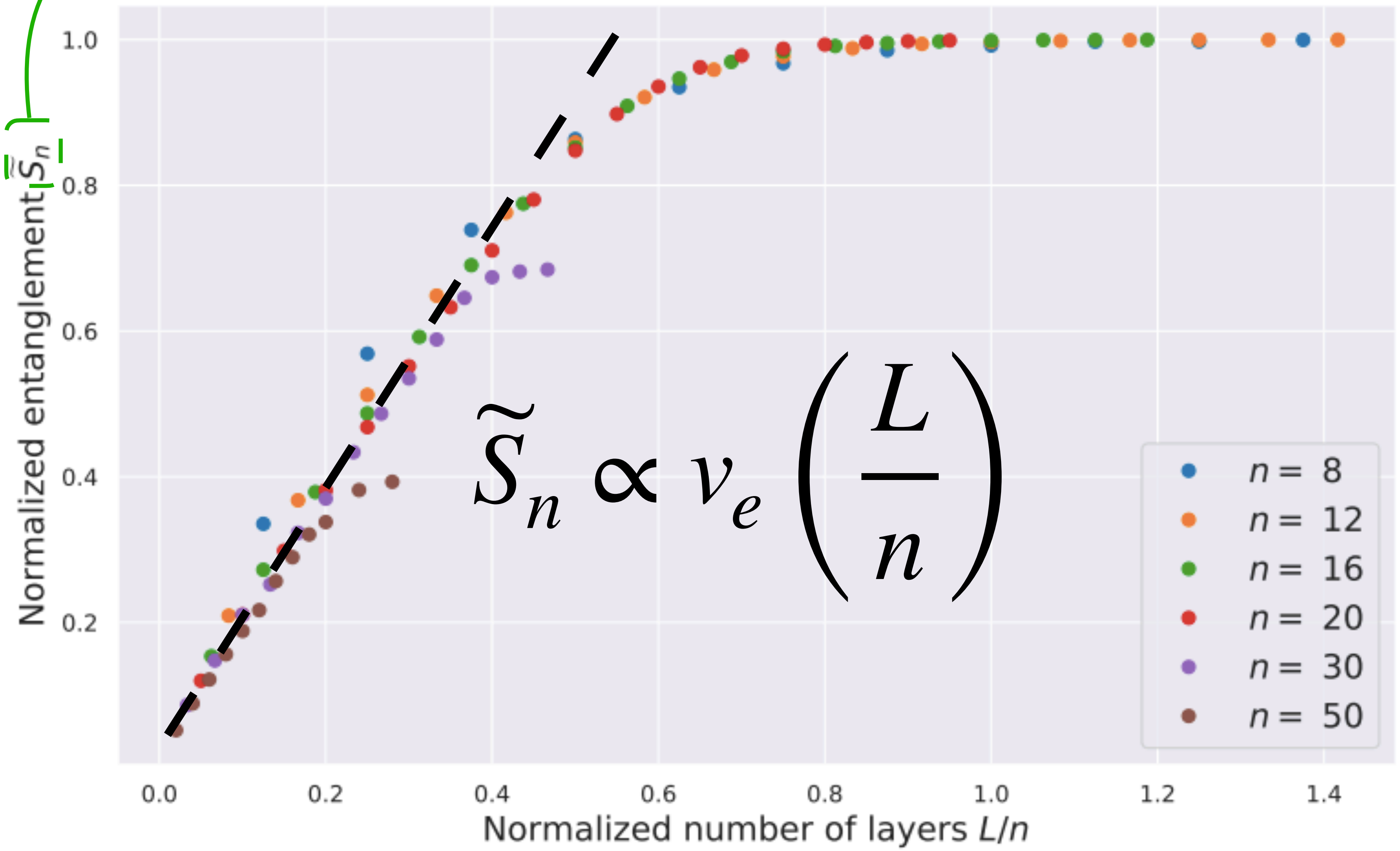

$$\widetilde{S}_n \propto v_e\left(\frac{L}{n}\right)$$

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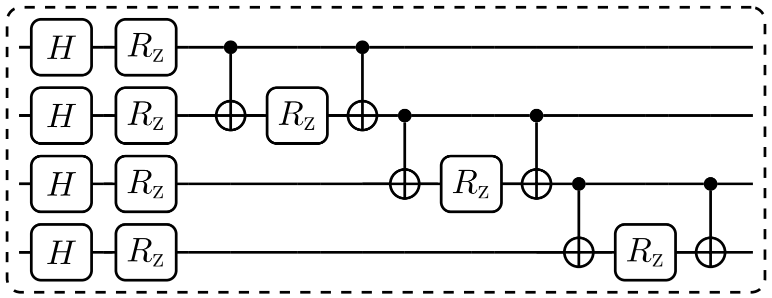

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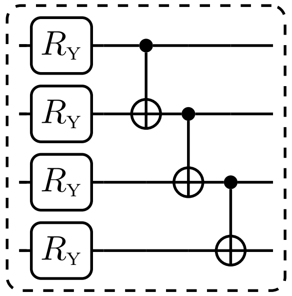

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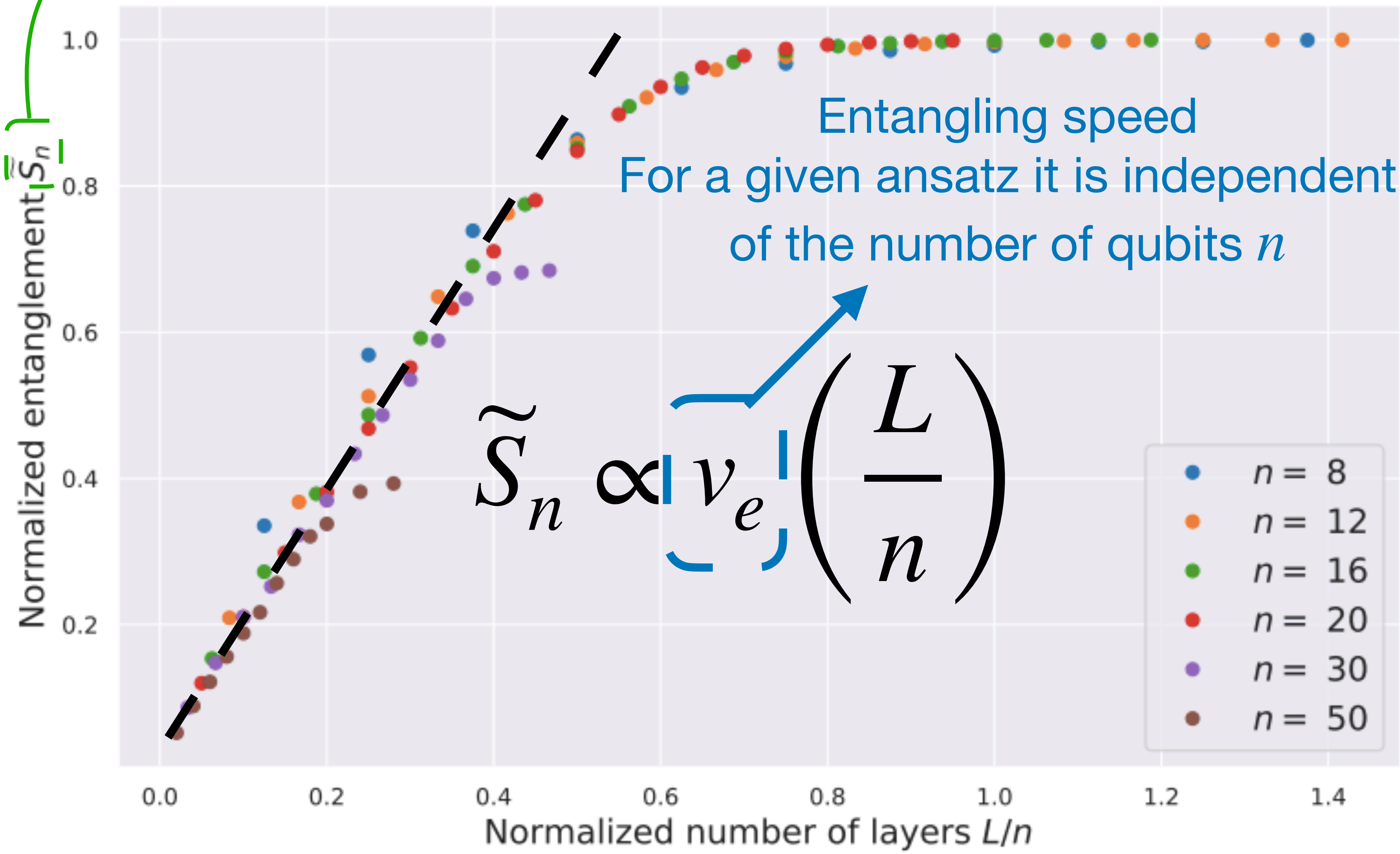

Entangling speed

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

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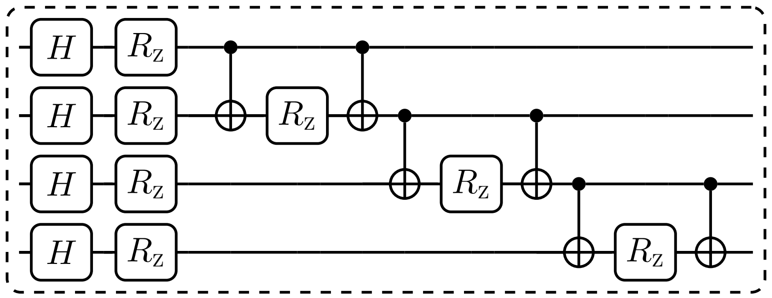

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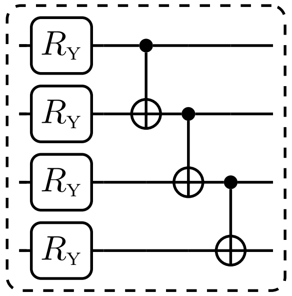

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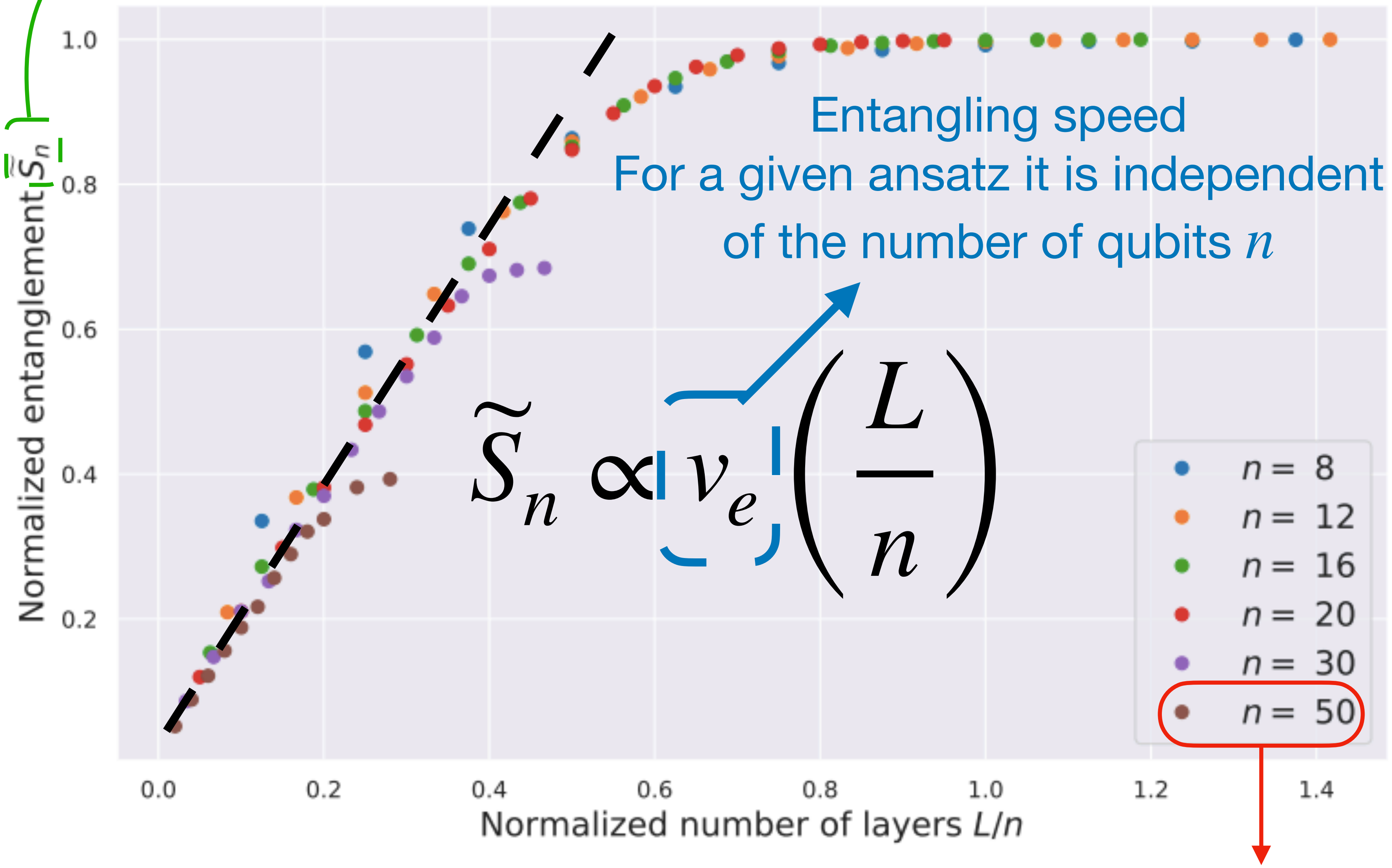

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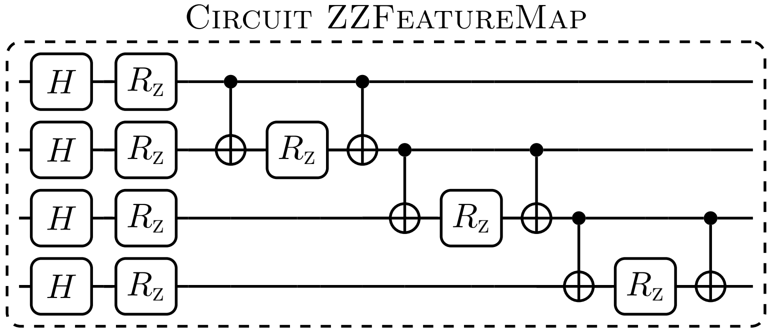

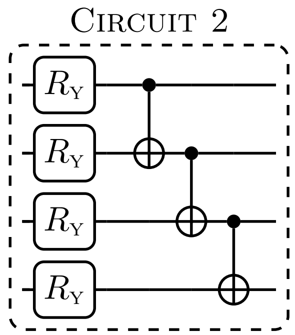

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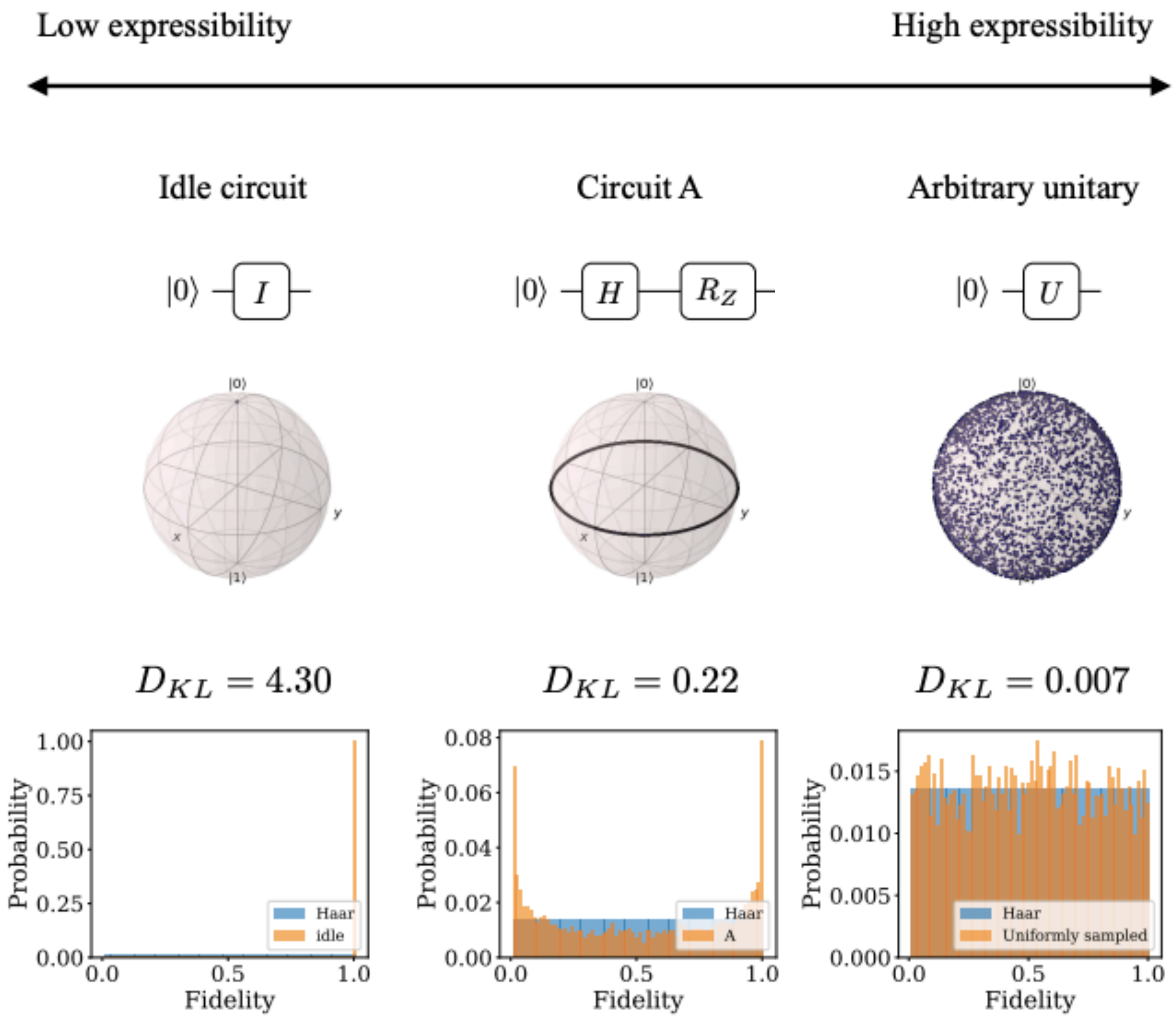
Using Galileo100 HPC from CINECA

Expressibility



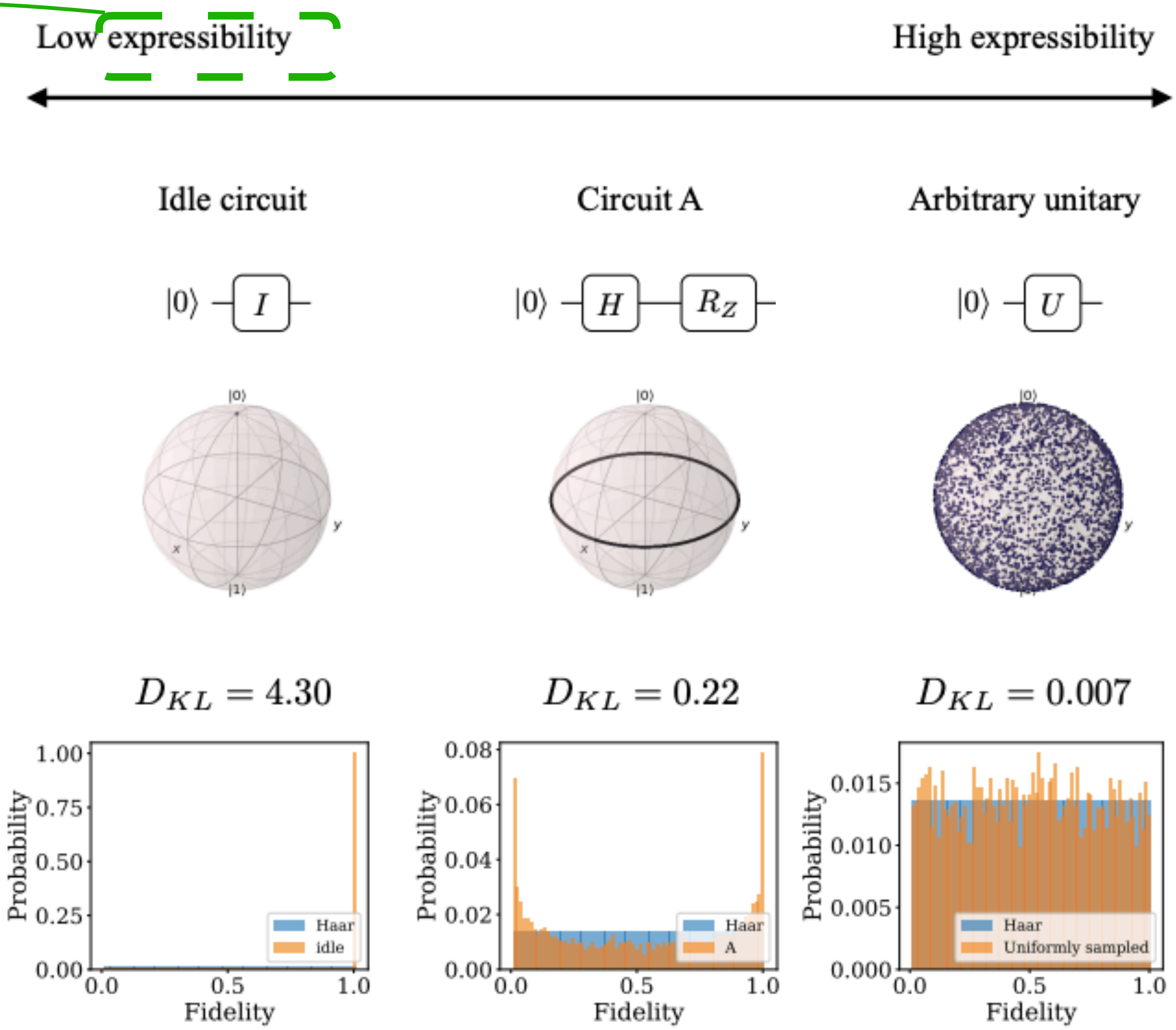
[6] Sim, Sukin, Peter D. Johnson, and Alán Aspuru-Guzik. "Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms." *Advanced Quantum Technologies* 2.12 (2019): 1900070.

Expressibility

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

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



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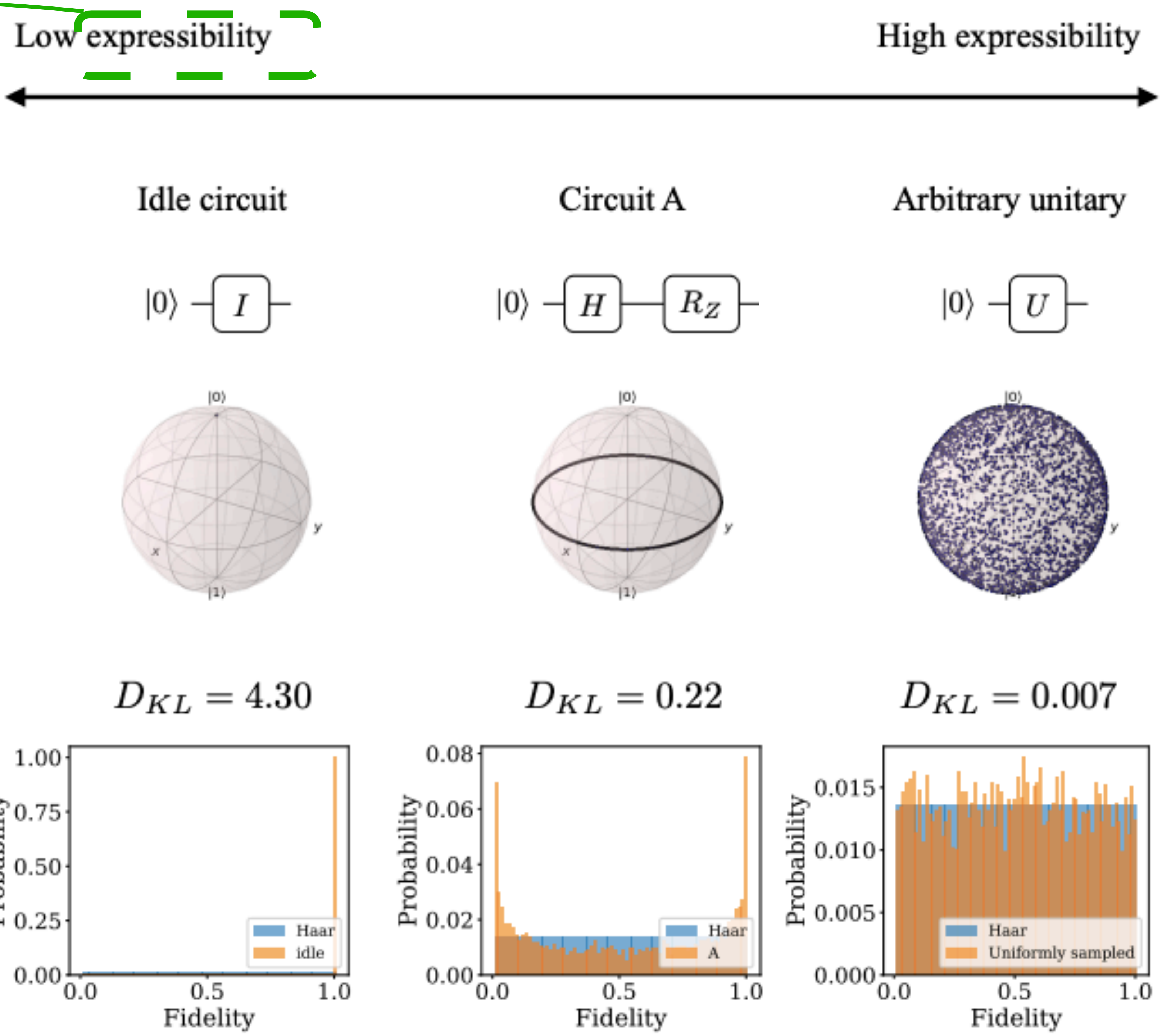
2. Compute the overlap $F = |\langle\psi_\gamma|\psi_\phi\rangle|^2$
3. Repeat many times to obtain statistics



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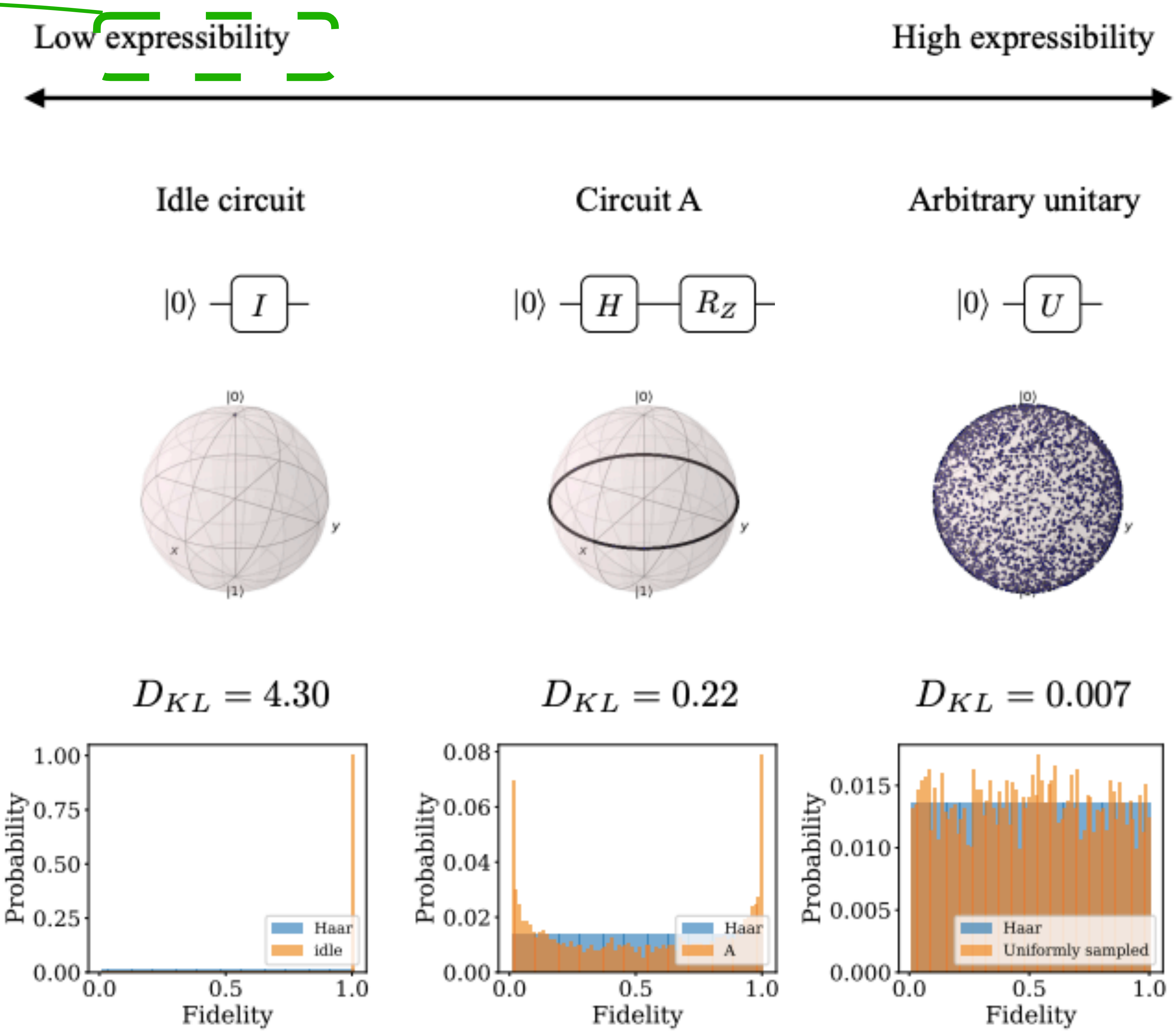
Uniformly distributed fidelity
$\Rightarrow$ address the full space



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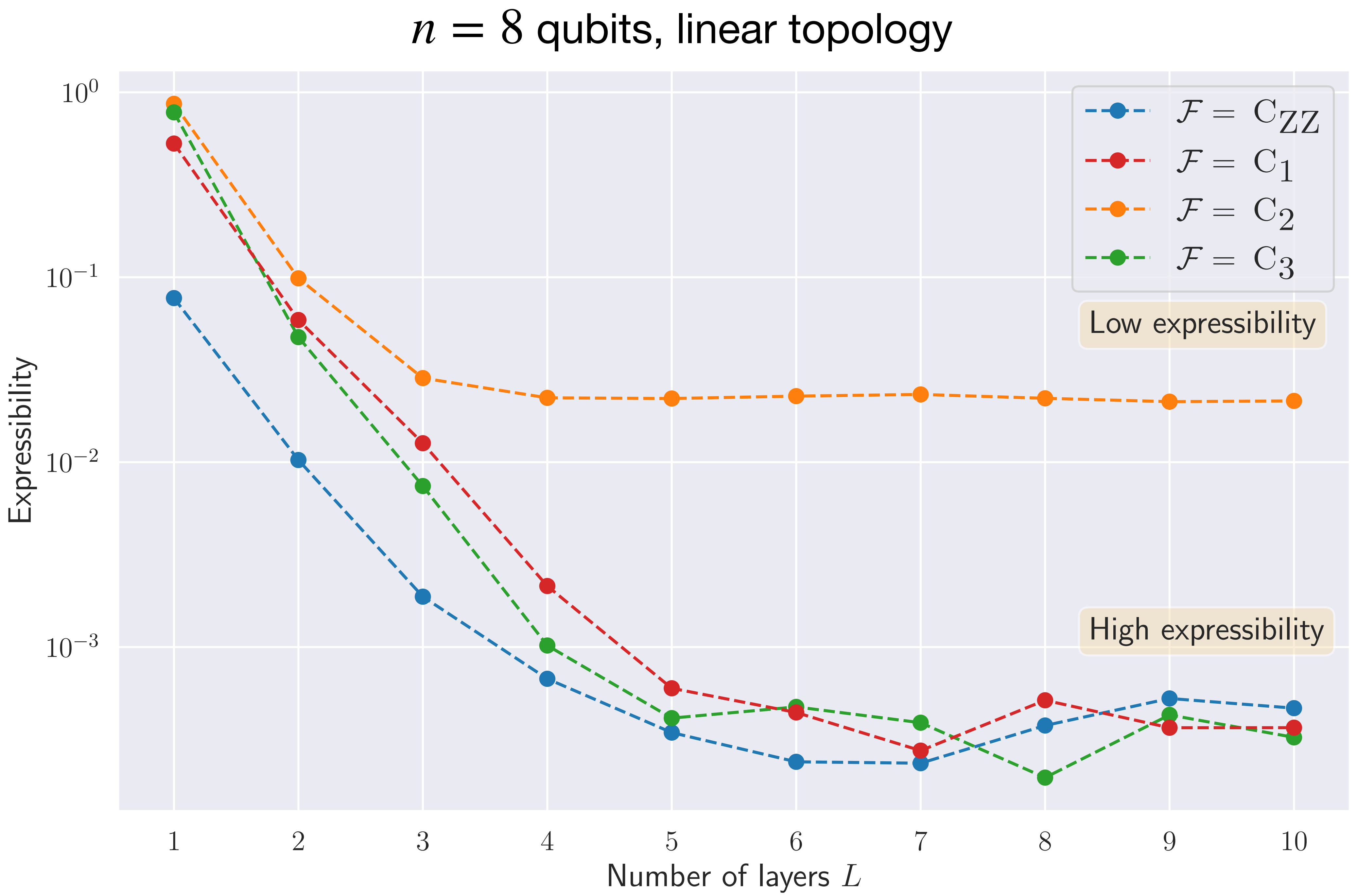
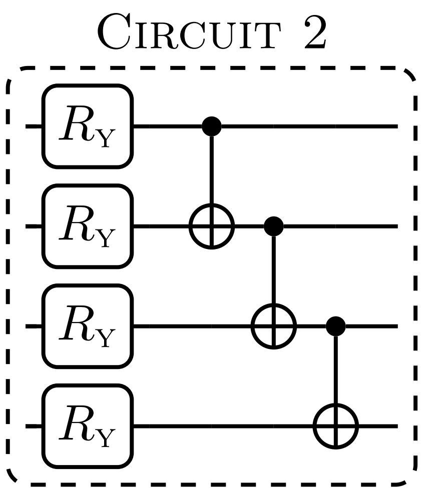

$n = 8$ qubits, linear topology

Variational ansatz



[3] Abbas, Amira, et al. "The power of quantum neural networks." *Nature Computational Science* 1.6 (2021): 403-409.

Expressibility

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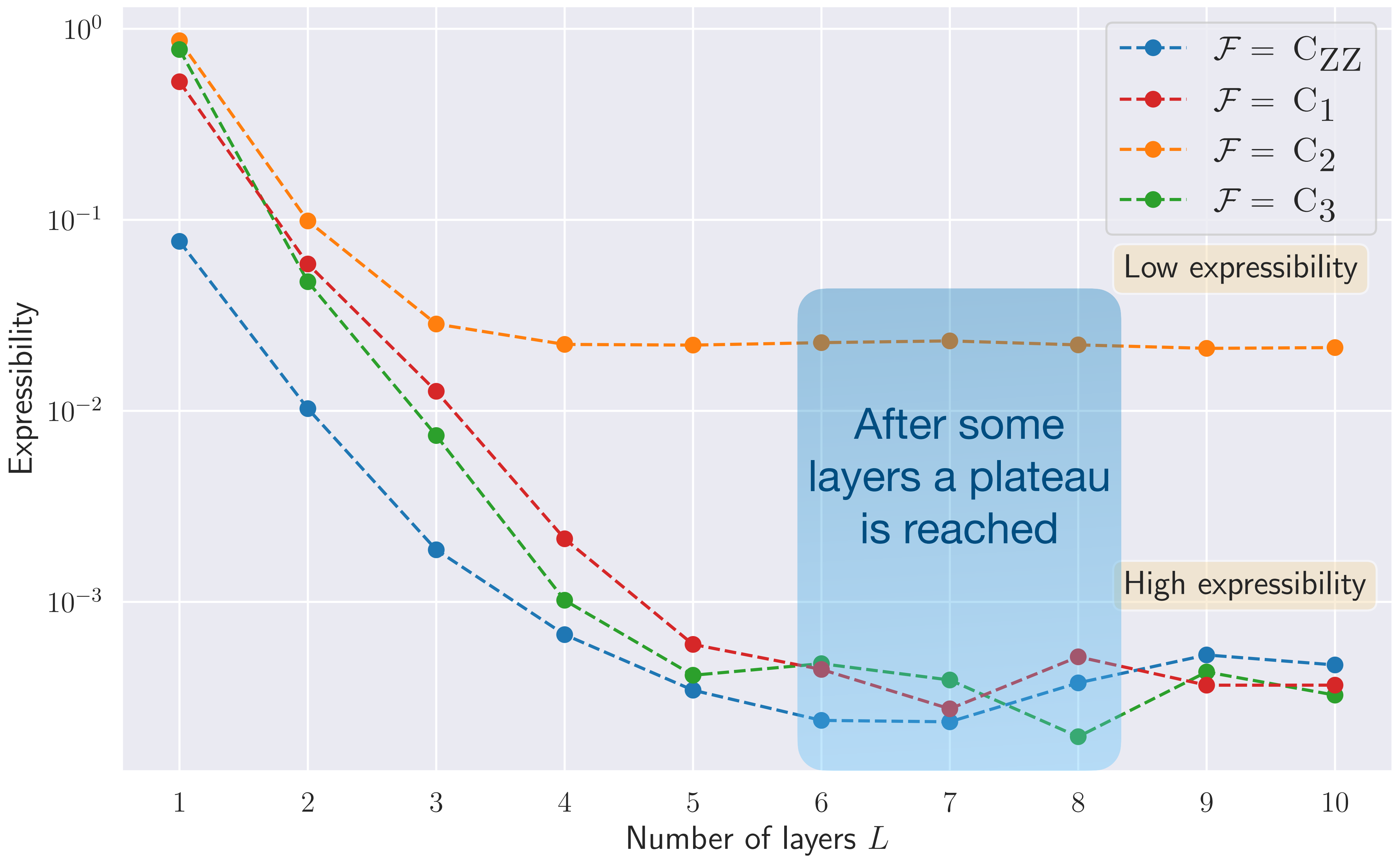


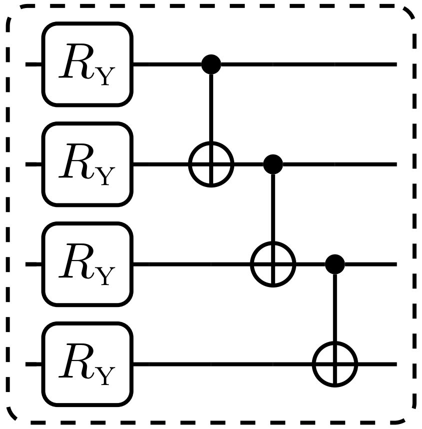
Low expressibility

After some layers a plateau is reached

High expressibility

Variational ansatz

CIRCUIT 2



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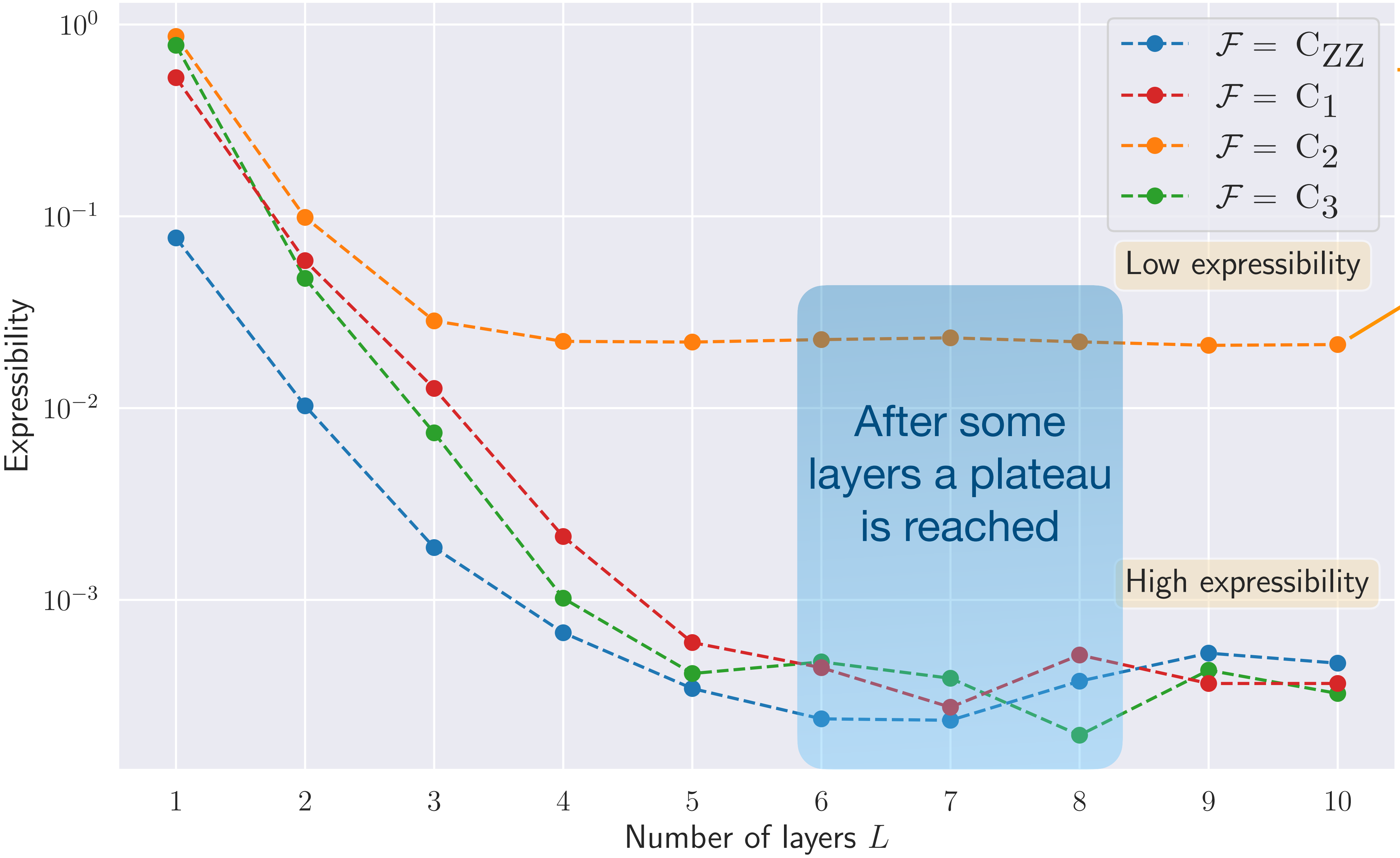


Low expressibility

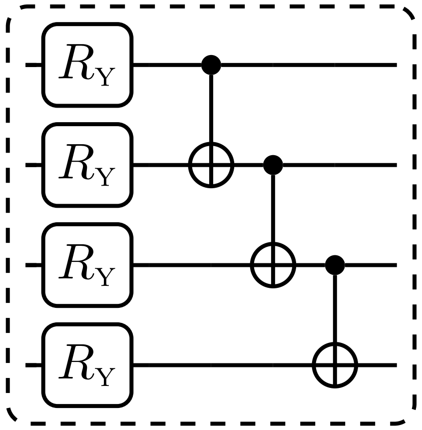
High expressibility

After some layers a plateau is reached

The circuit that builds entanglement faster has the worst expressibility

Variational ansatz

Circuit 2



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Expressibility

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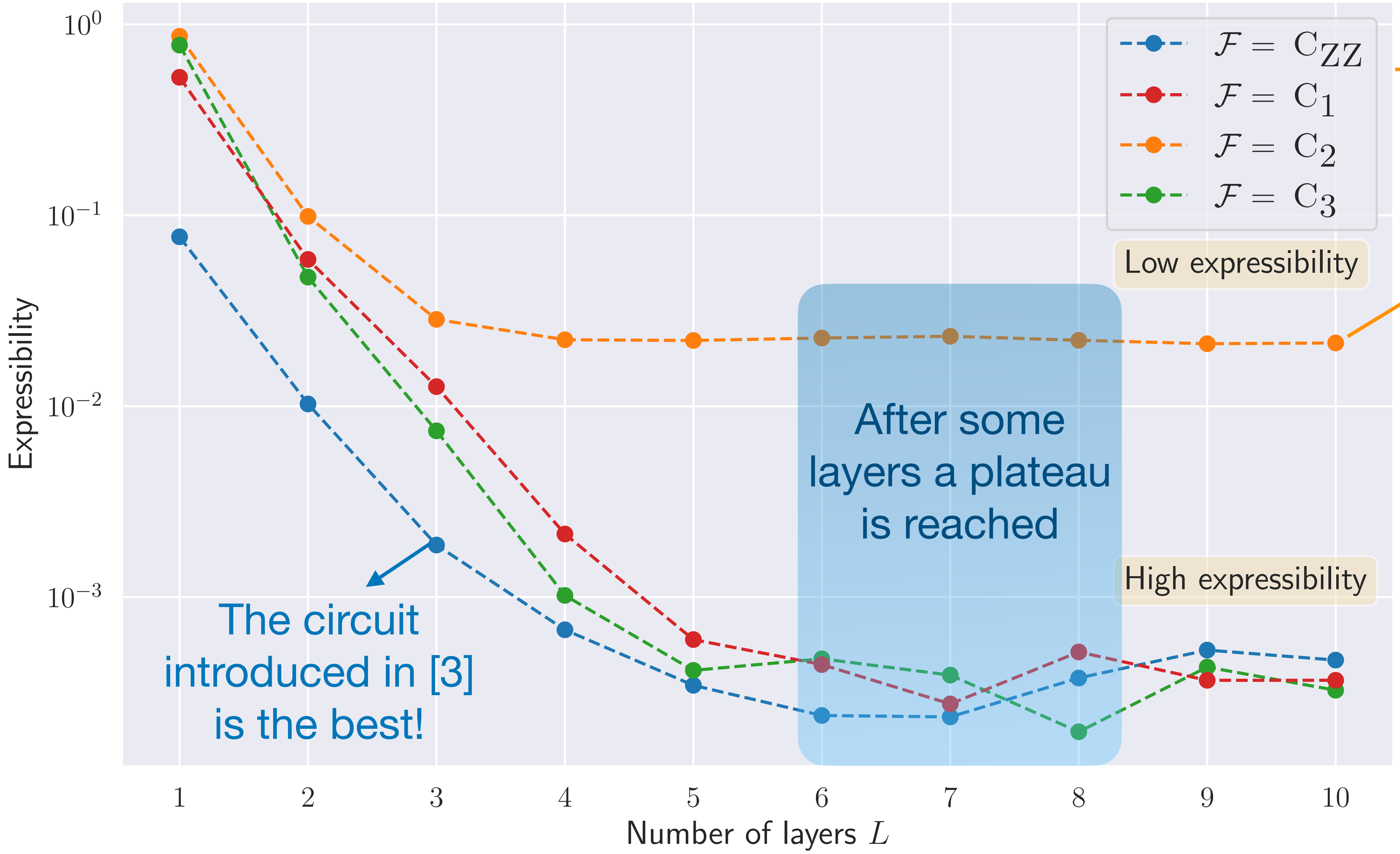


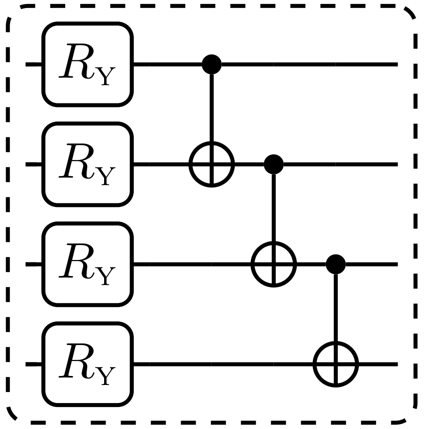
After some layers a plateau is reached

The circuit introduced in [3] is the best!

The circuit that builds entanglement faster has the worst expressibility

Variational ansatz

Circuit 2



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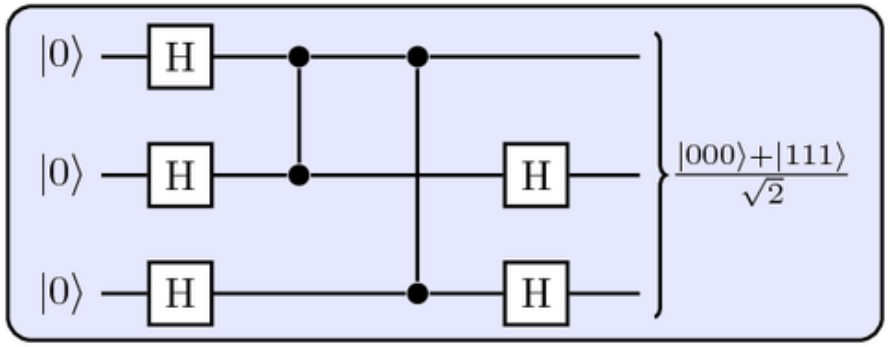
Quantum Matcha Tea

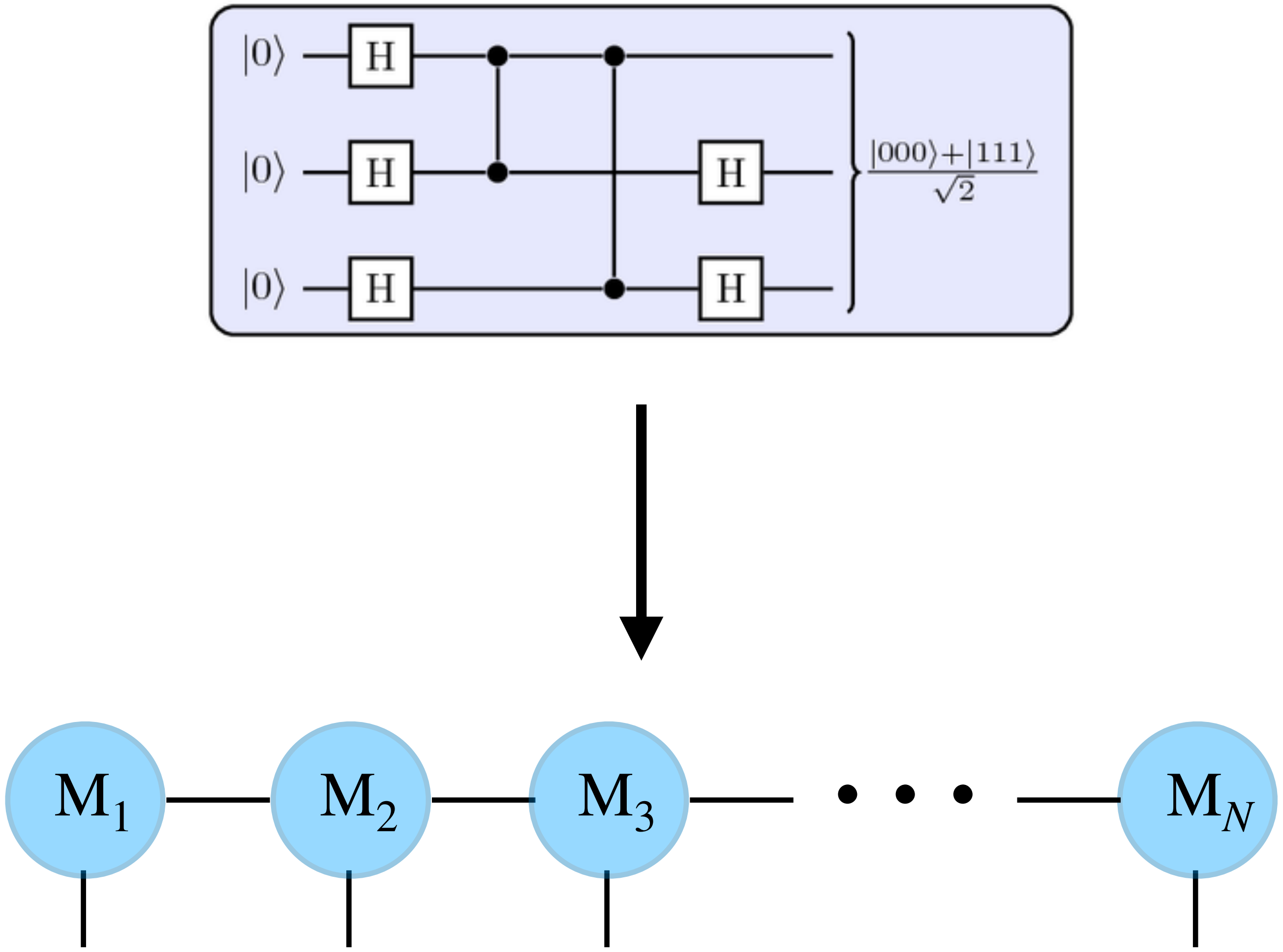
Tensor network emulator



Input:
Quantum circuit

Quantum Matcha Tea

Tensor network emulator



Input:
Quantum circuit

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

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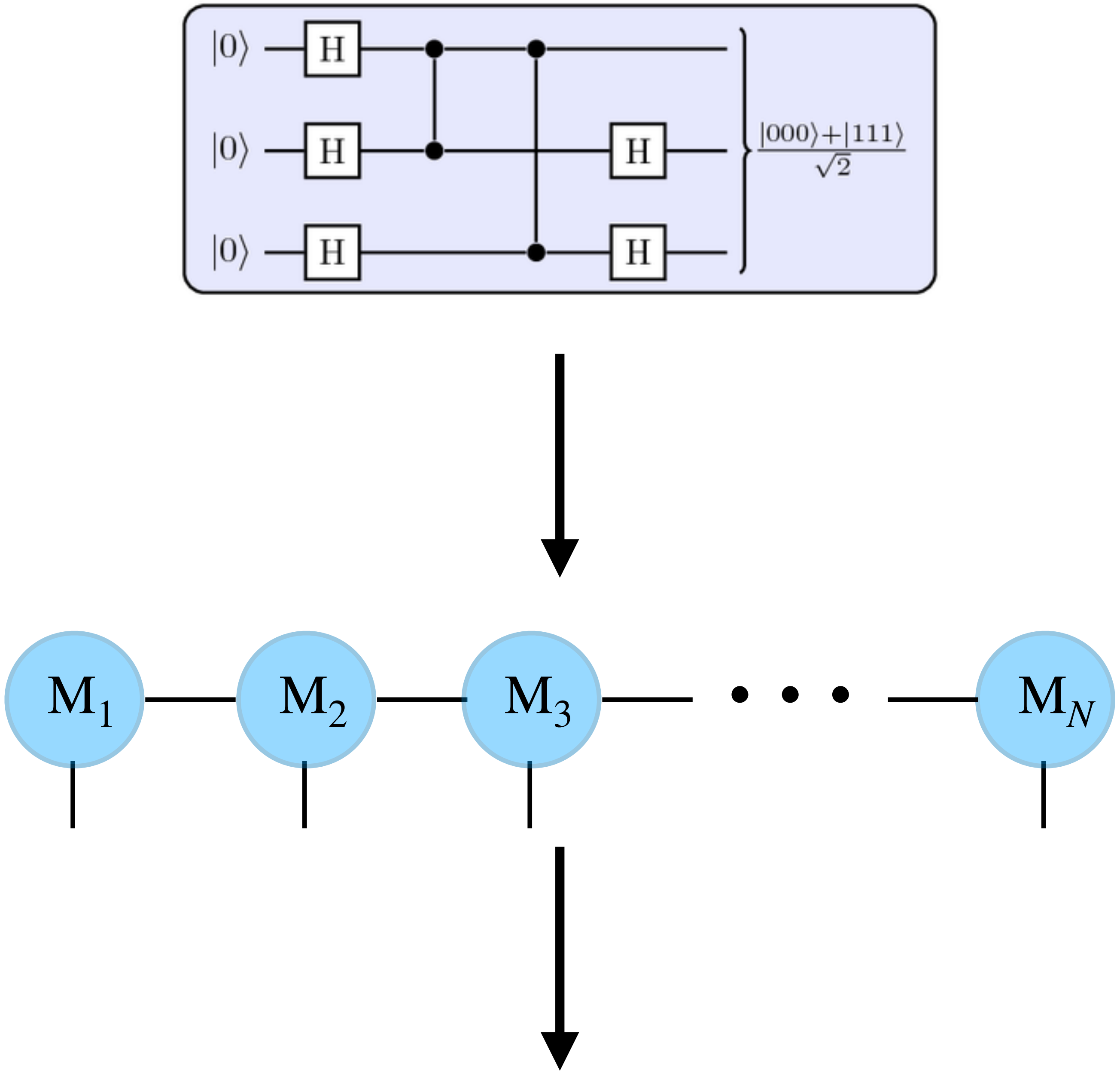

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Output:
Expectation values of observables

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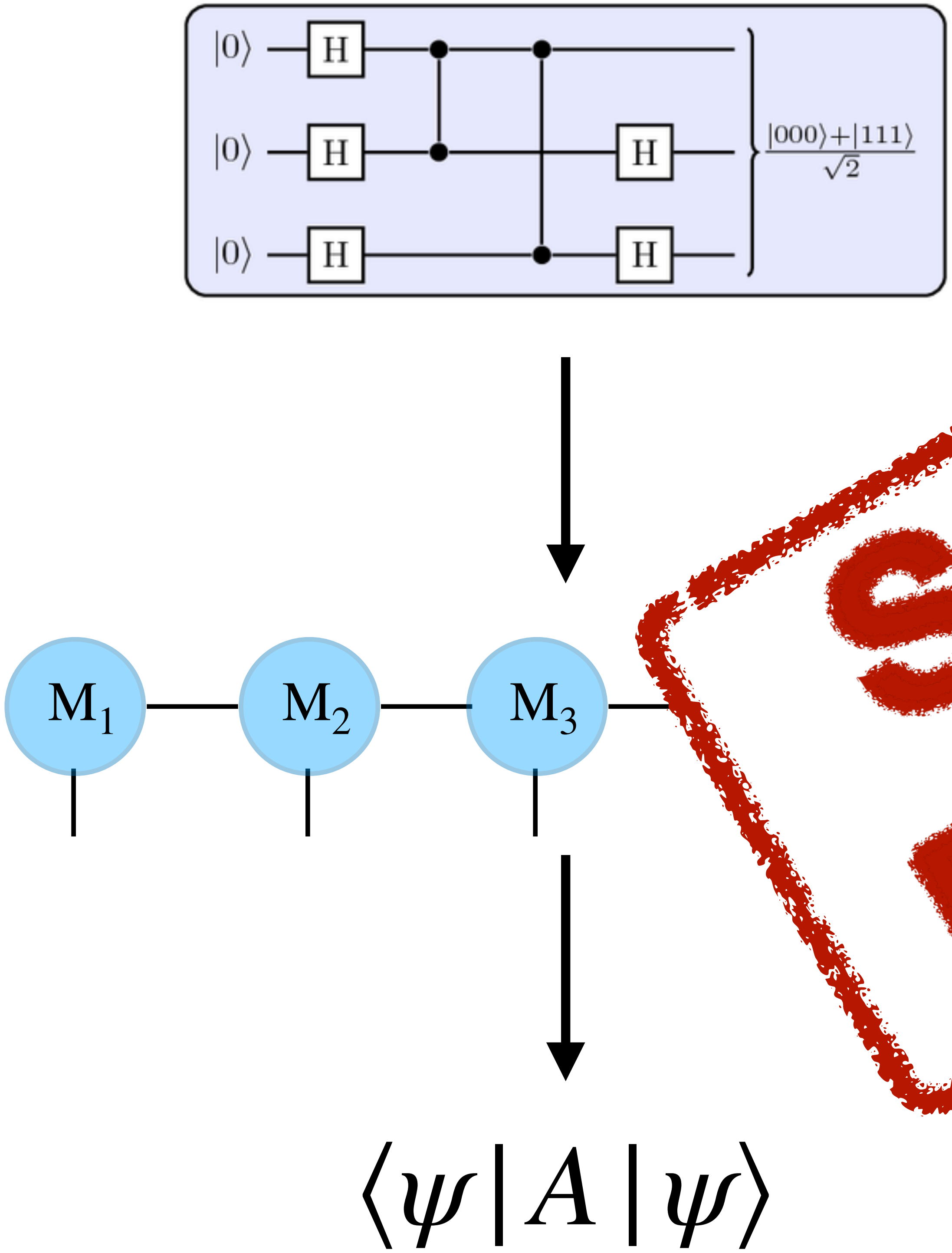

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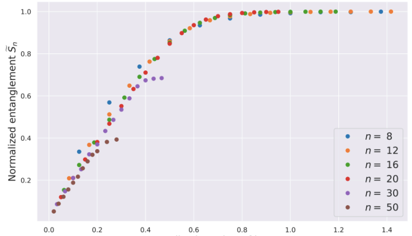
Conclusions and outlook

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



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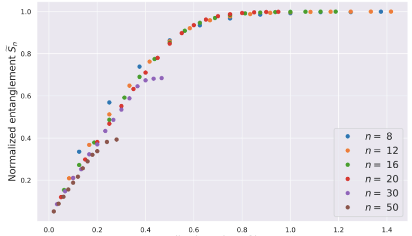
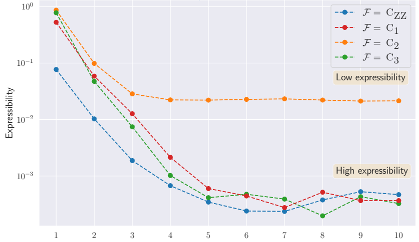


Expressibility: necessity of finding a sweet spot between the entanglement production and the expressibility of the QNN



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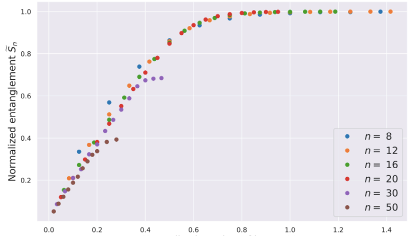

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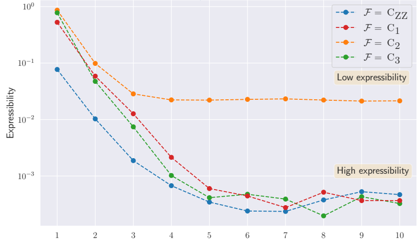
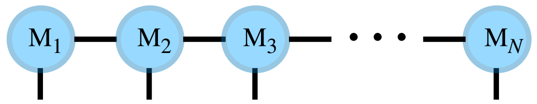


Tensor network methods: use of efficient methods to simulate large system (up to 50 qubits) to investigate the limiting behaviour. **Quantum matcha tea!**



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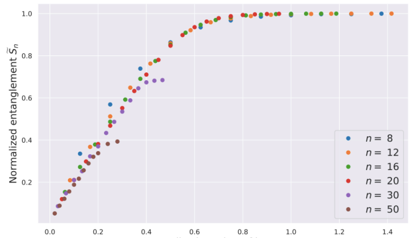

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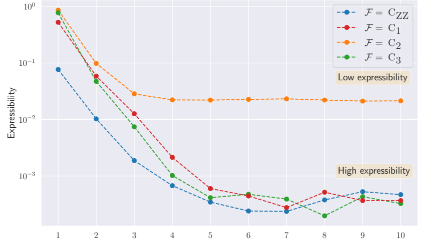

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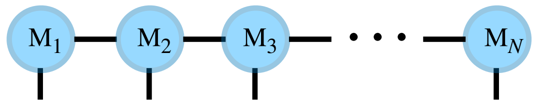

Training: Extend the analysis of the paper to the entanglement produced during the training.

How much entanglement is really needed?

Conclusions and outlook

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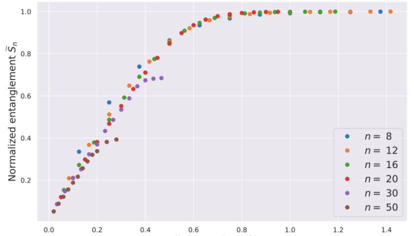

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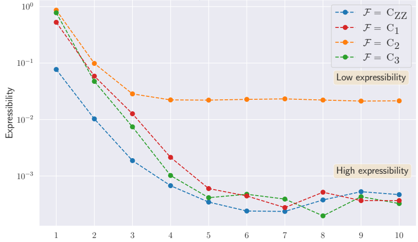

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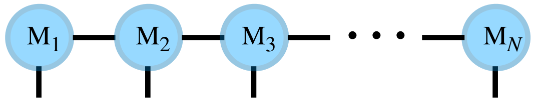

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Using different distribution: how is the entanglement changing when we draw the random parameters from a gaussian distribution? Can we observe a “critical” behavior?

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Thank you
for your attention

References

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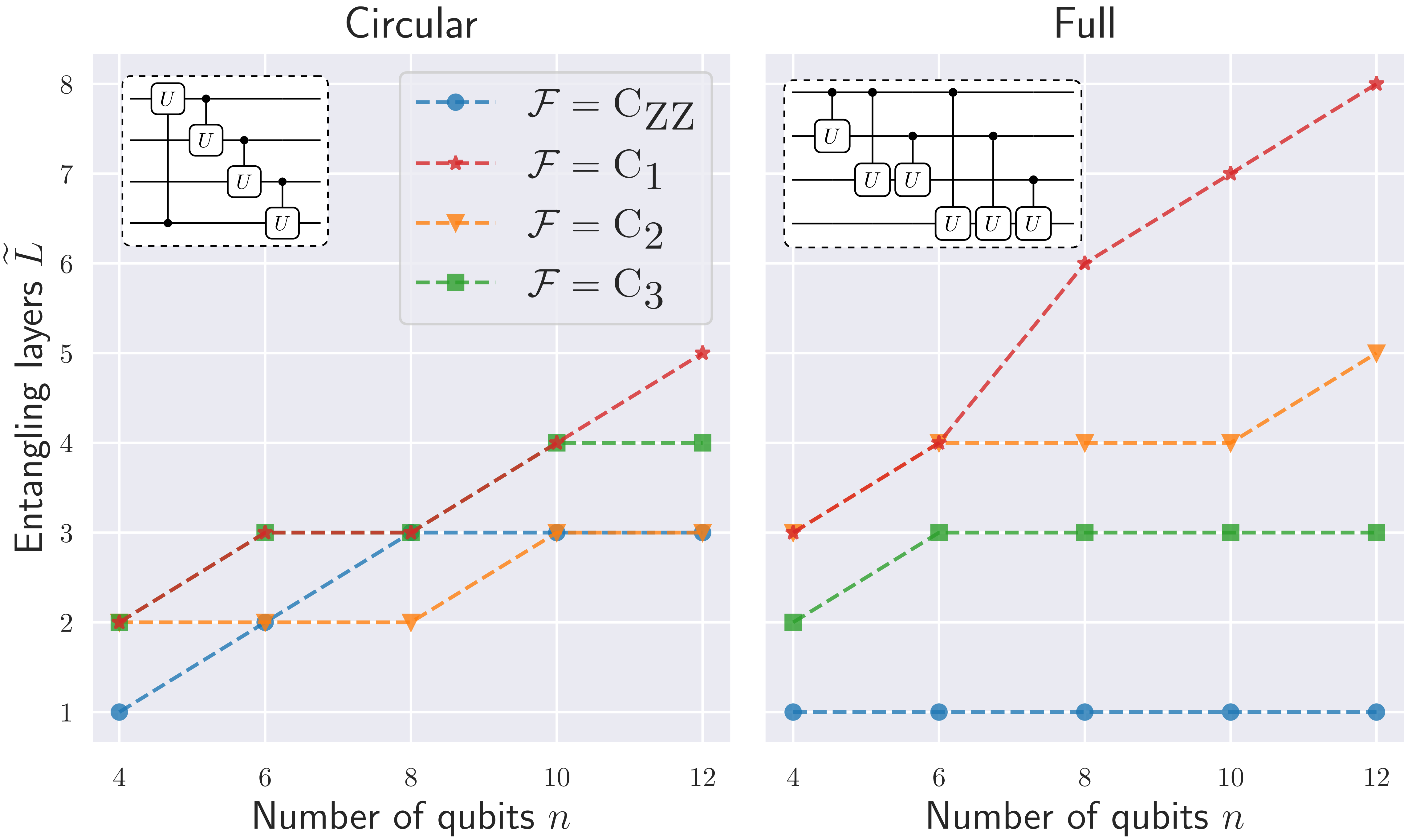
Entanglement scaling with depth



As expected, entanglement increases much faster in these cases!