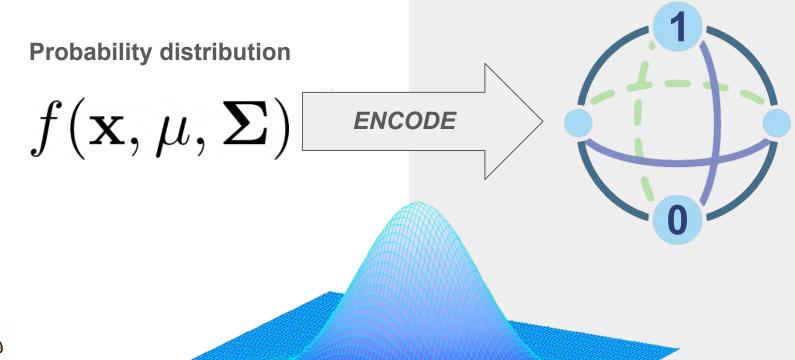
# Ta Os

Encoding of Probability Distributions for Quantum Monte Carlo Using Tensor Networks



## Problem statement

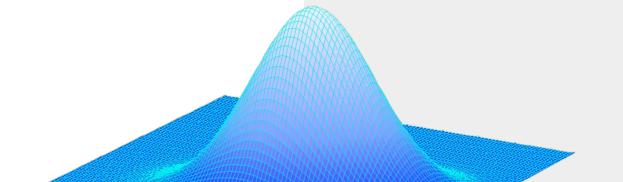
**Challenge on Quantum Monte Carlo (QMC)** 





## **Motivation**

- Useful for solving high-dimensional integrals that arise in Many Body Physics and other domains of science.
- Real-world applications like Quantum Finance,
  optimization, and risk assessment.

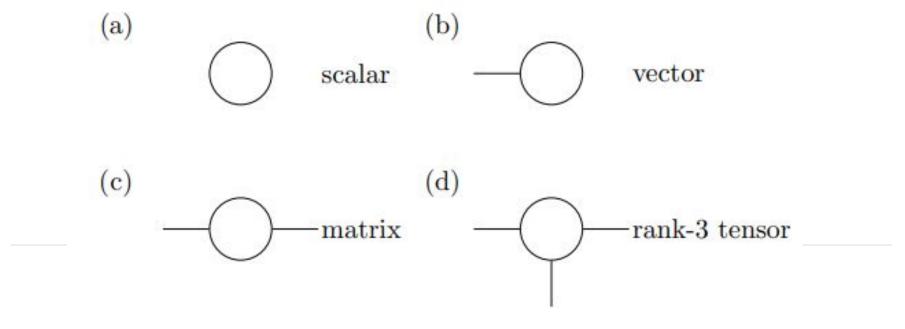




# **Tensor Networks**

Represents and manipulates **high-dimensional data**.

Let us **decompose complex tensors** into simpler ones.

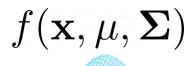




### Data Encoding ("quantization")

#### Approach:

- Define number of qubits  $n \text{ qubits} \Rightarrow 2^n \text{ values}$
- Define dimensions
- Create a volume to sample



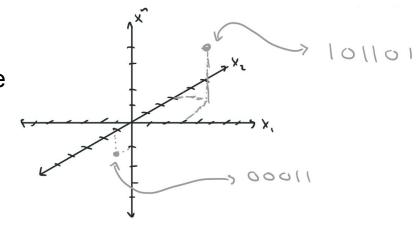


#### Data Encoding ("quantization")

#### Approach:

- Map one bitstring to one volume coordinate
  - Different maps are different quantizations

$$m:b\to i \text{ in } \mathbf{x}_i$$





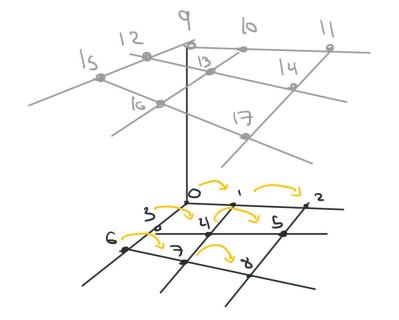
## Data Encoding ("quantization")

#### Approach:

Sequential Quantization

$$f: \mathbb{R}^d \to \mathbb{R}$$

$$p(x_i) = A(i_1, i_2, ... i_d)$$



Interleaving Quantization (braiding)



#### Quantum tensor train (TT) approximation

$$A(i_1,\ldots,i_d) = \sum_{r_0,r_1,\ldots,r_d} G_1(r_0,i_1,r_1)G_2(r_1,i_2,r_2)\cdots G_d(r_{d-1},i_d,r_d),$$

High Dimensional Array



Sequence of lower-dimensional tensors

10D TT tensor:

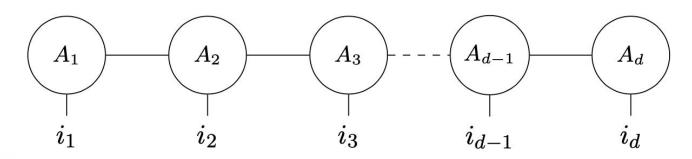
- Define "physical dimensions" = single qubit dimension
- Create a domain space from each qubit



#### Tensor train (TT) approximation

#### Approach:

- Cross TT approximation usage
  - Define bond-dimension (max amount of interacting qubits)
  - Samples probability distribution over random subset of domain
  - Optimizes contractions to form tensor which represents data
  - Output tensor has indices corresponding to the physical dimensions

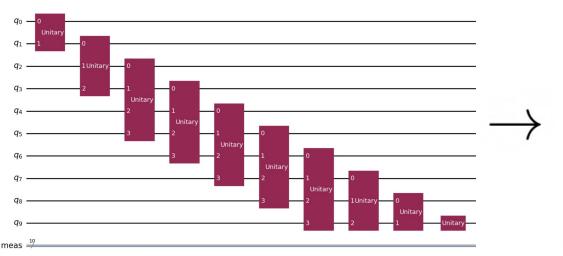


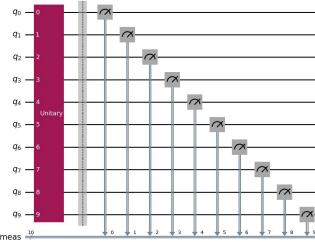


#### Mapping TT to circuit

#### Approach:

- Very smart reshaping per tensor core and SVD decompositions
- Get's unitary matrices which recreate tensor
- Can then map to one single unitary :)

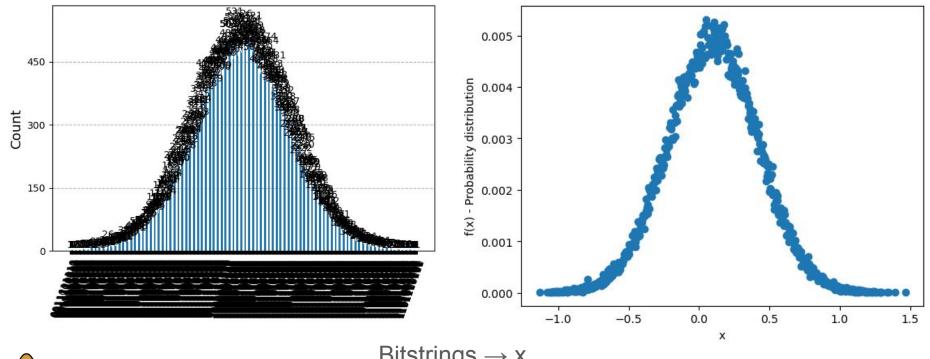




# 1D results



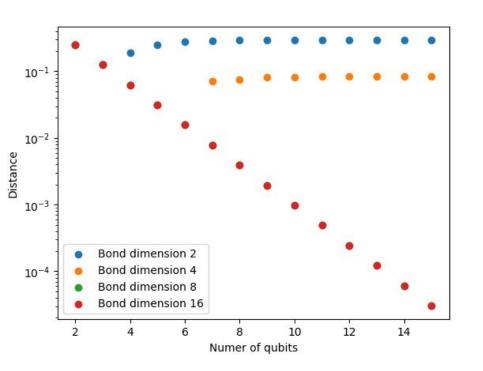
#### Results 1D

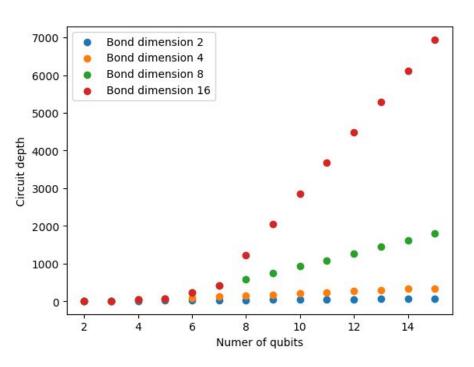




Bitstrings  $\rightarrow x$ Counts  $\rightarrow f(x)$ 

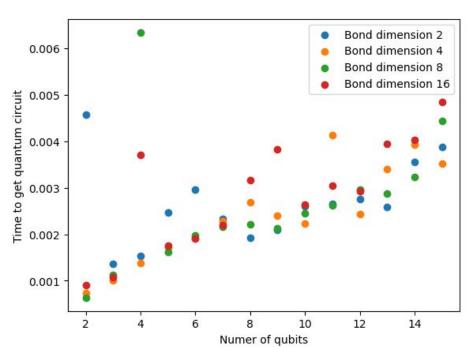
#### Distance and scaling

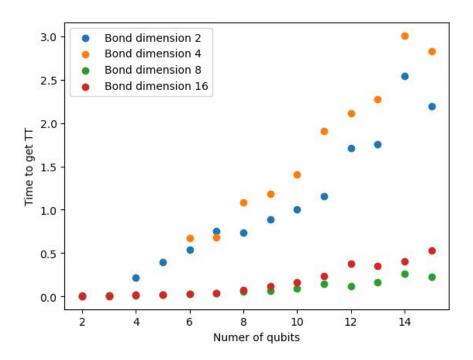






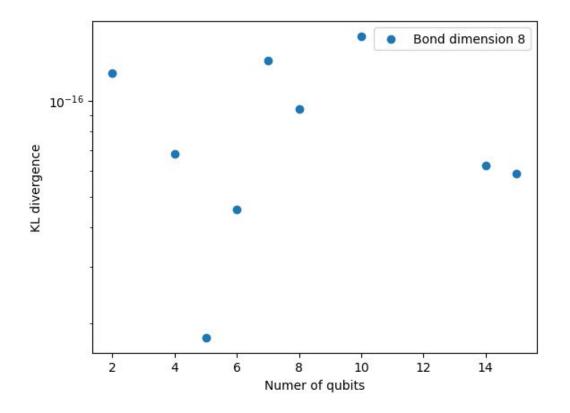
#### Time scaling







## KL Divergence

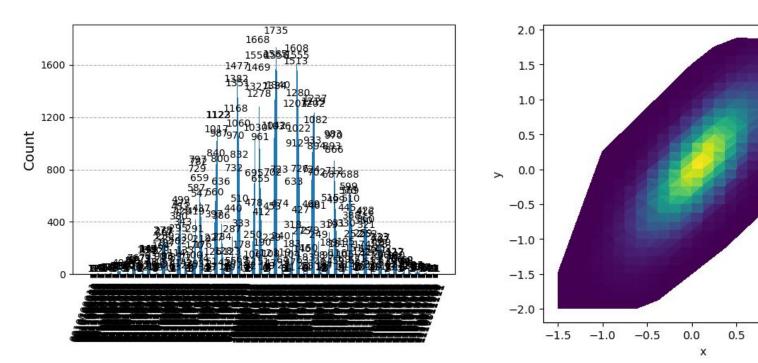




# 2D results



#### Results 2D





Bitstrings  $\rightarrow$  (x, y) Counts  $\rightarrow$  f(x, y)

0.016

0.014

0.012

- 0.010

- 0.008

0.006

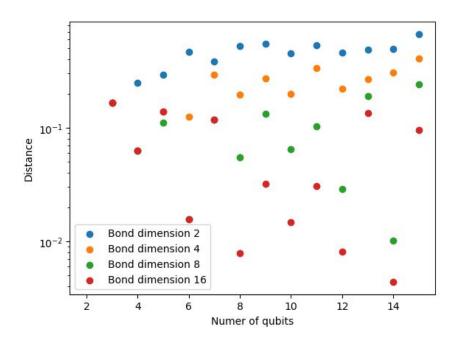
0.004

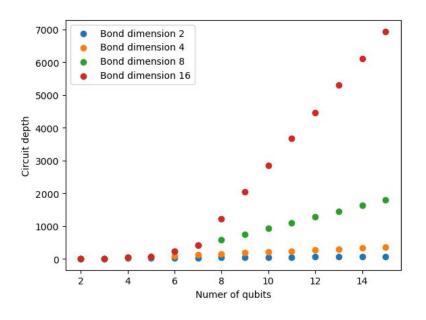
- 0.002

1.5

1.0

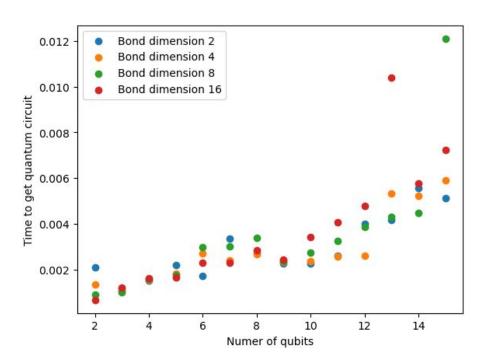
## Distance and scaling

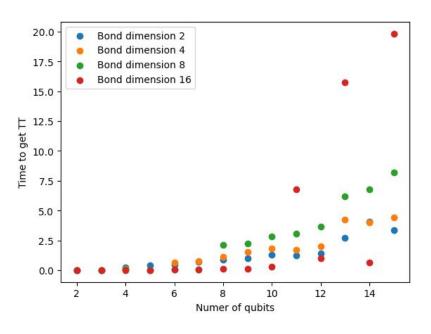






#### Time scaling

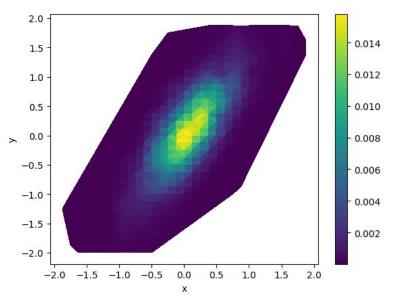


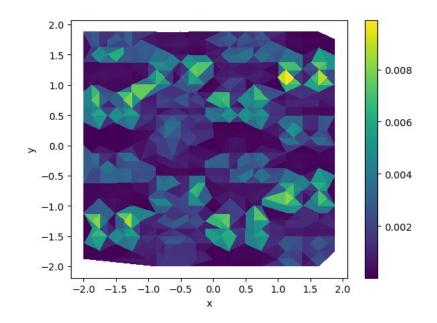




#### Comparison: different quantizations

Interleaving pattern & some weird pattern



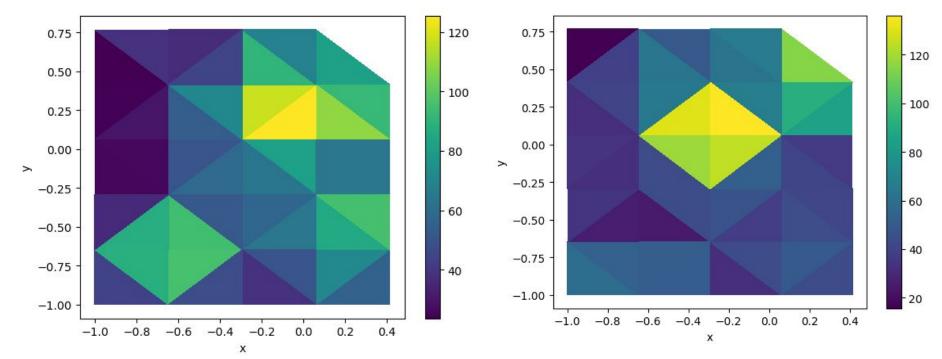




# 4D results

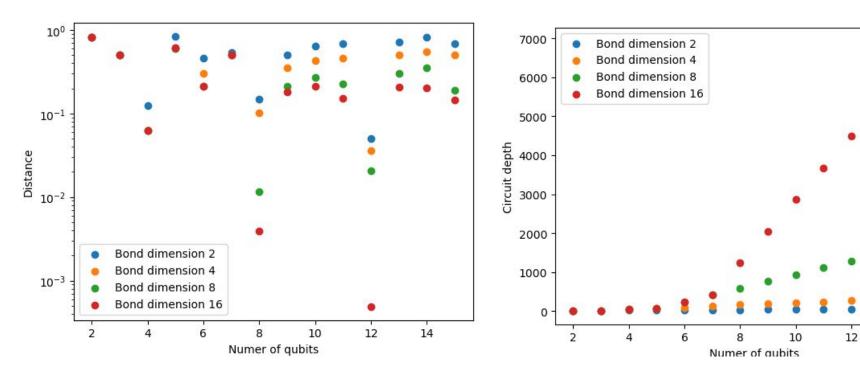


#### Results 4D sequenced vs interleaved



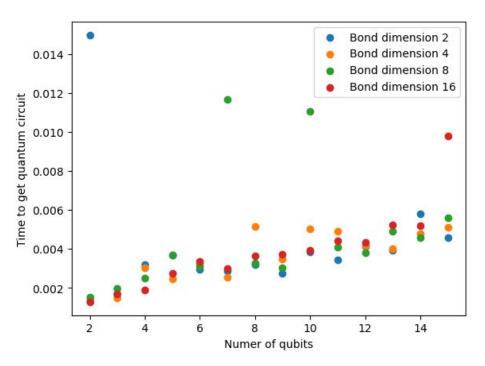


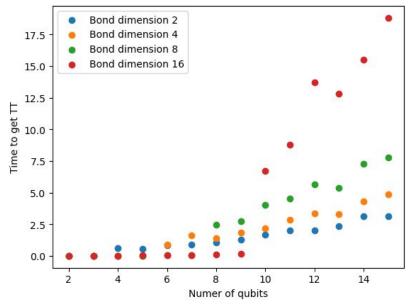
#### Distance and scaling (sequenced)





#### Time scaling (sequenced)







# Analysis

#### TT train & QC prep time

- Linear scaling with number of qubits
- Quasi-linear with bond dimension

#### **Quantum Circuit depth**

- Linear scaling with number of gubits
- Quasi-linear with bond dimension.

#### **Distance**

- Sequenced data worsens for more dimensions as expected
- Interleaved performs better
- Often improves with high bond dimension

#### Conclusion

- Can prepare d-dimensional distribution function, scaling linearly (time and depth) with number of qubits
- Only hard task → Good quantization
- Trade-off between resources vs good approximation (time,depth vs bond dimension)



## Discussion

# Algorithms assume state-preparation

- Examples:
  - Topological invariant calculations in condensed matter physics.
  - Adiabatic simulations
- Don't work without effective density matrix upload.

# Probability distribution preparation

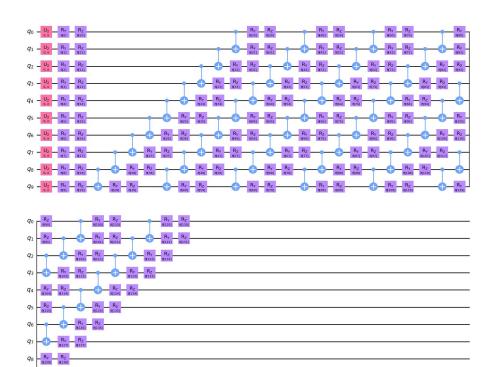
- In many-dimensional systems not one single method works for all.
- Encoding method open to creativity.
- Usually big trade-off between precision and resources.



## Bonus



# qGAN 2D

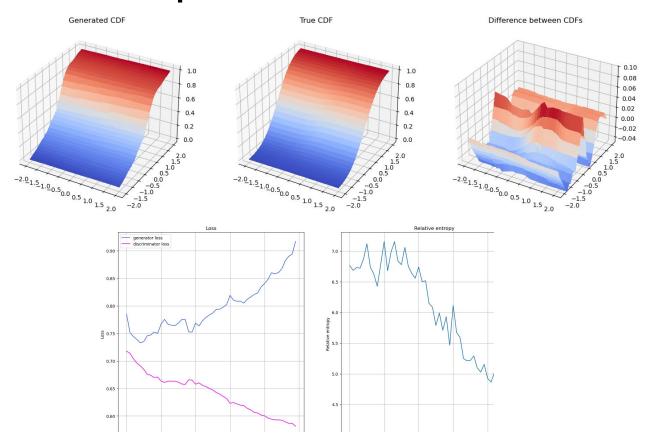


#### General idea

- Optimize a parametrized quantum circuit to map a probability distribution to a state.
- A neural network tries to discriminate the circuit's output from the real distribution and gives feedback.

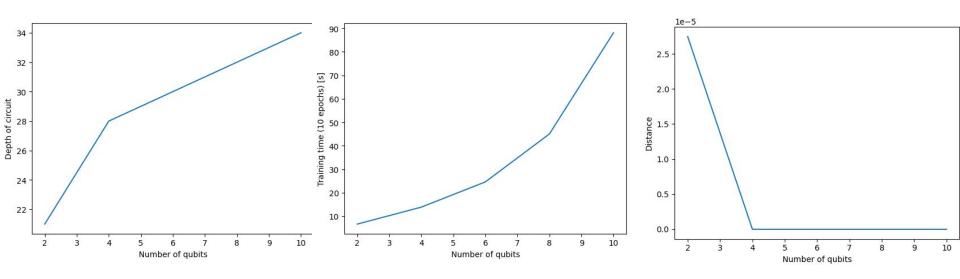


# qGAN 2D results





## Scaling





## Discussion

- Training time longer than TT-train circuit
- Time seems to have quadratic scaling with qubits → Very bad
- Circuit depth good (but iterations are not accounted for)
- Very good distance



## Thank you for your attention!

