# الگوریتم‌های کوانتومی وردشی
## مروری بر پیشرفت‌ها و چالش‌ها

سید علی حامد موسویان
دانشگاه فردوسی مشهد
مدرسه پاییزه الگوریتم‌های کوانتومی و کاربردهای آن‌ها
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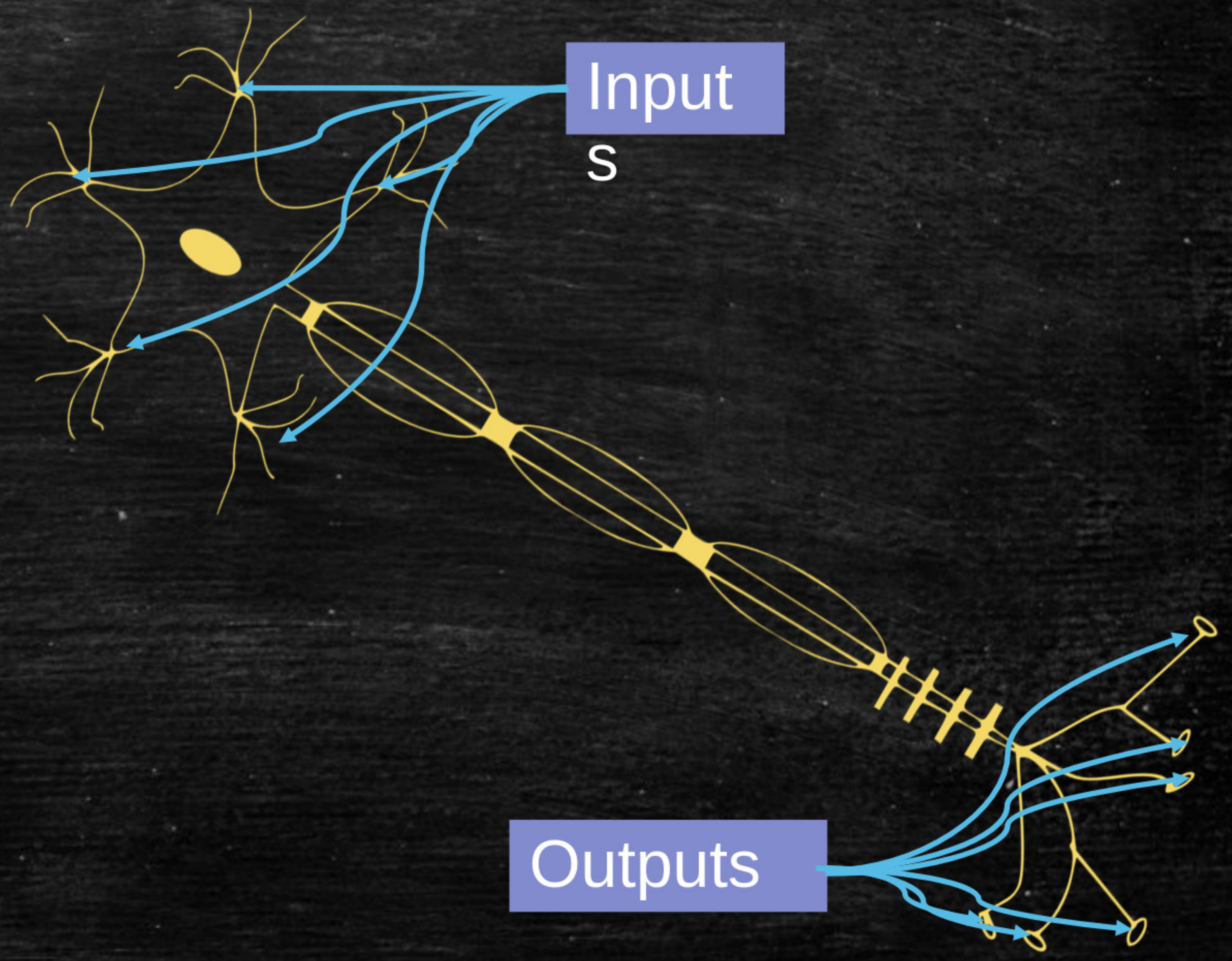
# Contents

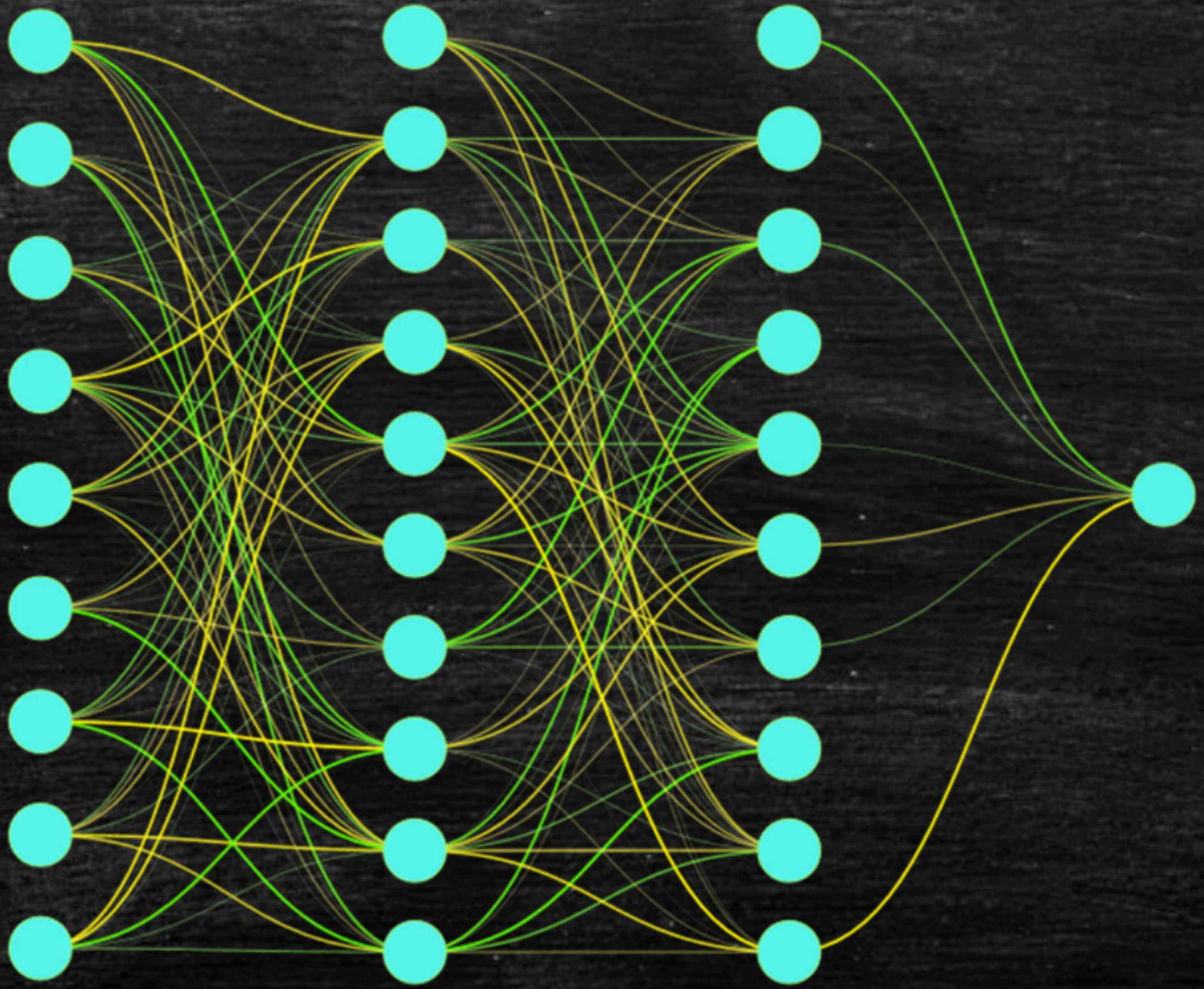
- What are VQAs?
- Applications
- Challenges
- Solutions

# Machine Learning, a bit of history

- 1943: Artificial Neuron
- Input Signal > Threshold
  - -> Output
- Activation function
  - ReLU (Rectified Linear Unit)



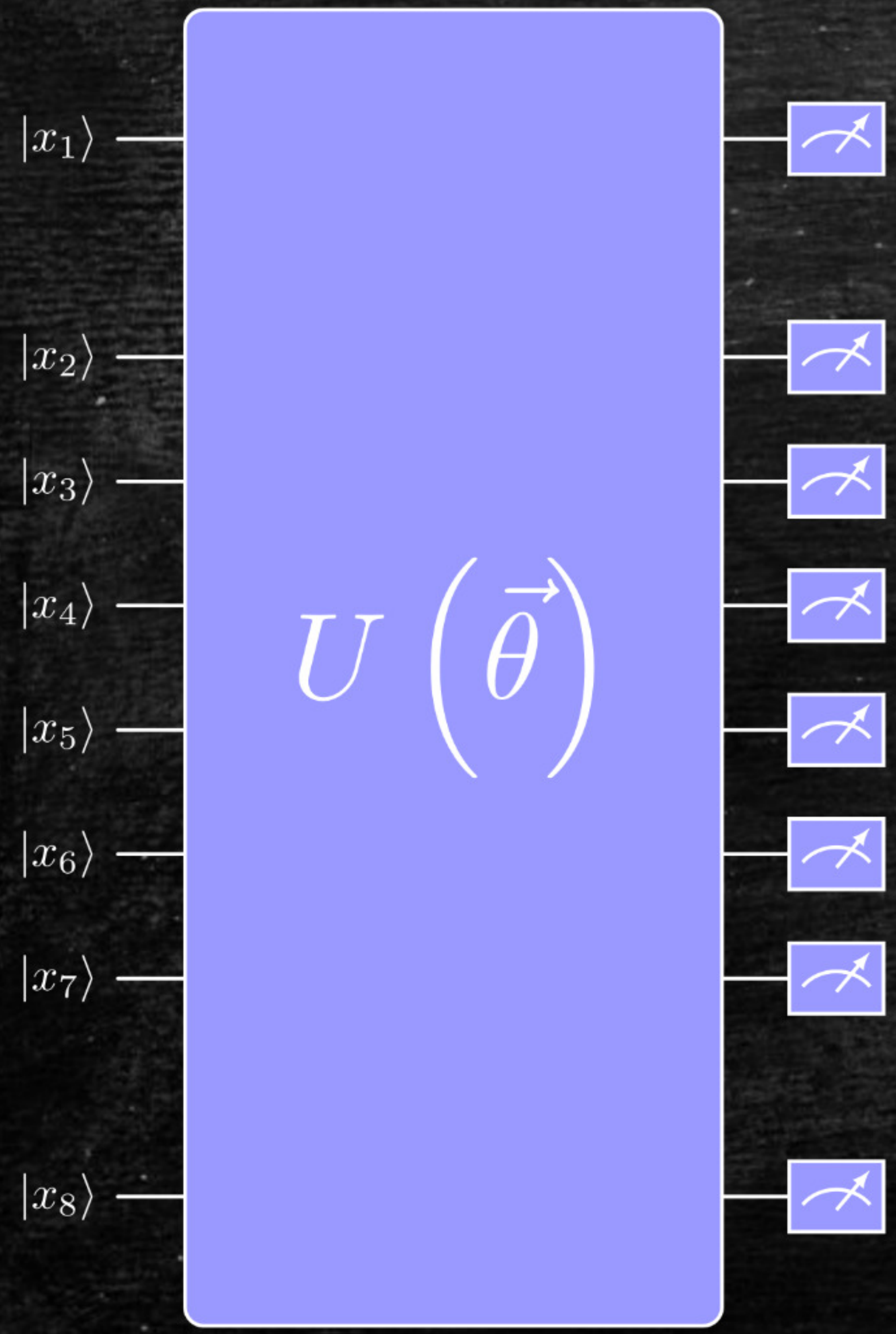
# Machine Learning, neural networks



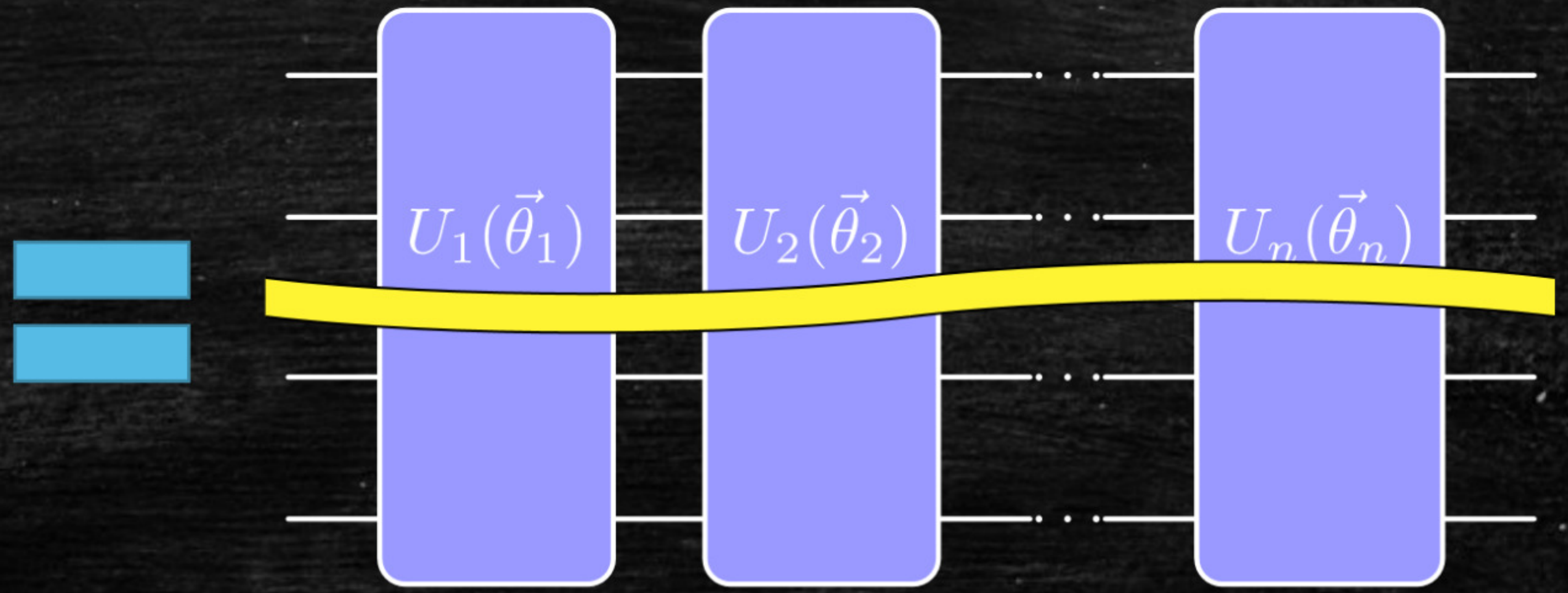
0.98 : yes

Is this a Cat?

# Variational Quantum Algorithms



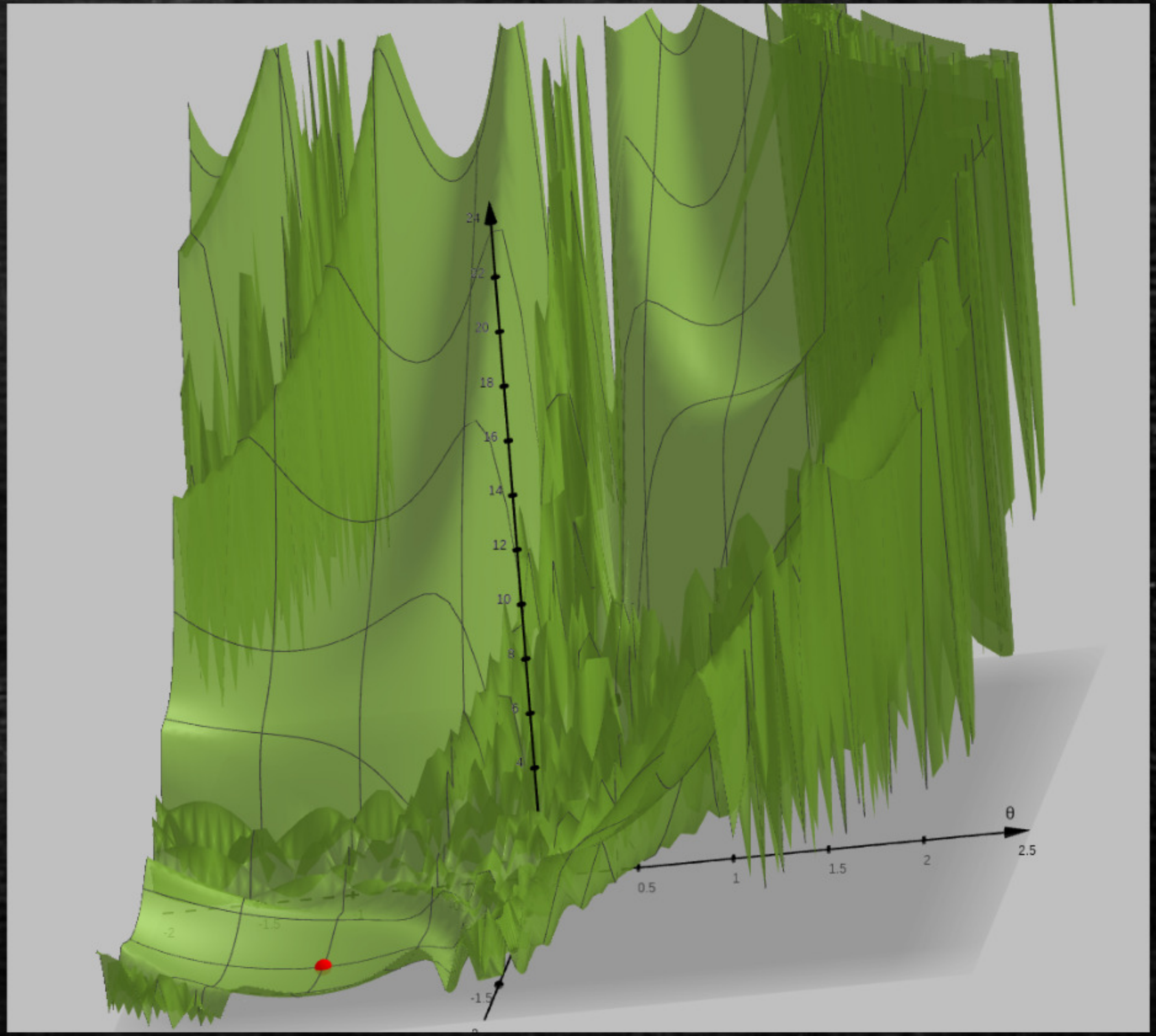

- We have a parameterized *quantum* circuit!
- Training means finding the right set of parameters



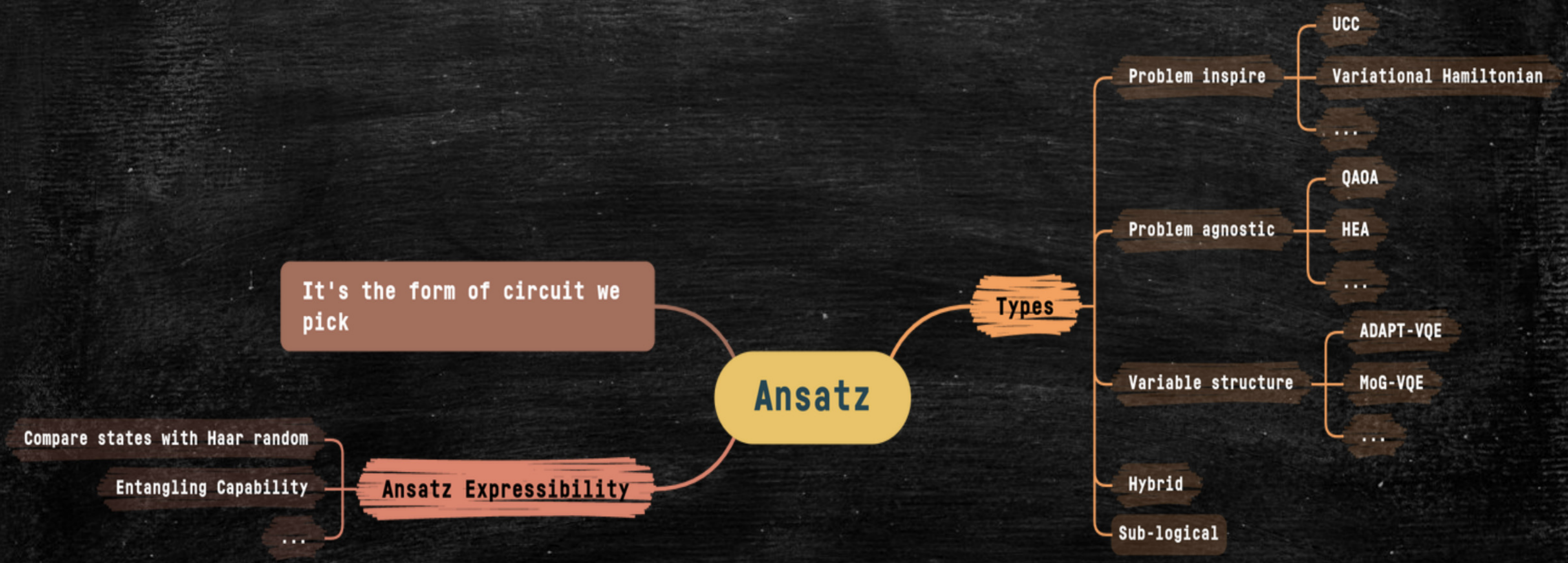
## VQA: Cost function

- Cost function:
  - The circuit $U(\vec{\theta})$
  - States from a training set $\{\rho_k\}$
  - A set of Observables $\{O_k\}$

$$C(\vec{\theta}) = \sum_k f_k \left( \mathrm{Tr} \left[ O_k U(\vec{\theta}) \rho_k U^\dagger(\vec{\theta}) \right] \right)$$

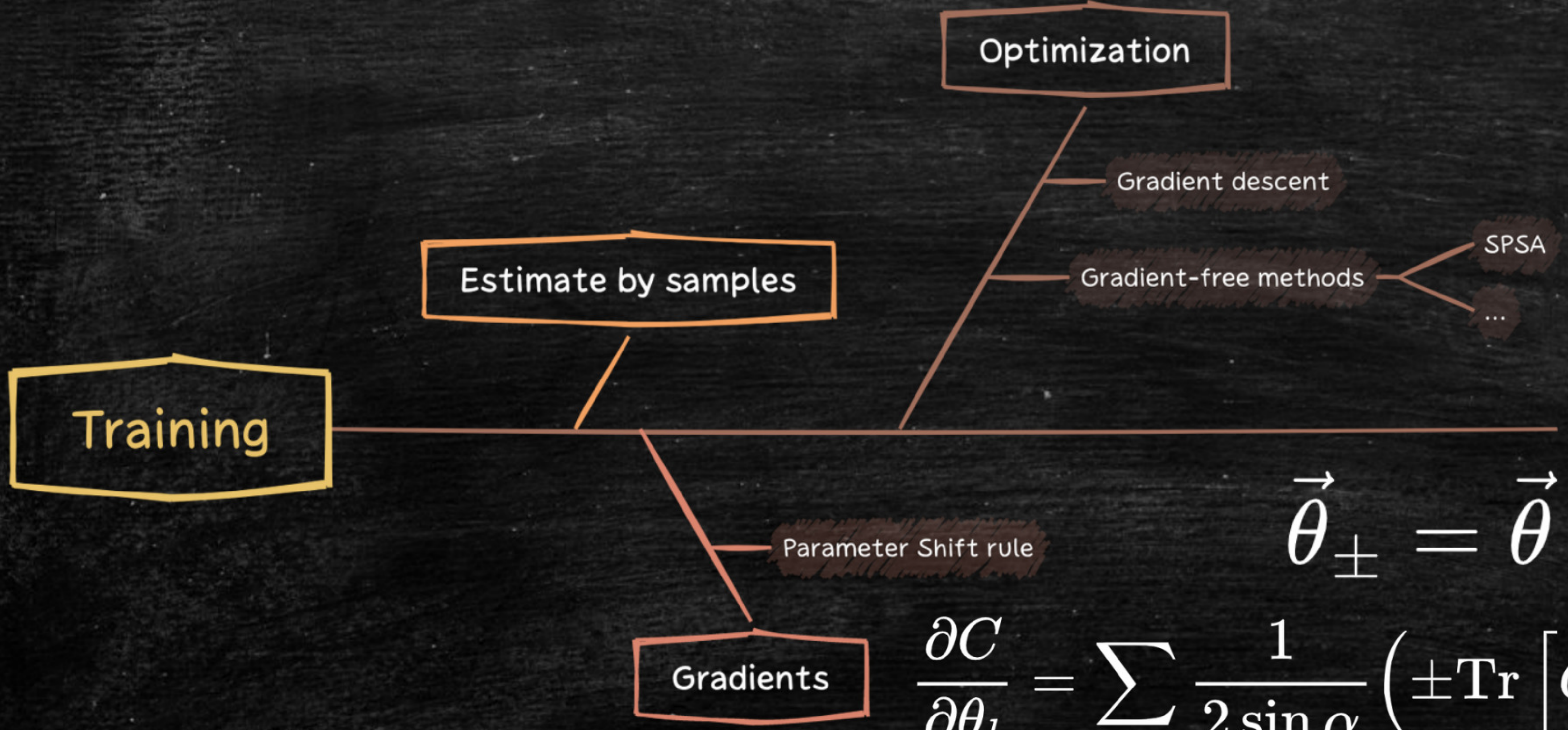


# VQA: Ansatz



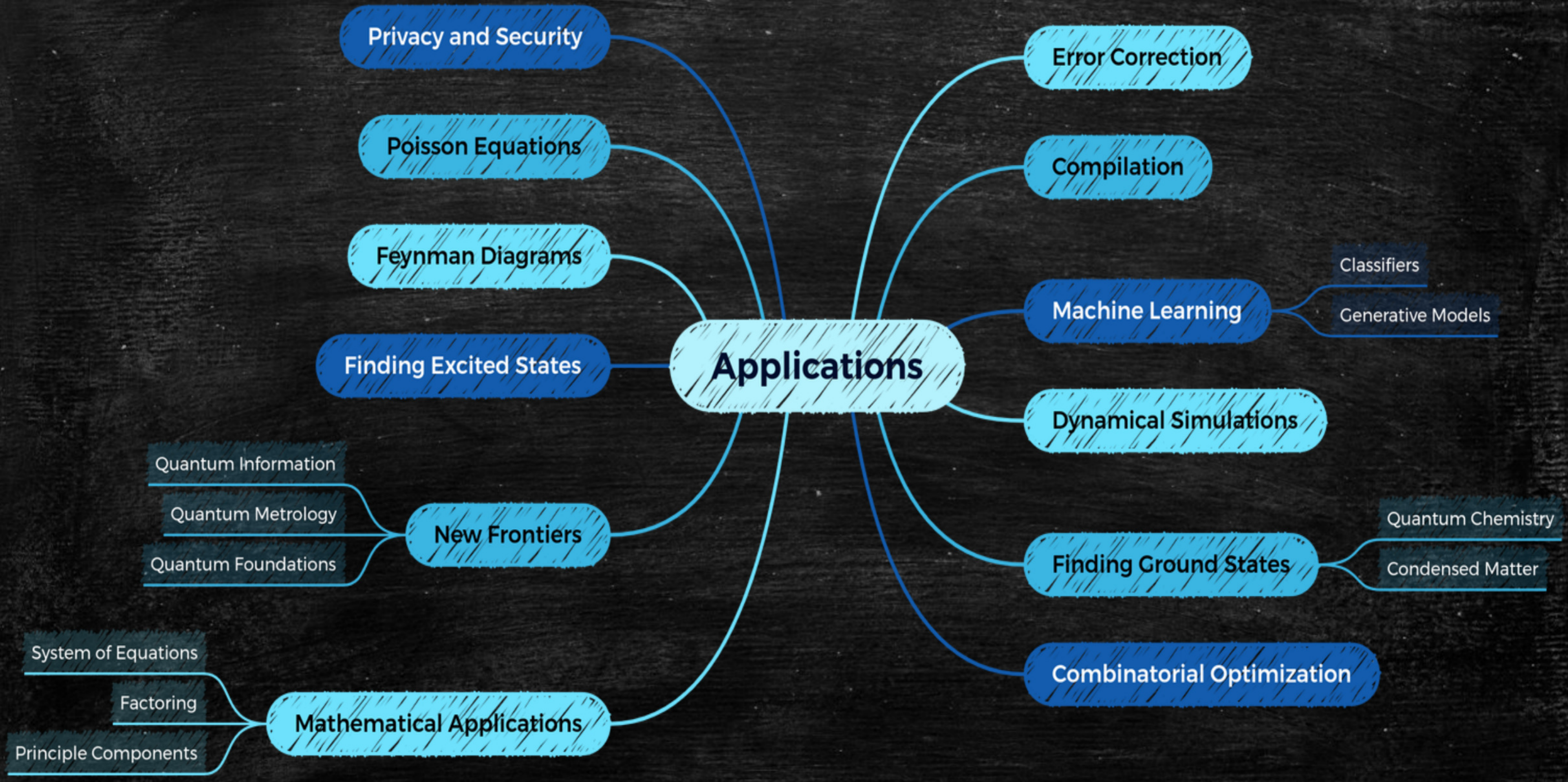
Ansatz
It's the form of circuit we pick
Types
Problem inspire
UCC
Variational Hamiltonian
...
Problem agnostic
QAOA
HEA
...
Variable structure
ADAPT-VQE
MoG-VQE
...
Hybrid
Sub-logical
Ansatz Expressibility
Compare states with Haar random
Entangling Capability
...

# VQA: Training




$$\vec{\theta}_{\pm} = \vec{\theta} \pm \alpha \vec{e}_l$$

$$\frac{\partial C}{\partial \theta_l} = \sum_k \frac{1}{2 \sin \alpha} \left( \pm \mathrm{Tr} \left[ O_k U^\dagger(\vec{\theta}_\pm) \rho_k U(\vec{\theta}_\pm) \right] \right)$$




https://www.nature.com/articles/s42254-021-00348-9

# Ex. 1: Variational Quantum Eigensolver

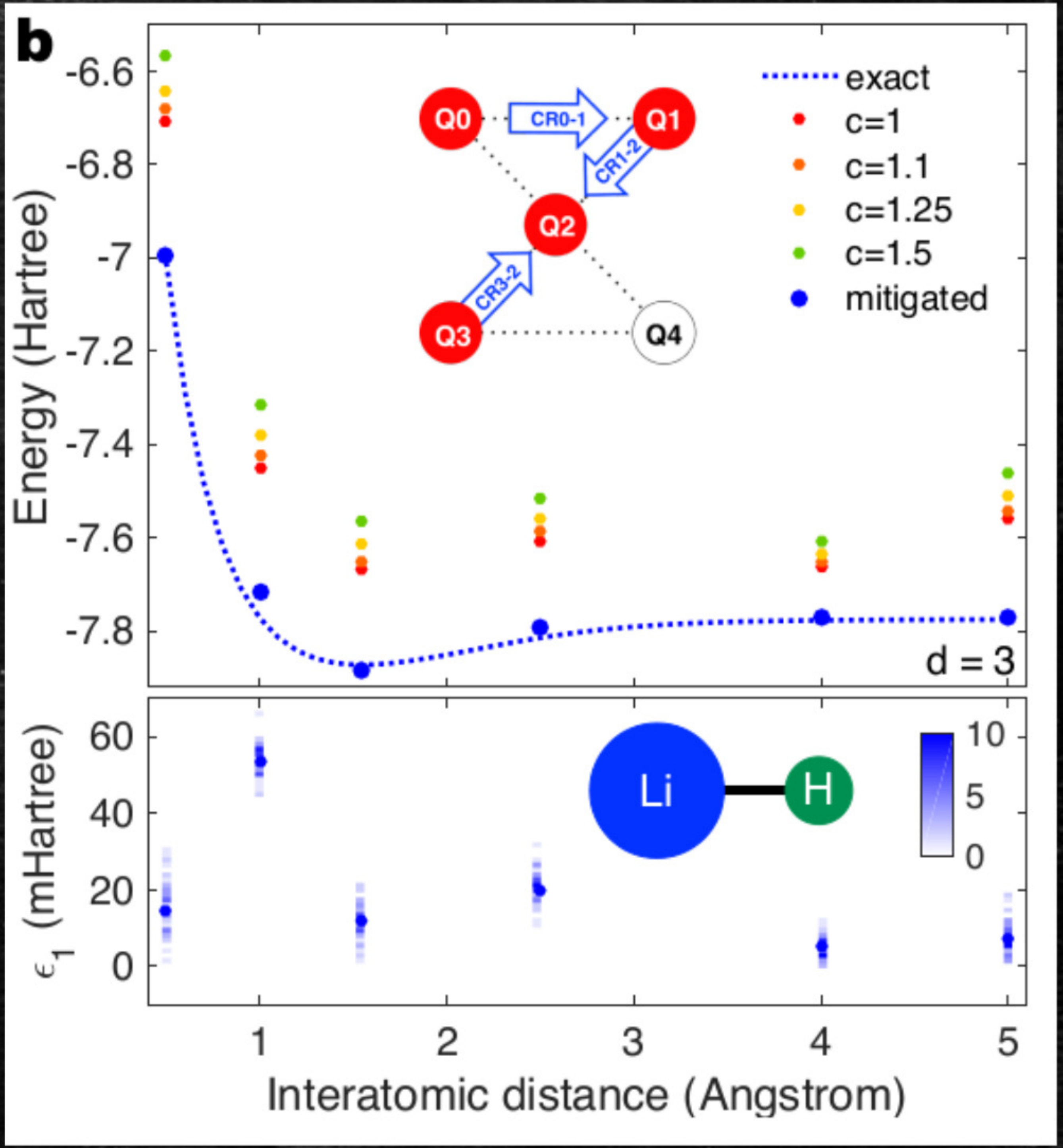
- Cost function

$$C(\vec{\theta}) = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle \,,$$

$$|\psi(\vec{\theta})\rangle = U(\vec{\theta}) |\psi_0\rangle$$

- The Hamiltonian usually has the form:

$$H = \sum_k c_k \sigma_k$$




https://www.nature.com/articles/s41586-019-1040

# Ex. 2 Dynamical Quantum Simulation

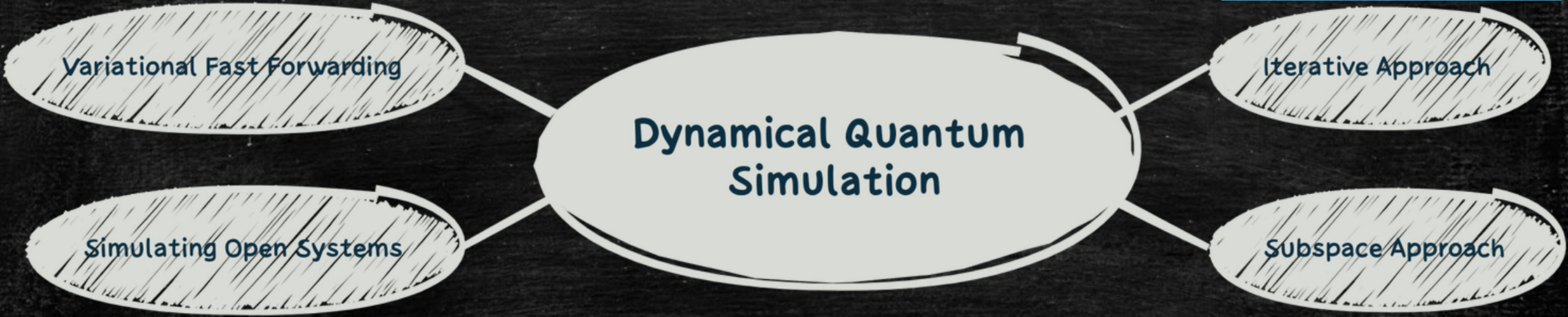
Increase fidelity between:

$$\exp(-iH\delta t)\,,U(\vec{\theta}^*)\mathcal{T}(E,\delta t)U^\dagger(\vec{\theta}^*)$$

$$\min_{\dot{\vec{\theta}}} \delta \left\| \left( \frac{d}{dt} + iH \right) \left| \psi(\vec{\theta}) \right\rangle \right\|$$

$$\Rightarrow M(\vec{\theta}).\dot{\vec{\theta}} = V(\vec{\theta})$$

$$\vec{\theta} \rightarrow \vec{\theta} + \dot{\vec{\theta}} \cdot \Delta t$$




Map the state to comp. basis.

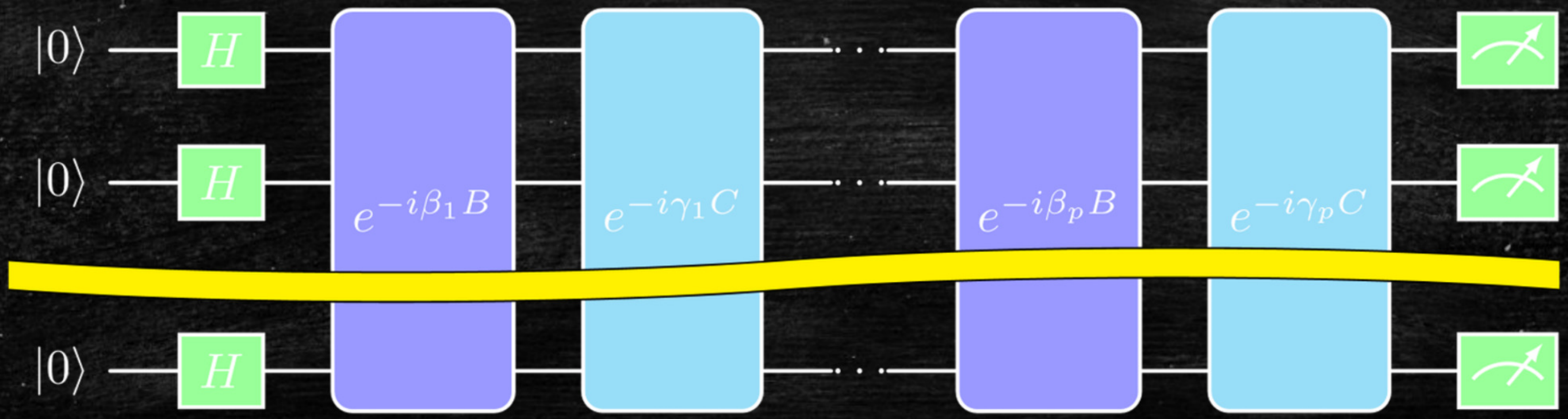
$$\exp(-iHt) \approx U(\vec{\theta}^*)\mathcal{T}(t)U^\dagger(\vec{\theta}^*)$$

# Ex. 3: Optimization, e.g. QAOA

- Map a classical optimization problem to a Hamiltonian:

$$C(z) = \sum_{\alpha=1}^{m} C_\alpha(z)$$

- A mixer operator $B = \sum_{j=1}^{n} \sigma_j^X$
- Optimize angles $\vec{\beta}\,, \vec{\gamma}$



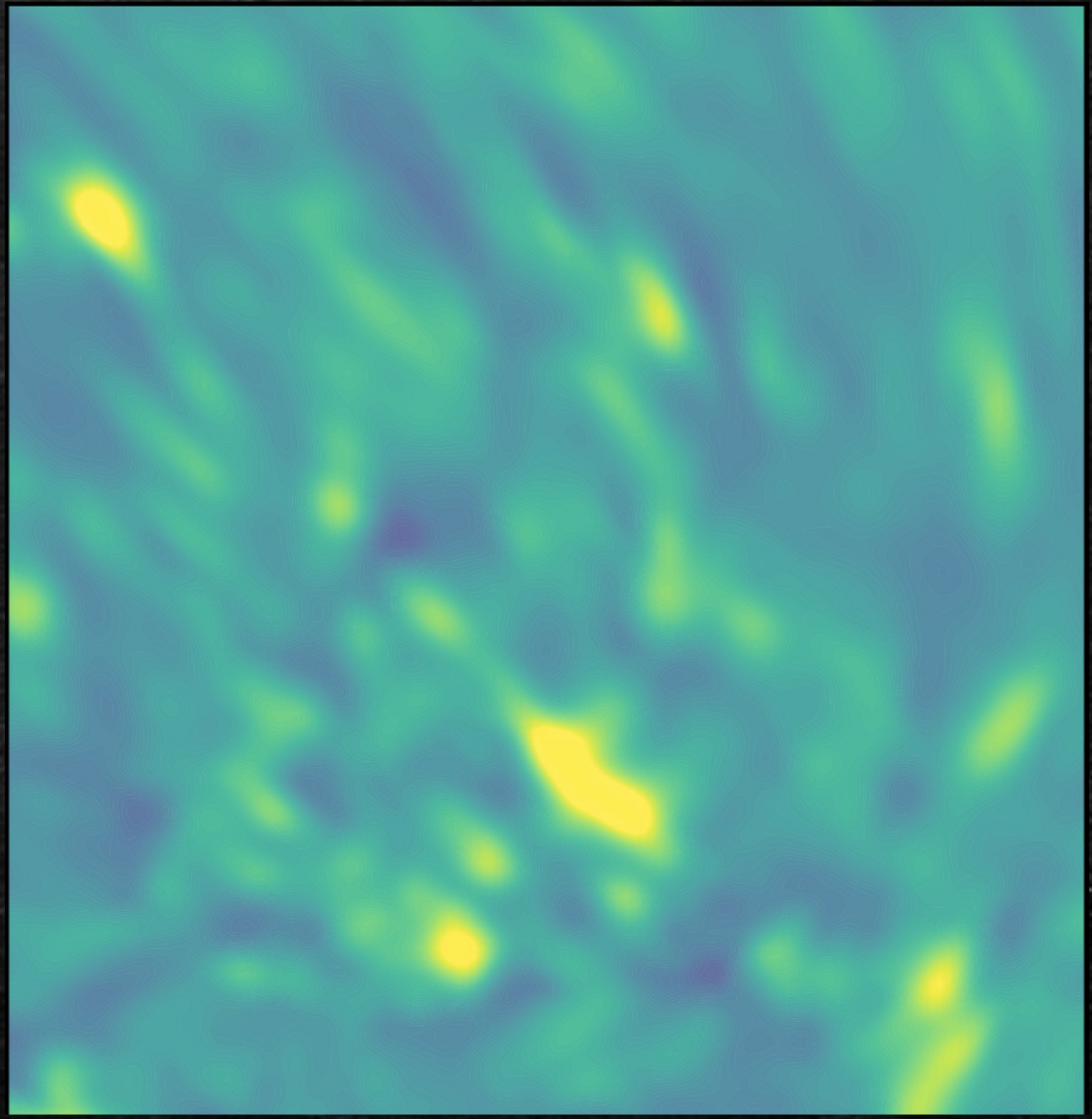
# Doubts: Overview

**Challenges**

- Getting stuck in local minima
- Barren Plateaus (Vanishing gradients)
- Are there any improvements?

# Local minima

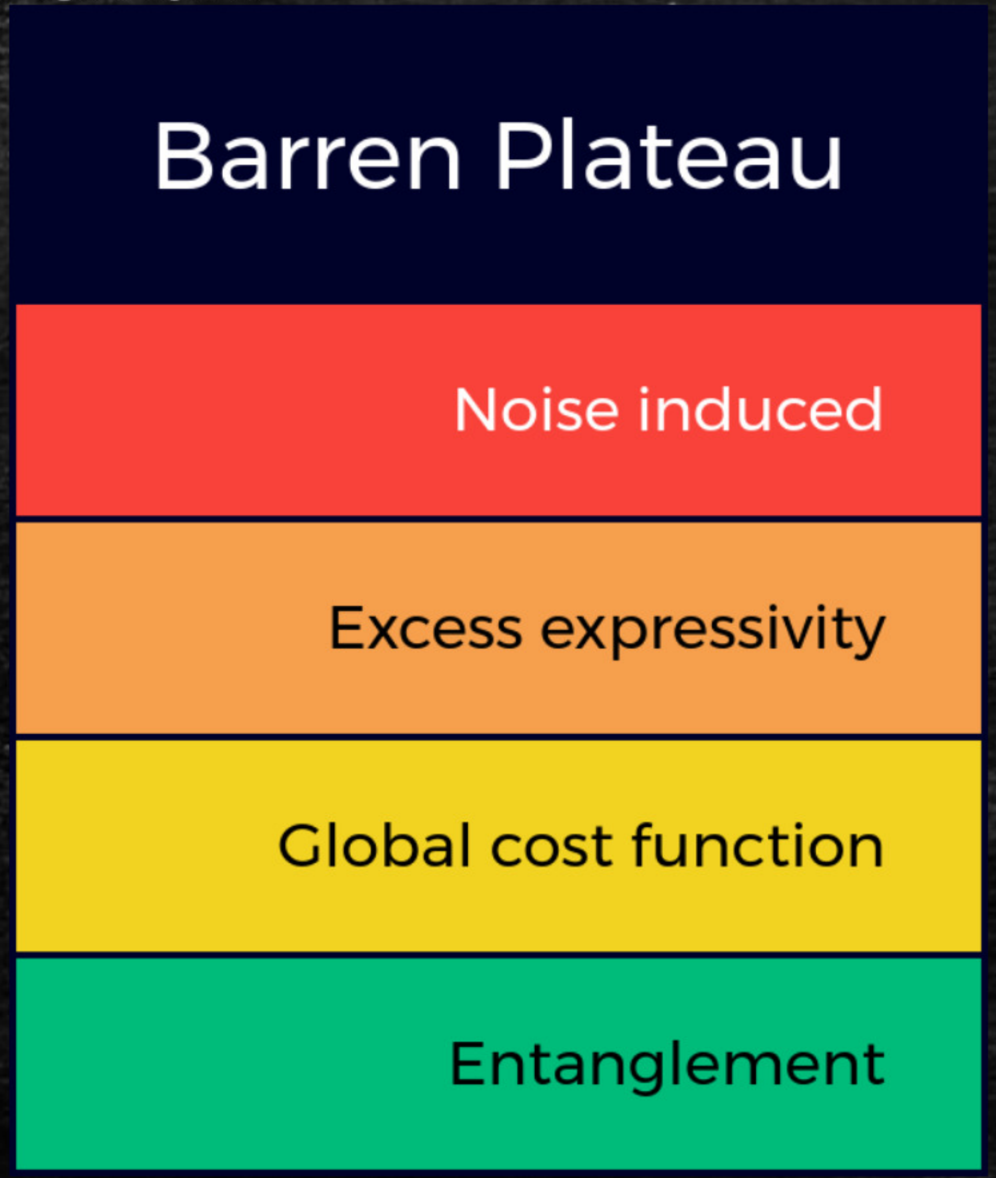
- There is evidence that the parameter hyperspace is not smooth!
  - "Beyond Barren Plateaus: Quantum Variational Algorithms Are Swamped With Traps", 2022
  - "Training Variational Quantum Algorithms Is NP-Hard", 2021

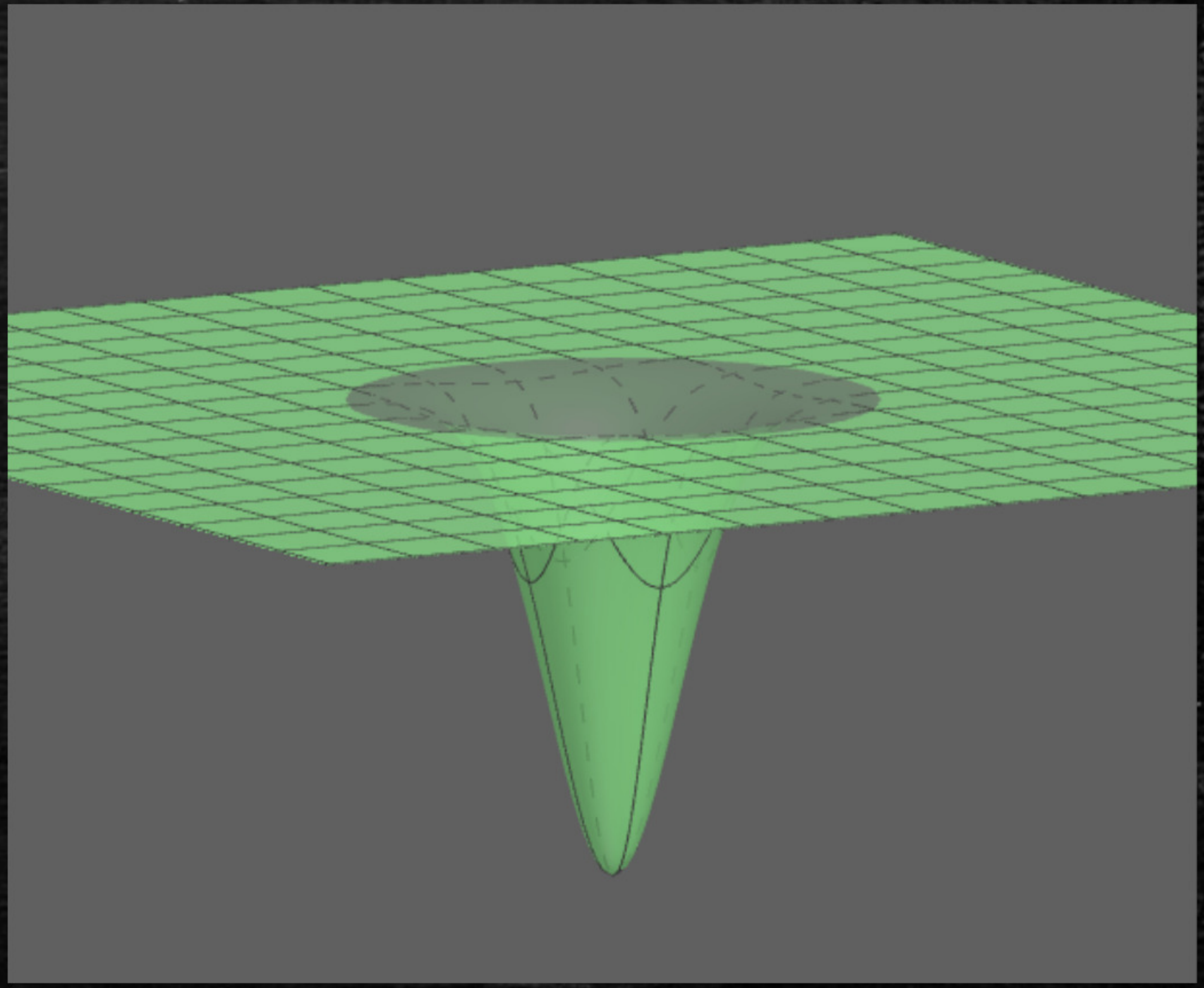


arXiv:2101.07267v1, arXiv:2205.05786v1

# Barren Plateau

- In many cases it has been proven that the gradients will be exponentially small.



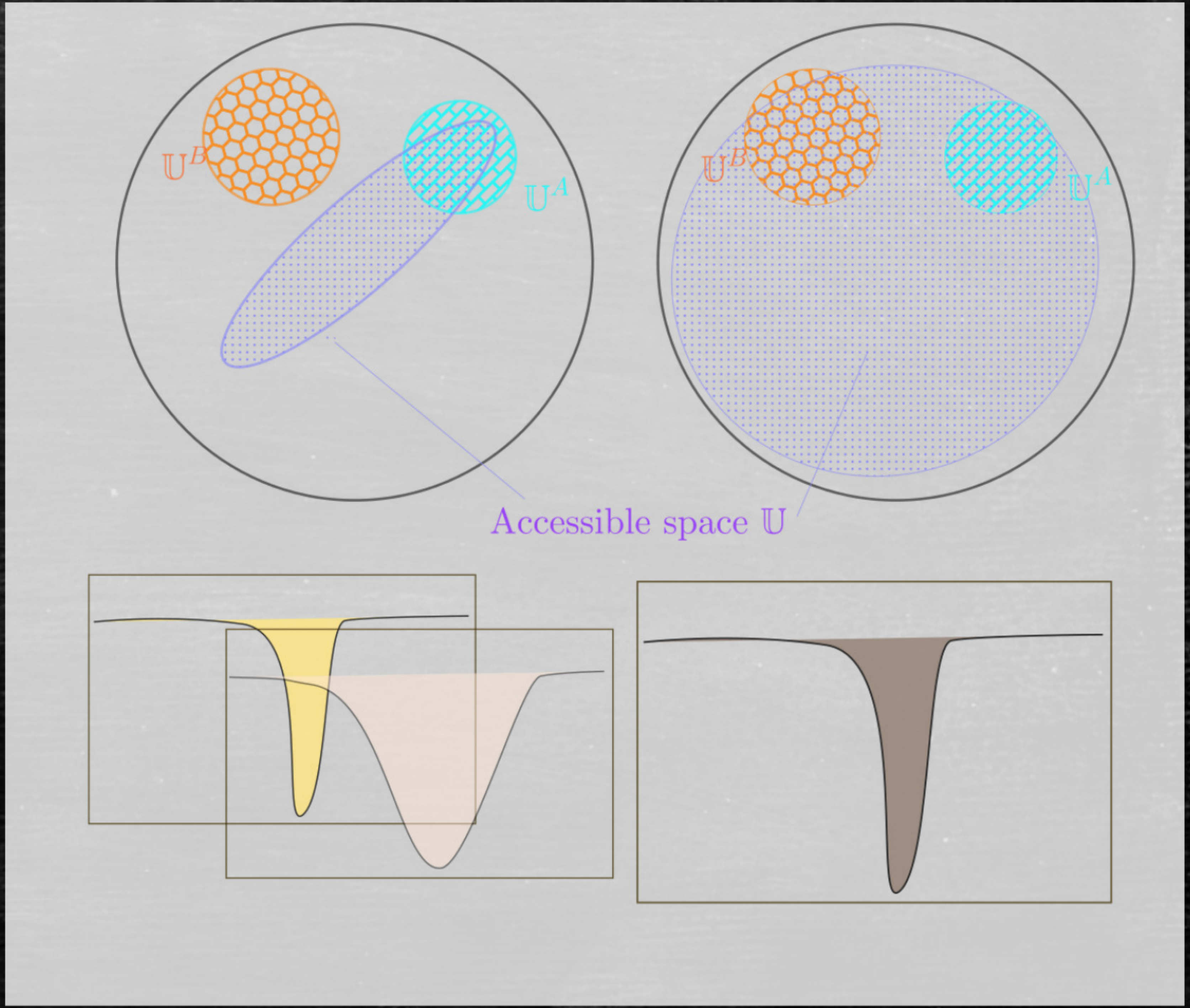
# Barren Plateau: Expressiveness

- We know:

$$C(\vec{\theta}) = \mathbf{Tr}\left[HU(\vec{\theta})\rho U(\vec{\theta})^\dagger\right]$$

$$P\left(\frac{\partial C}{\partial \theta_k} \geq \delta\right) \leq \frac{\mathbf{Var}(\partial_k C)}{\delta^2}$$

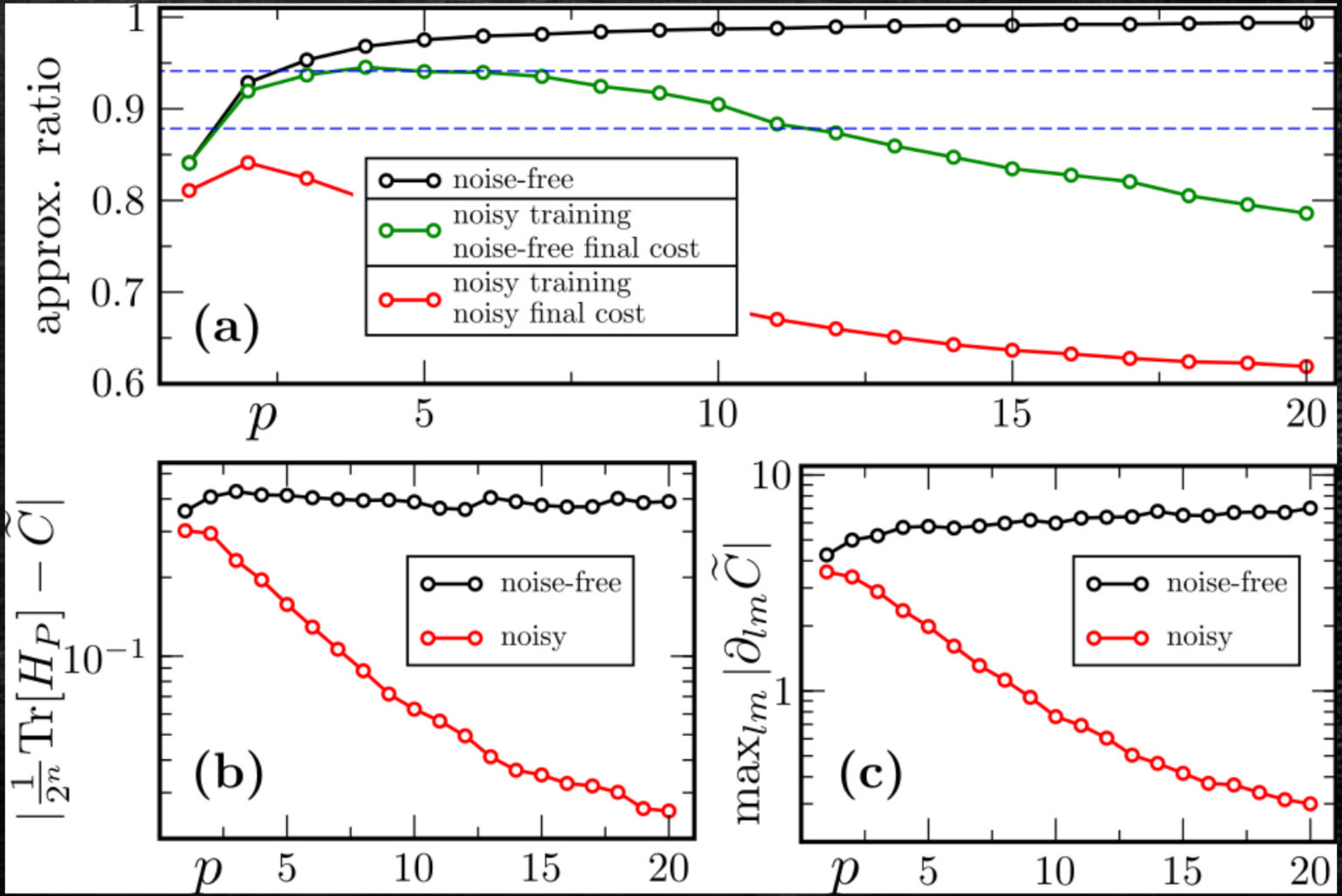
- As the expressibility of the circuit grows, the variance becomes exponentially smaller!




DOI: 10.1103/PRXQuantum.3.010313

# Barren Plateau: Noise Induced

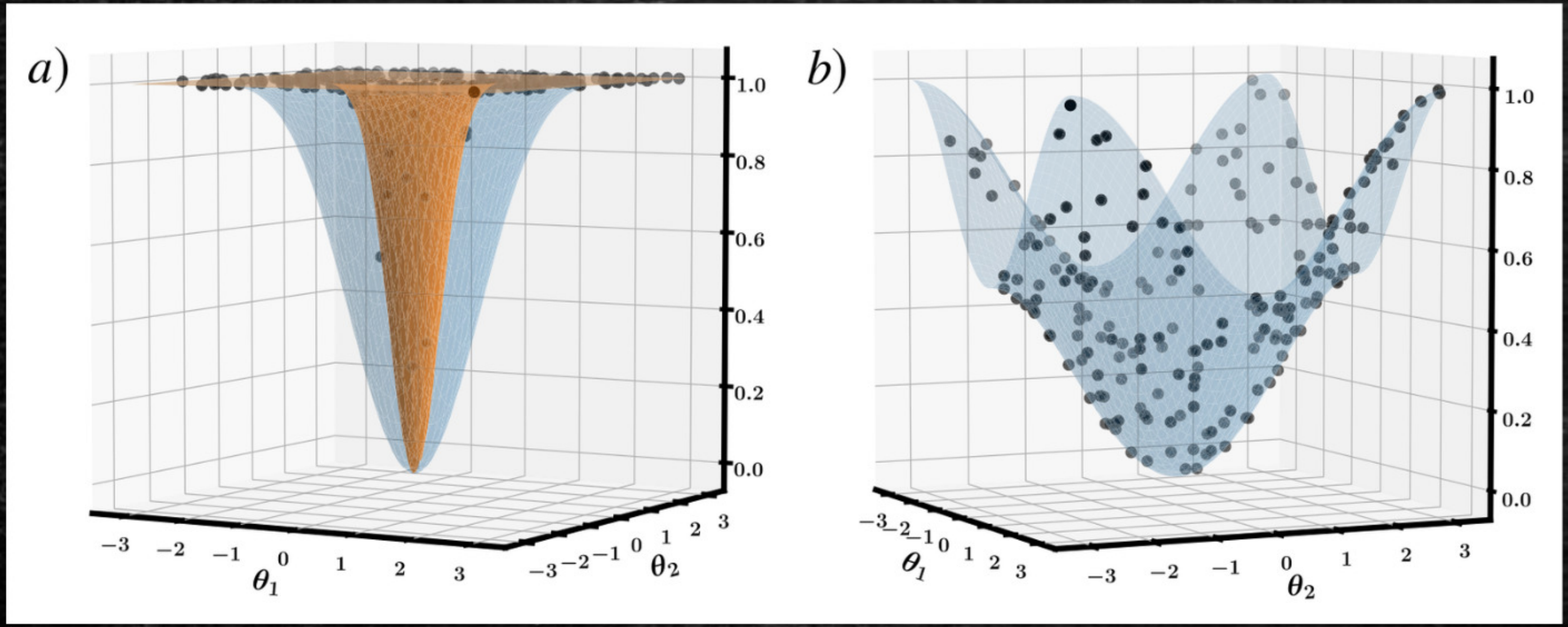
- Noise: Expectation value of an operators -> its average
- Flattens the parameter space
- E.g. QAOA for MaxCut

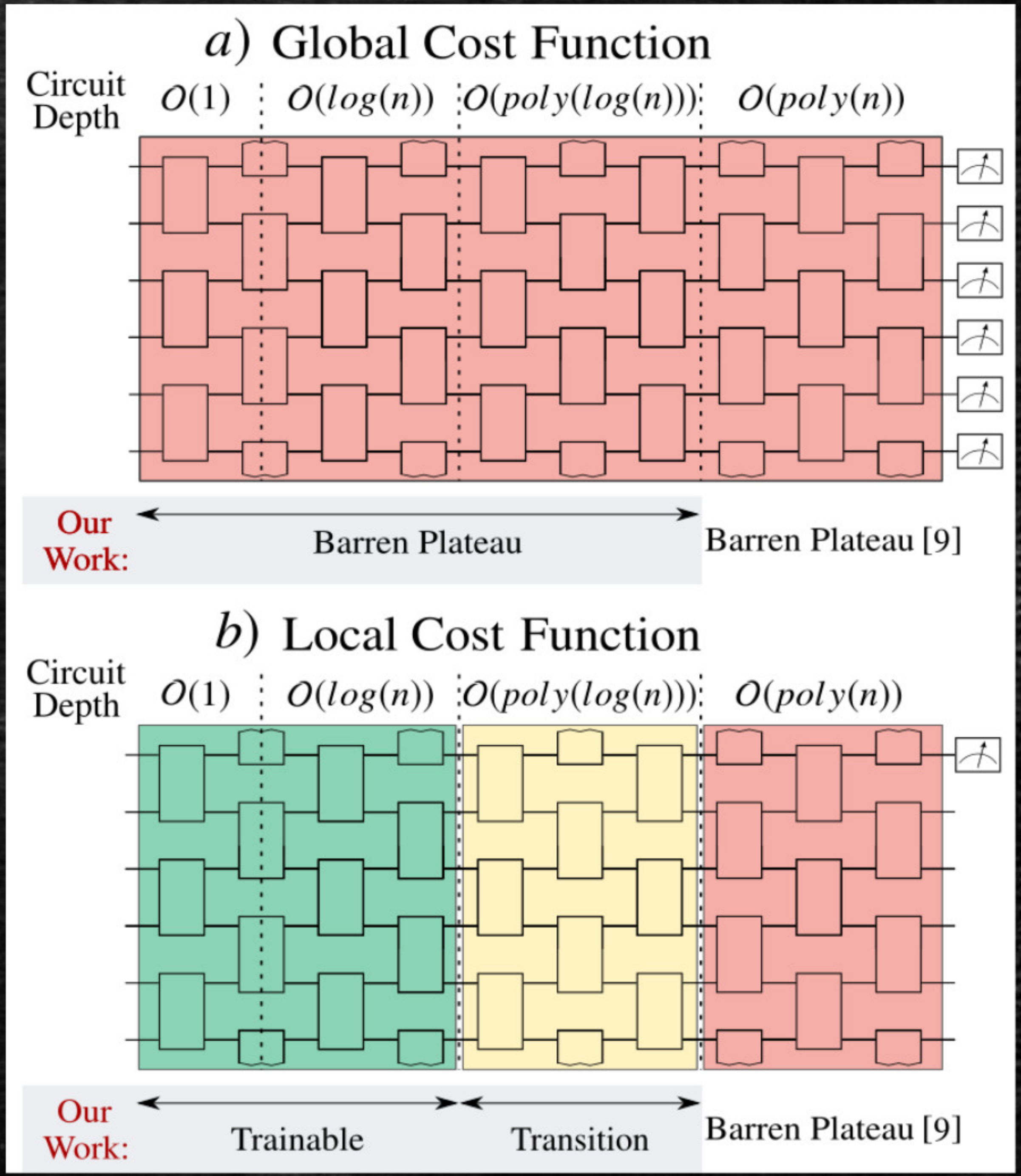



DOI: 10.1038/s41467-021-27045-6

# Barren Plateau: Global cost function

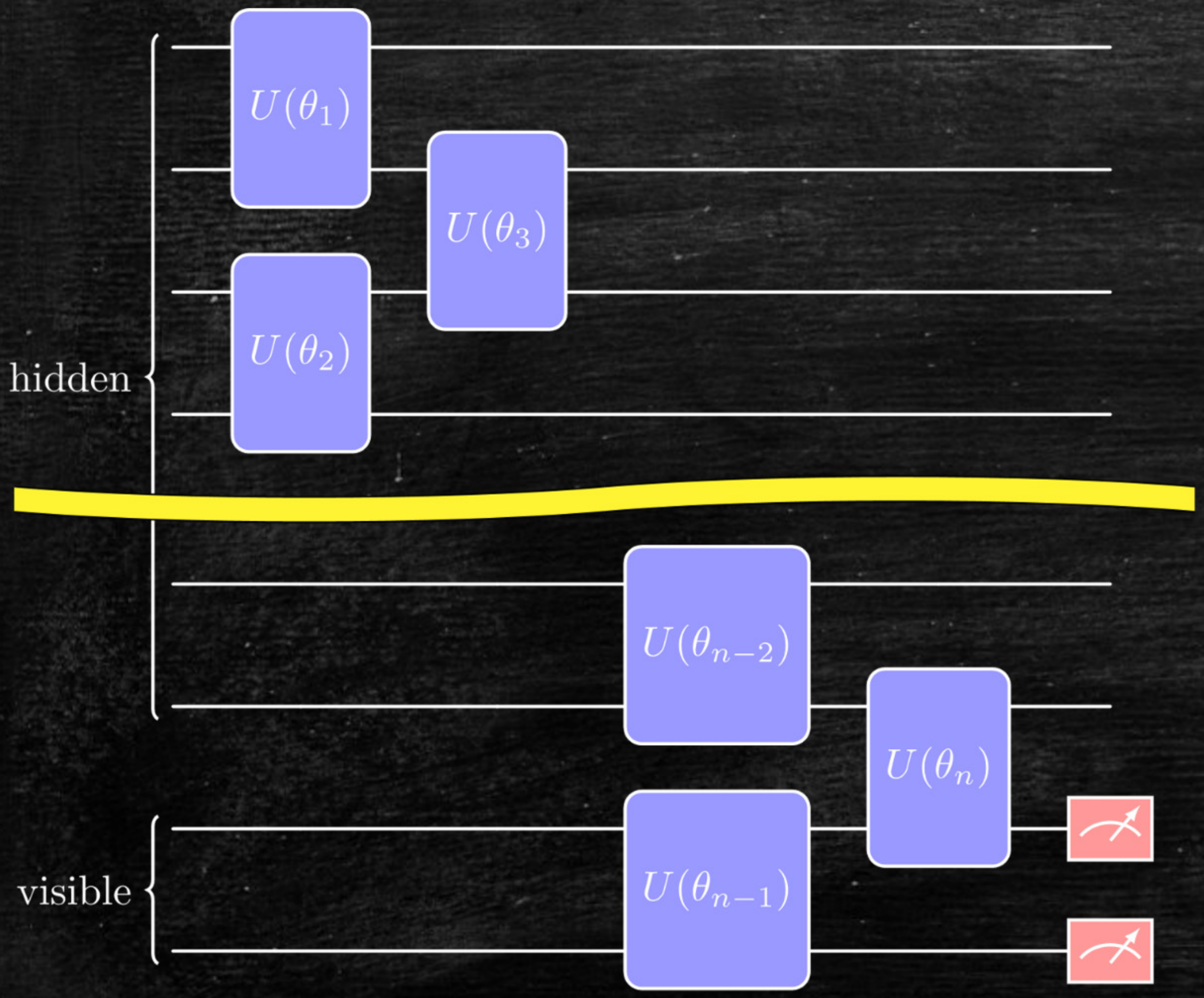
- Circuit depth as well as global cost function can cause BP.




DOI: 10.1038/s41467-018-07090-4
DOI: 10.1038/s41467-021-21728-w

# Barren Plateau: Entanglement

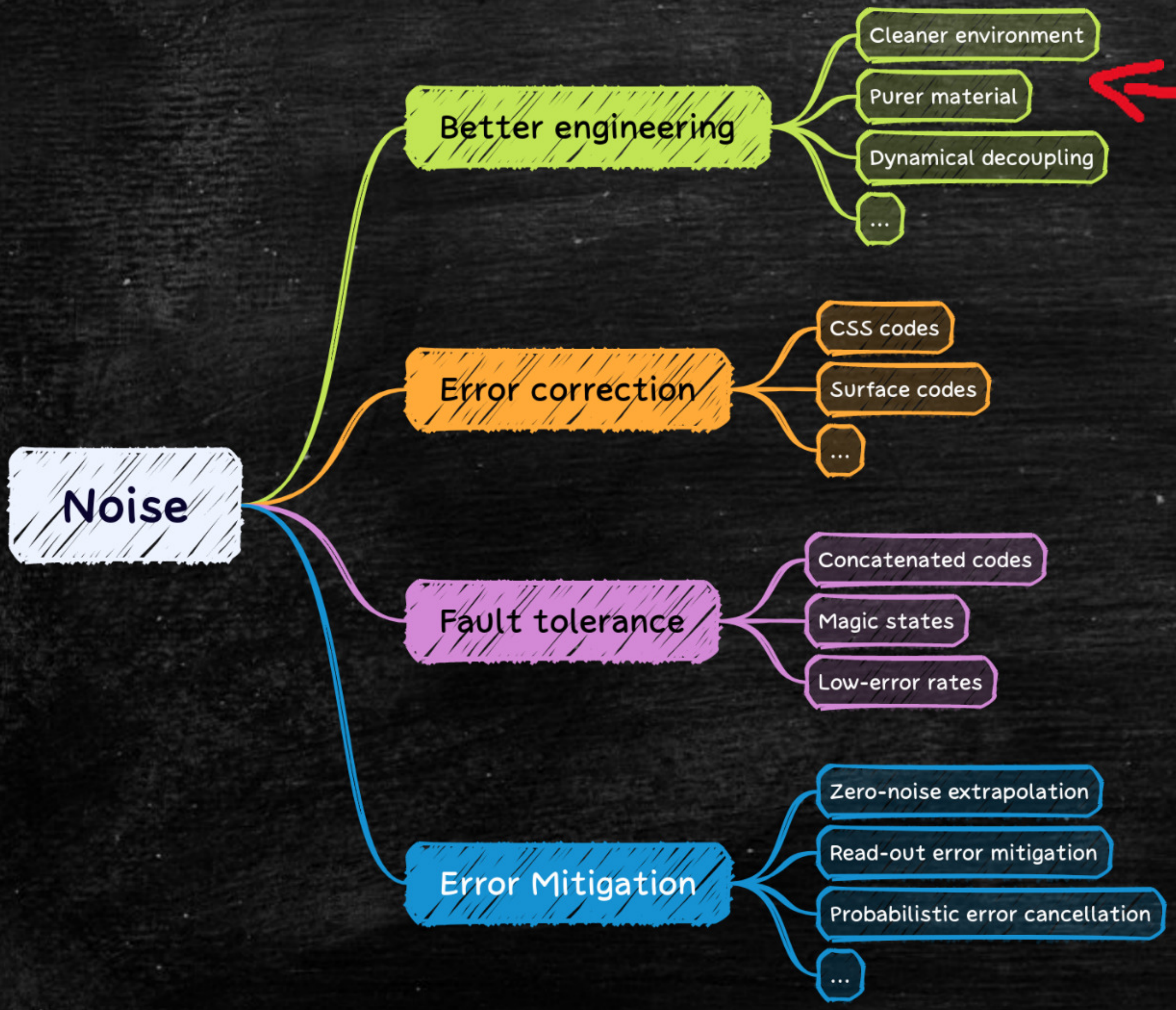



- B/w hidden and visible qubits (volume law)
- Entanglement in the training data
- => Barren Plateau


DOI: 10.1007/s42484-023-00103-6
DOI: 10.1103/PhysRevLett.128.180505
DOI: 10.1103/PRXQuantum.2.040316

# Solutions

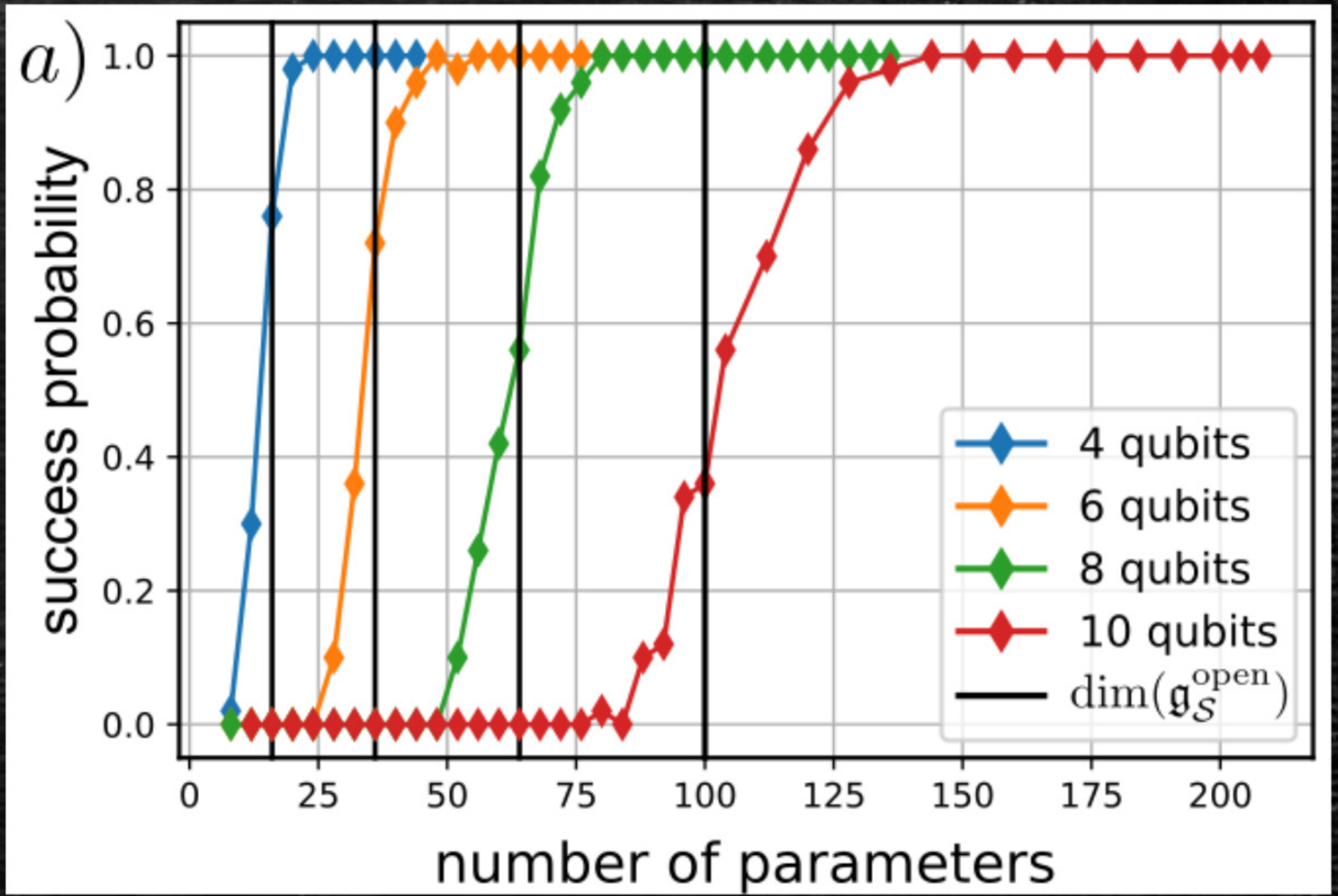
# Solutions: Noise




- NISQ-era VQA challenges!

# Solutions: LM -> Overparametrization

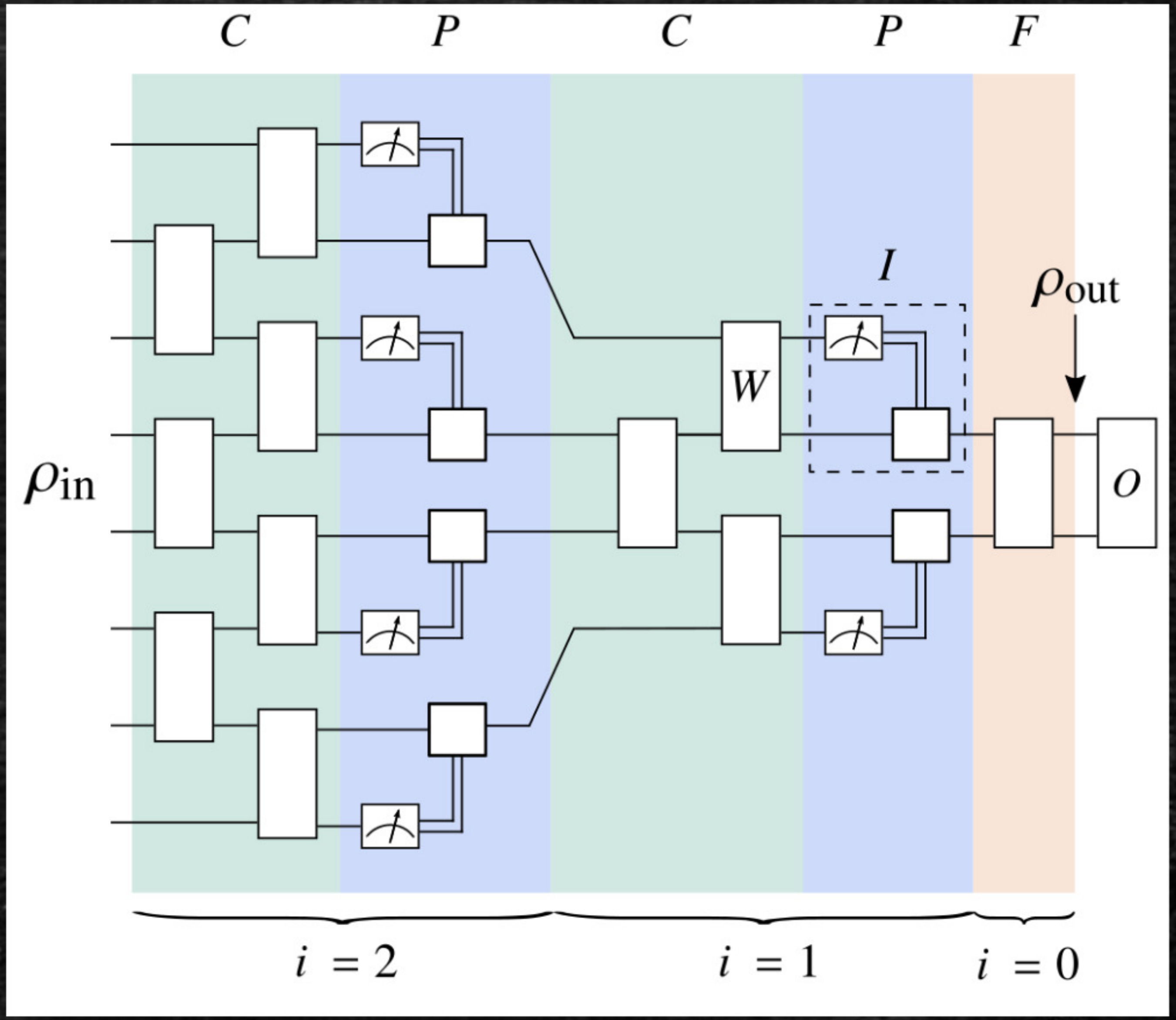
- Overparametrization can increase the success probability.
- The rank of the Quantum Fisher Information Matrix is a good threshold.
- Noise can affect these in a non-intuitive manner.
  - Increases the rank of QFIM
  - Eigs. exponentially small, insensitive to change




DOI: 10.1038/s43588-023-00467-6
https://arxiv.org/abs/2302.05059v1

# Solutions: BP -> Careful design

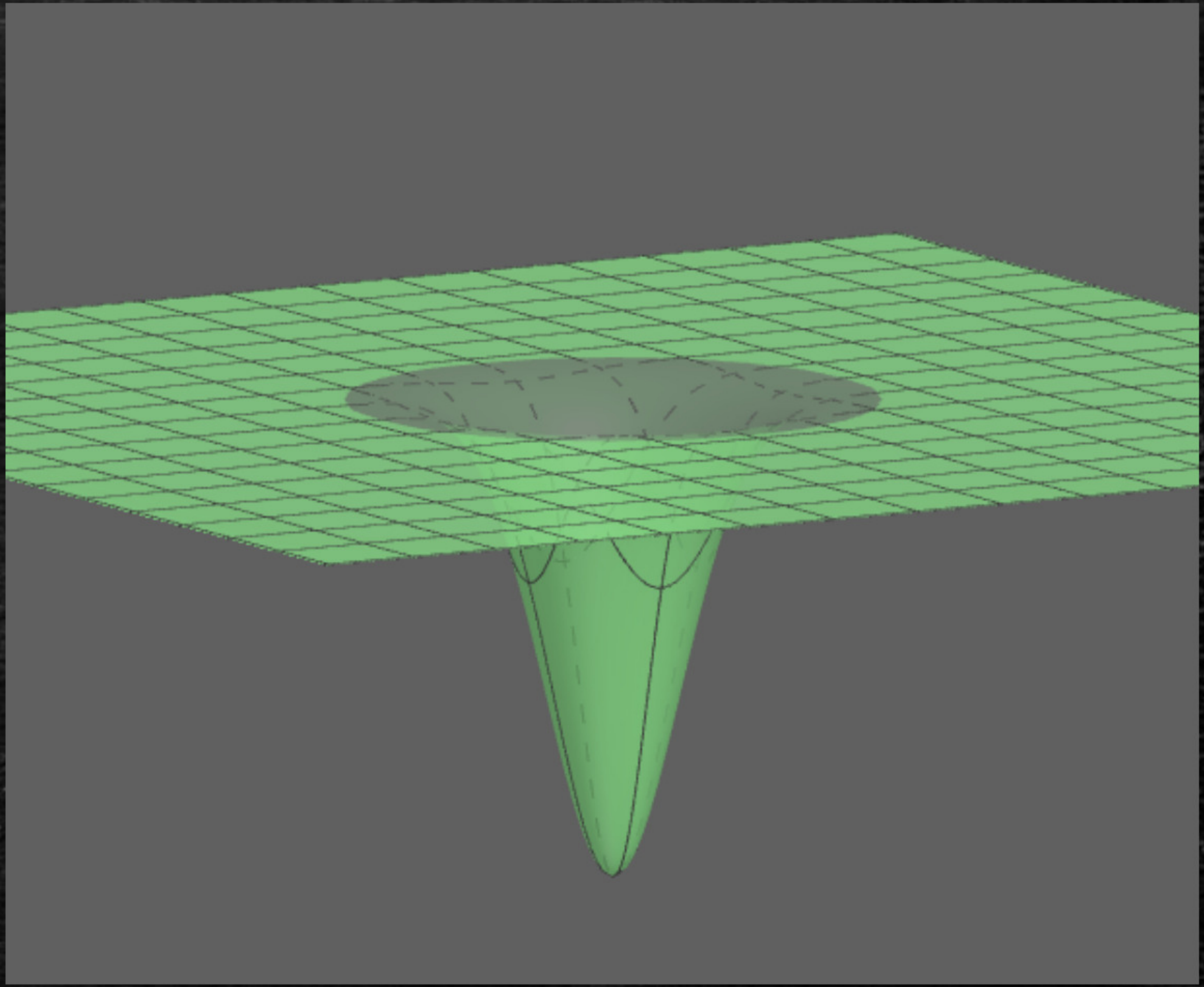
- It is very important to choose a good ansatz.
- Some ansatz do not exhibit Barren plateaus.
- There are also techniques one can use in the design of the ansatz to avoid barren plateaus.




DOI: 10.1103/PhysRevX.11.041011
DOI: 10.1103/PRXQuantum.3.020365

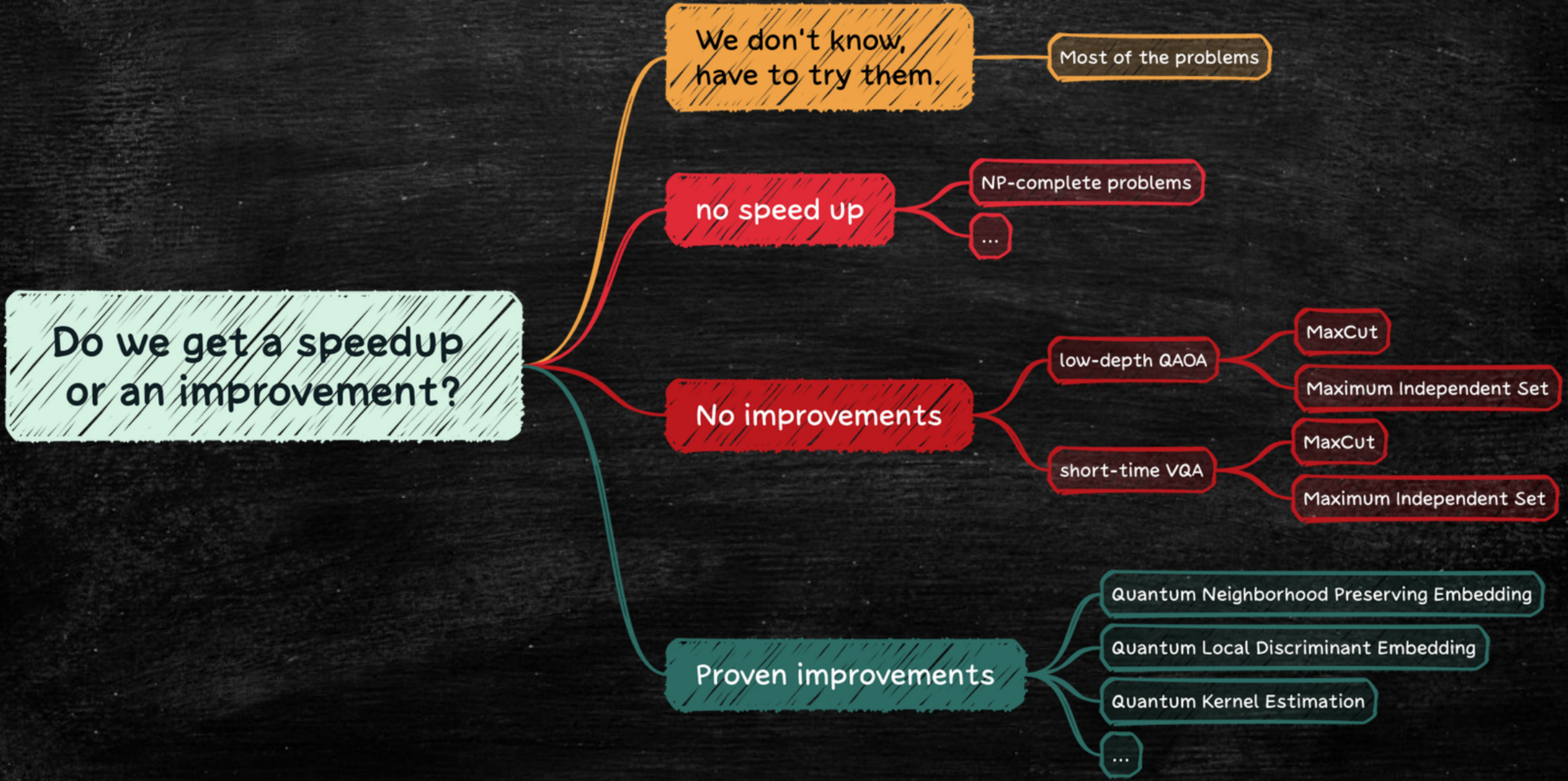
# Solutions: BP -> Hot start

- There are proposals to use techniques such as:
  - Classical machine learning
  - MPS
  - Classical Shadows
  - ...
- Start from:
  - Good initial states.
  - Good set of parameters
  - …
- Avoid the BP region.



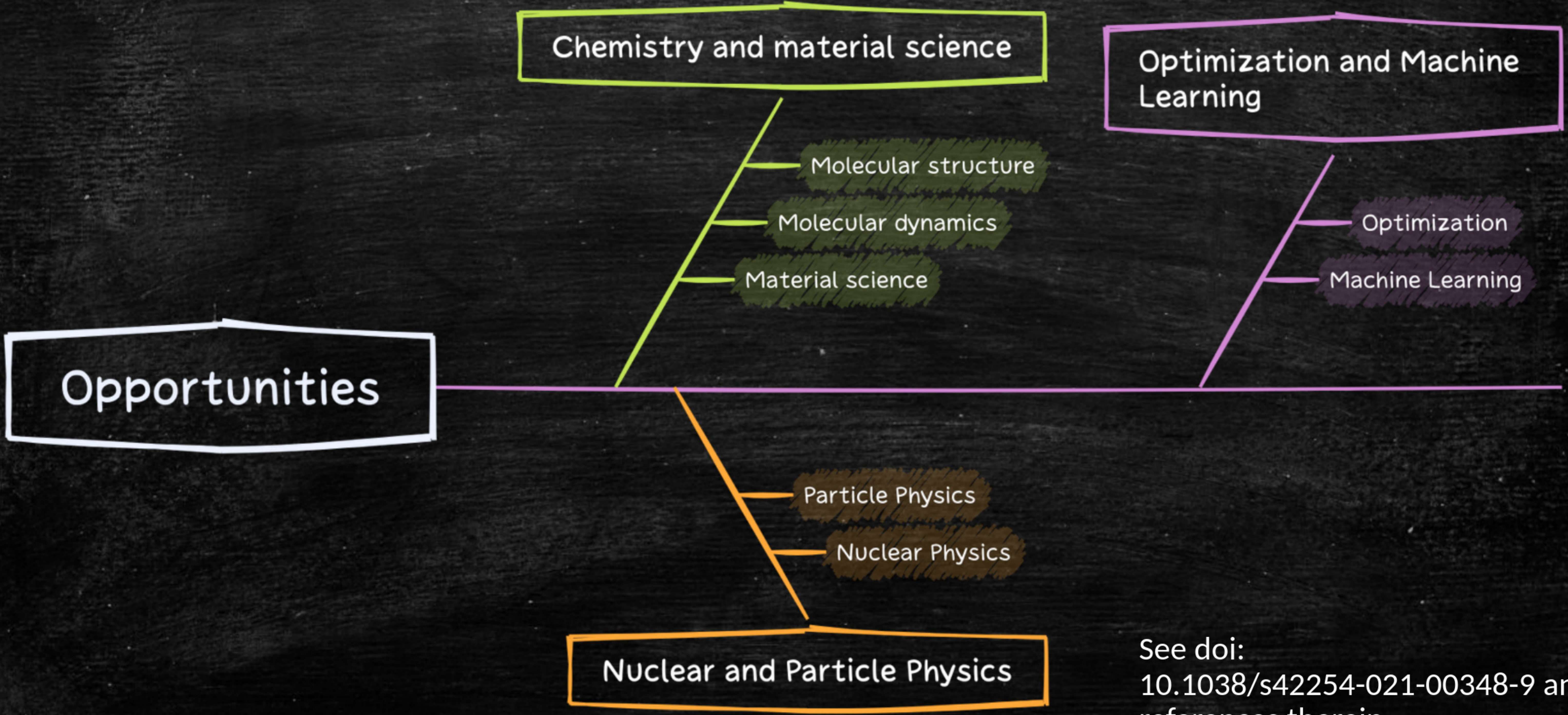
DOI: 10.1088/1367-2630/acb58e, DOI: 10.1103/PRXQuantum.3.020365

# Speed-up



Do we get a speedup or an improvement?
We don't know, have to try them.
Most of the problems
no speed up
NP-complete problems
...
No improvements
low-depth QAOA
MaxCut
Maximum Independent Set
short-time VQA
MaxCut
Maximum Independent Set
Proven improvements
Quantum Neighborhood Preserving Embedding
Quantum Local Discriminant Embedding
Quantum Kernel Estimation
...

# Promising Possible Applications




See doi: 10.1038/s42254-021-00348-9 and references therein.

# Summary

- Variational Quantum Algorithm is a promising approach for getting quantum improvements in NISQ-era.
- There are certain pitfalls one should avoid.
- Its true power is likely to become apparent as more powerful quantum computers emerge.

# Thank you!