Quantum Circuit Generation for Combinatorial Optimization Problems

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arXiv:2501.16986

Quantum Circuit Generation/Synthesis

Paper: arXiv:2501.16986

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■ Quantum circuit generation is the process of automatically generating a quantum circuit that implements a desired quantum operation.

Input

What to achieve

Quantum state

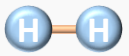
$$|\psi\rangle = \sum_{k=0}^{N-1} a_k |k\rangle$$

Unitary

$$U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1N} \\ u_{21} & u_{22} & \cdots & u_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ u_{N1} & u_{N2} & \cdots & u_{NN} \end{bmatrix}$$

Task description

```
Quantum circuits for the
prime factorization of 100.
```



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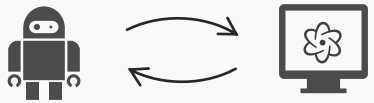
AI / ML

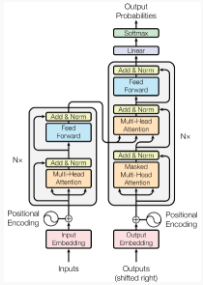
How to generate

Reinforcement learning



Diffusion model

Transformer



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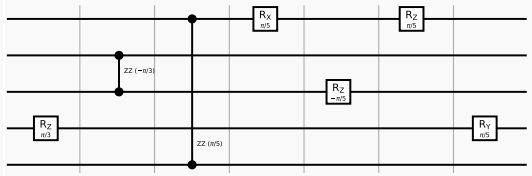
Quantum Circuit

What to generate

Gate



Code

```
qc = QuantumCircuit(3, 3)
qc.h(0)
qc.cx(0, 1)
qc.cx(0, 2)
qc.rx(0.5, 2)
qc.measure([0, 1, 2], [0, 1, 2])
```

⋮

Transformer-Based Quantum Circuit Generation

Paper: arXiv:2501.16986

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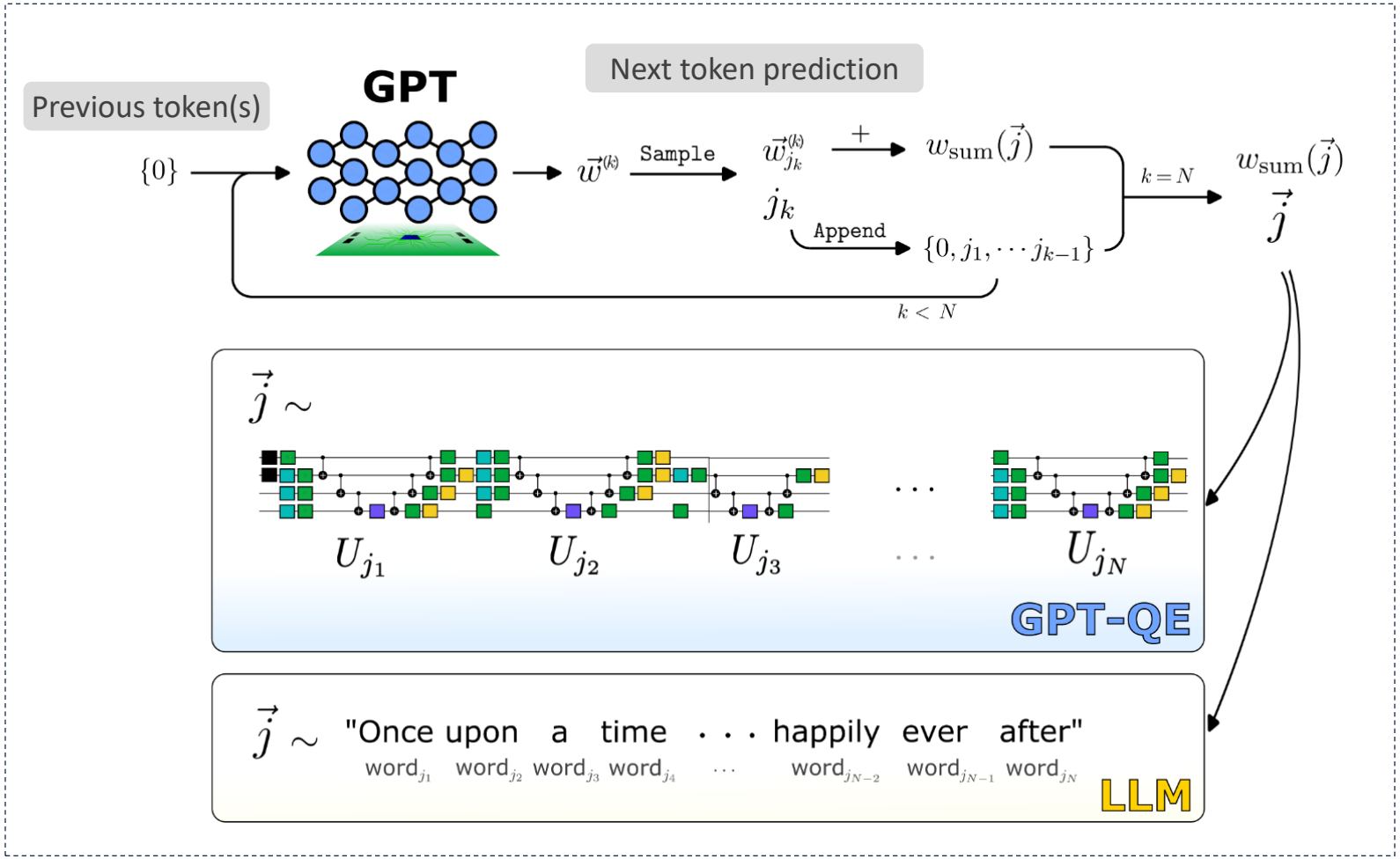
GQE: Generative Quantum Eigensolver [Nakaji+ 2024]

- GQE generates sequences of quantum gates in the same manner as LLMs.



GQCO: Generative Quantum Combinatorial Optimization

Paper: arXiv:2501.16986

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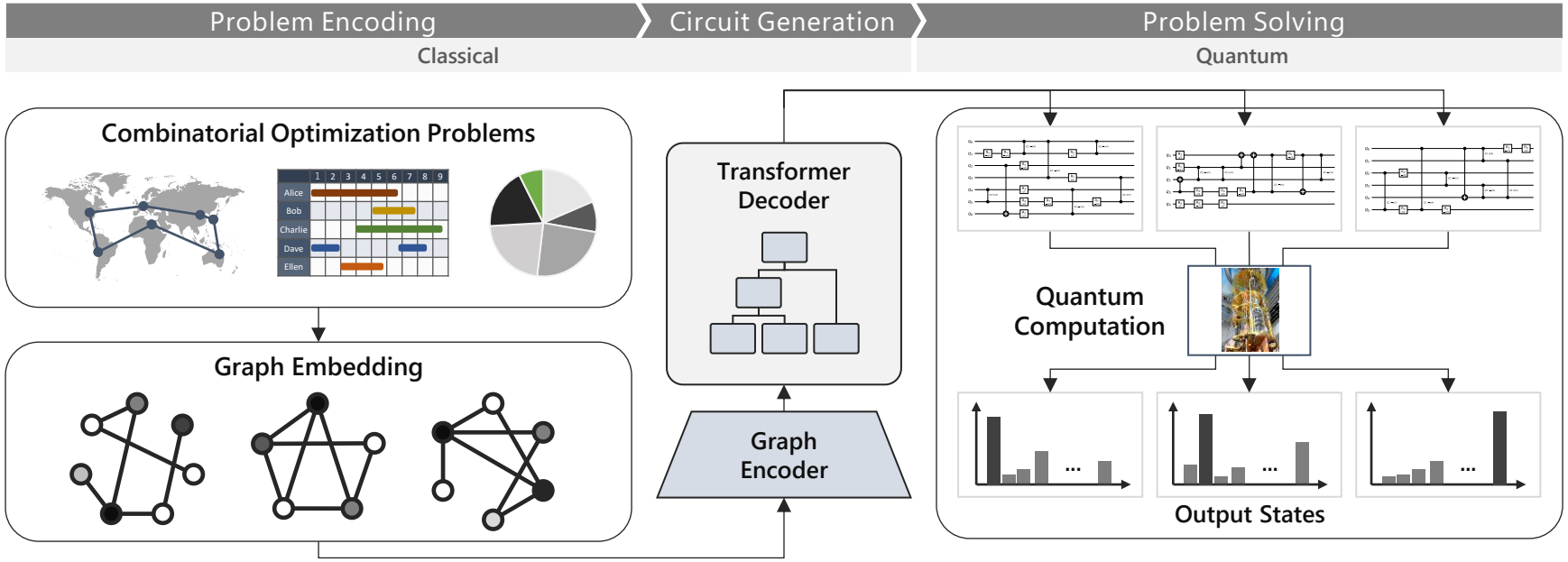
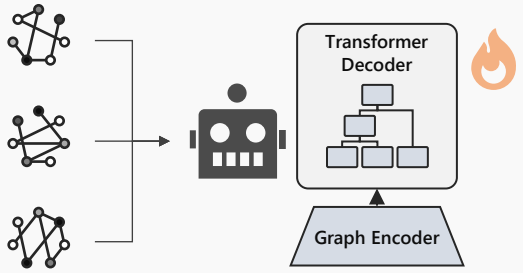
■ GQCO is a context-aware quantum circuit generator powered by an encoder-decoder Transformer.



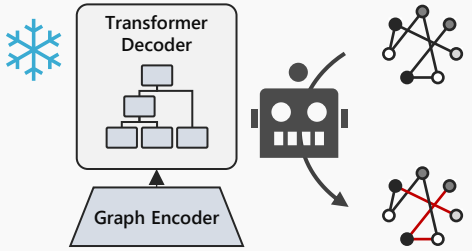
Training phase

Train a model on huge number of problems.



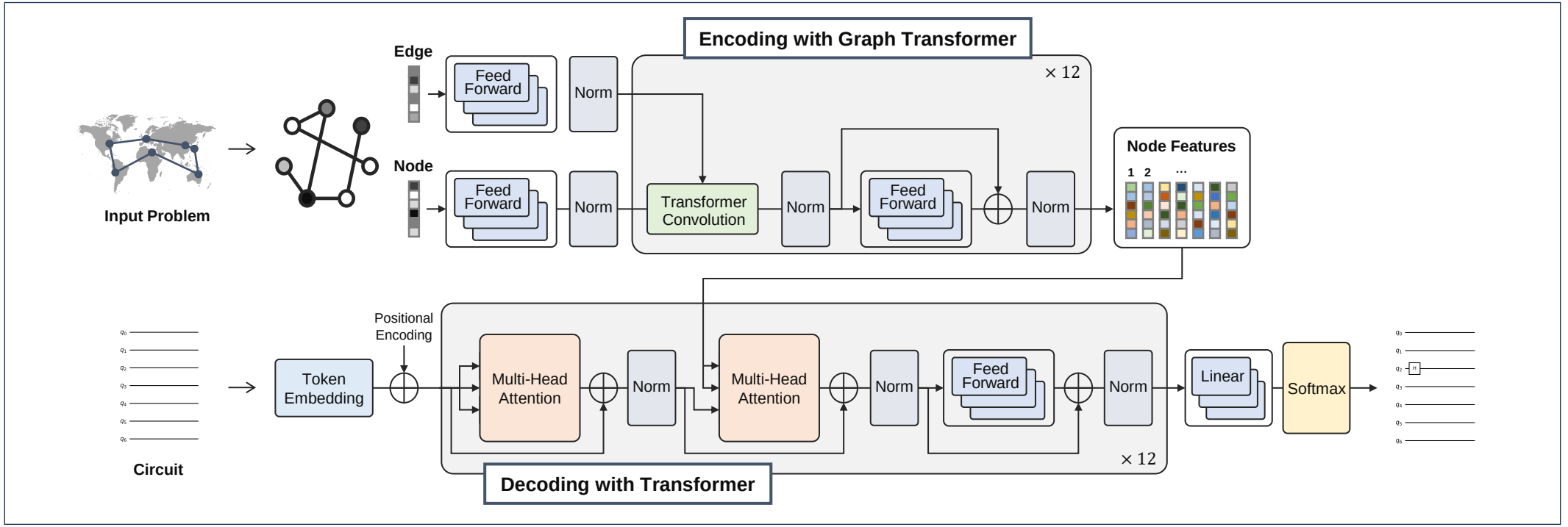
Inference phase

Solve new problems using the trained model.

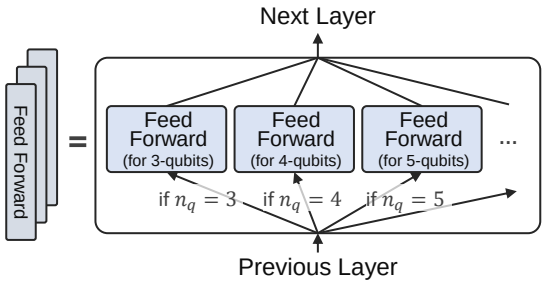


Model Architecture

Paper: arXiv:2501.16986



Qubit-based mixture of experts

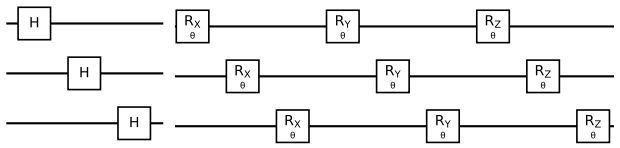


Gate pool (= vocabulary)

1-qubit gates

Hadamard

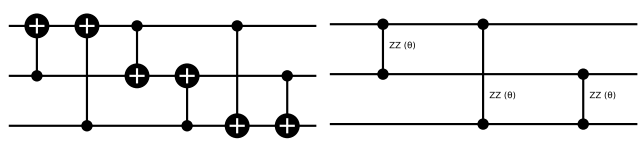
Rotation



2-qubit gates

CNOT

Rzz

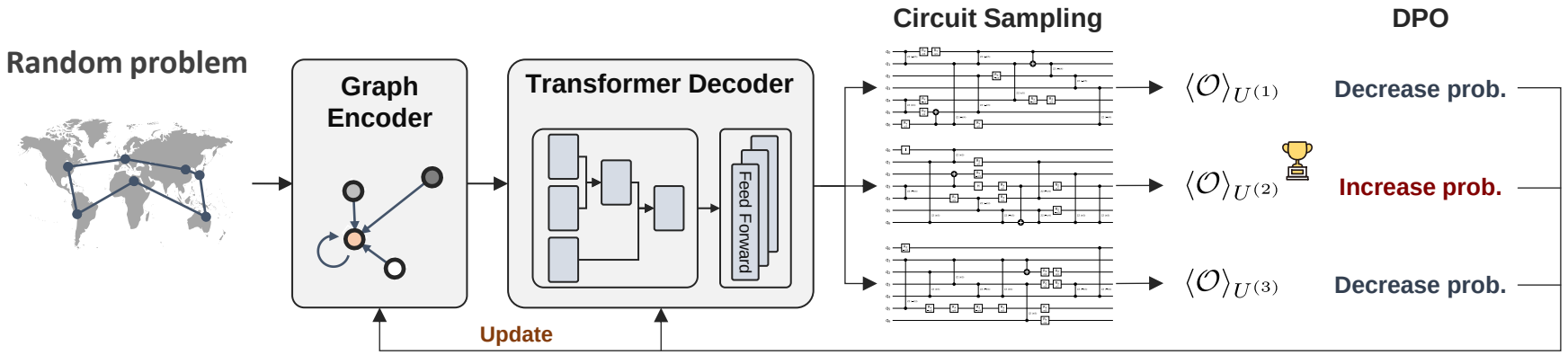


Training Procedure

Direct Preference Optimization + Negative Log-likelihood (= Contrastive PO) [Rafailov+ 2023, Xu+ 2024]

Loop

1. **Randomly generate coefficients of an Ising Hamiltonian**
2. **Generate multiple circuits for the input problem**
3. **Update the parameters to …**
   - increase the probability of generating a good circuit (one with lowest cost)
   - decrease the probability of generating the other circuits

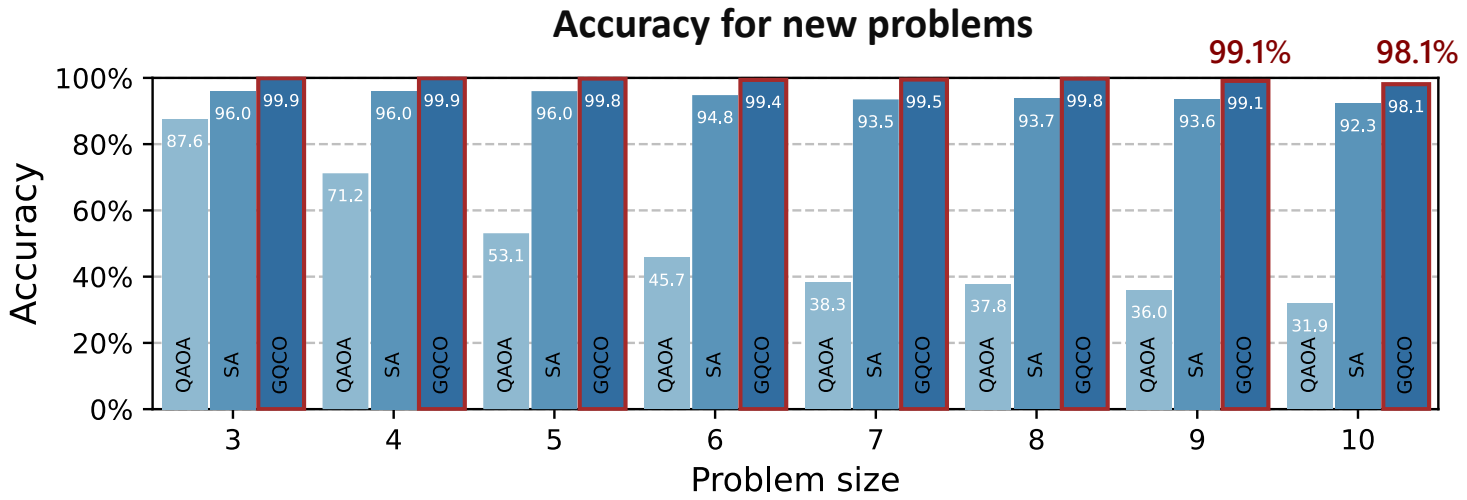


Loss function

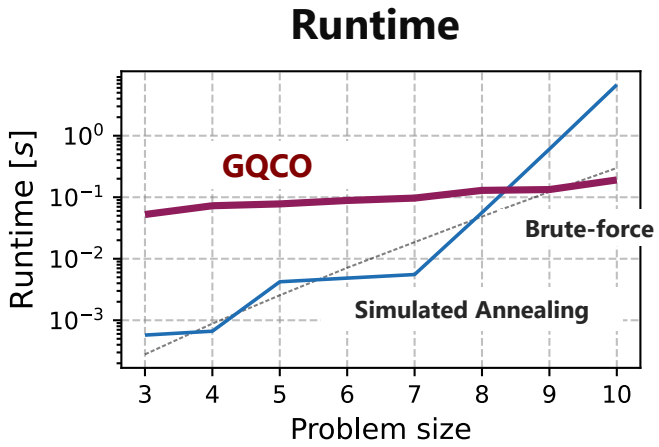
$$\log\left\{1+\exp\left\{-\beta\left(\log\frac{p(C_{best})}{\exp\{-E(C_{best})\}}-\log\frac{p(C_i)}{\exp\{-E(C_i)\}}\right)\right\}\right\}-\log p(C_{best})$$

Results and Performance Highlights

Paper: arXiv:2501.16986



► GQCO shows **nearly perfect performance** for problems with up to 10 qubits.



► GQCO is expected to solve problems **much faster** than brute force.

Solving Procedure and Generated Circuits

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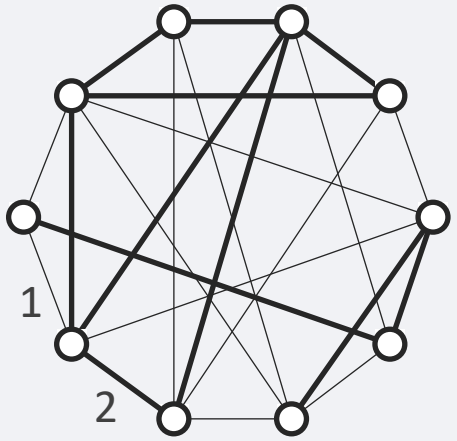
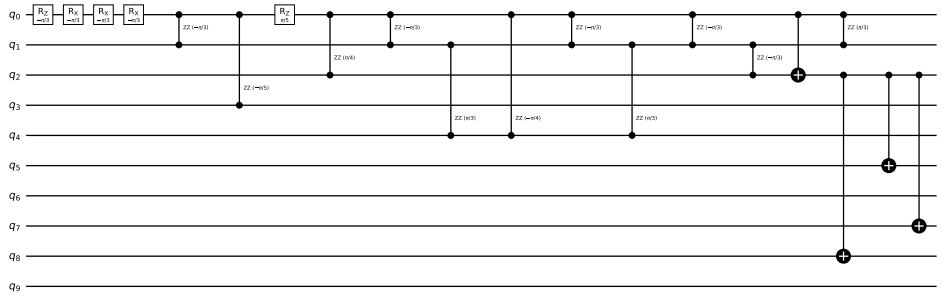
Input problem

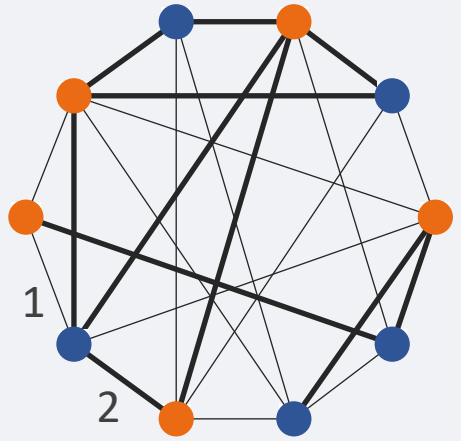


GQCO model

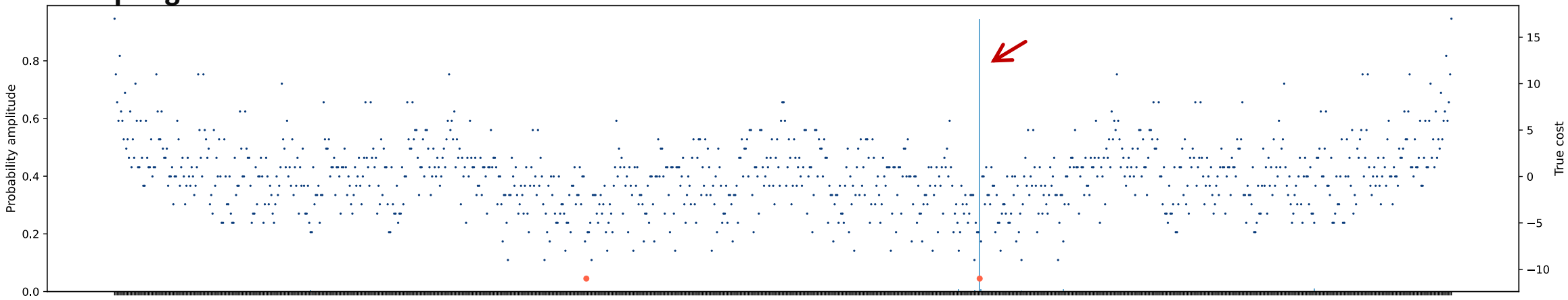
Generated circuit



Answer



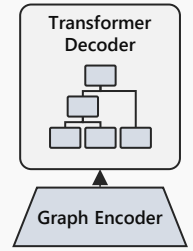
Sampling result



Summary and Future Perspectives

Summary

- We develop an input-dependent quantum circuit generator.
  - **Model architecture**: Encoder-decoder Transformer
  - **Training strategy**: DPO with randomly generated data

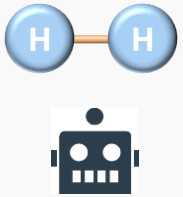


Future work: Scaling up

- We should **scale up the circuit size** for practical applications.
  - **Model architecture**: domain-guided encoder, optimal gate pool
  - **Training strategy**: Loss function, pre-training, …

Future work: Applications for other domains

- GQE for **ground state search of molecules**.
- GQE for **quantum machine learning**.
- GQE for **…**



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