QCircuitBench: A Large-Scale Dataset for Benchmarking Quantum Algorithm Design

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Motivation

Quantum Algorithm Design

- Deliver superpolynomial speedups.
- Challenging to design manually.

Large Language Models

- Abundant pre-training knowledge.
- Human-friendly interfaces.

Existing Benchmarks

- Target NISQ systems & tools—not AI training/evaluation.

Challenges

What challenges do we need to tackle?

Formulation: Natural Language? verbose, ambiguous (✗)
Math formulas? precise, but hard to verify automatically (✗)

Oracle Paradox: Theoretically: black-box.
Experimentally: explicit construction with quantum gates.

Classical Procedure: Quantum Algorithm = Quantum Circuit + Interpretation of Measurement Results.

Design Principles

Challenges

Formulation: Natural Language? (✗) Math formulas? (✗)

Oracle Paradox: Theoretically: black-box. Experimentally: explicit gates.

Classical Procedure: Quantum Algorithm = Quantum Circuit + Interpretation of Measurement Results.

Solutions

A code generation perspective

Represent quantum algorithms with quantum programming languages.

A Separate oracle.inc library

Preserve black-box abstraction while enabling compilation in OpenQASM.

Require post-processing functions

Include number of shots to characterize query complexity.

QCircuitBench

First large-scale benchmark for LLM-driven quantum algorithm design

- **Task Formulation**

  A general framework capturing the core aspects of quantum algorithm design.

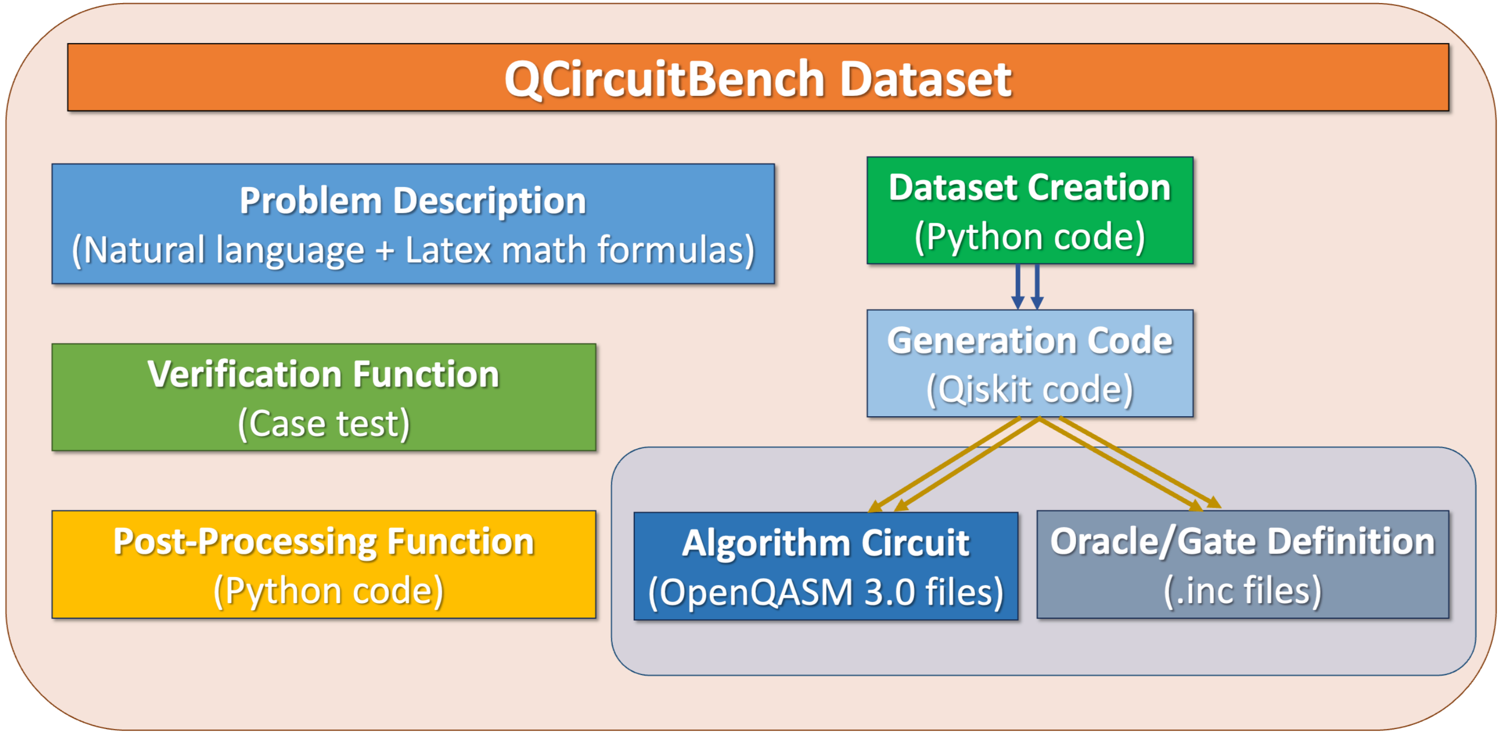
- **Rich Algorithm Coverage**

  Covering 3 task suites, 25 algorithms, 120,290 data points.

- **Automatic Verification**

  OpenQASM syntax, Python syntax, and task-specific semantic checks.

- **Training Potential**



Task Suite

❖ Oracle Construction

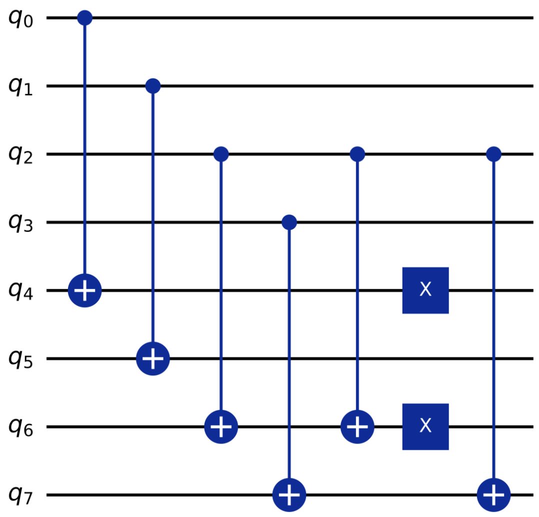
Encode Boolean function f as an oracle U_f such that $U_f|x\rangle|z\rangle = |x\rangle|z \oplus f(x)\rangle$.

❖ Quantum Algorithm Design

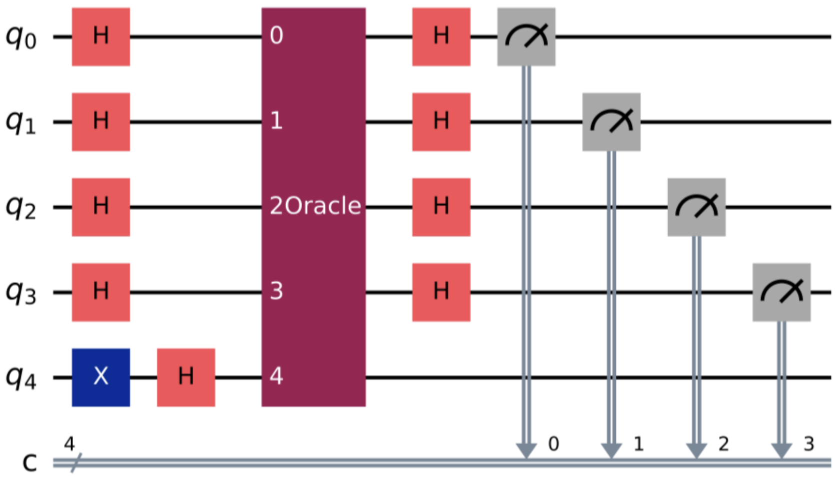
Covers textbook-level algorithms to advanced applications.

❖ Random Circuit Synthesis

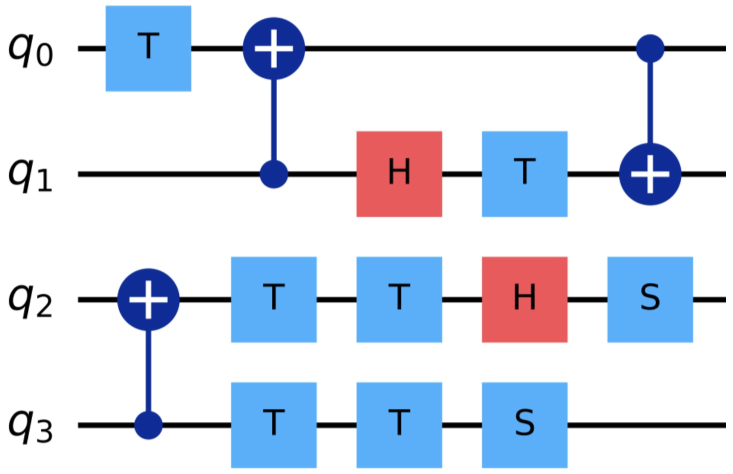
Reproduce quantum states from Clifford set {H, S, CNOT} / universal set {H, S, T, CNOT}.



(a) Simon's Problem (s=1100)



(b) Deutsch-Jozsa Algorithm



(c) Universal Circuits

Benchmark Results

Observations

- BLEU ≠ correctness: high BLEU score but low syntax/semantic accuracy.
- Few-shot > one-shot on structurally simple or template-like tasks; useless for hard ones.
- VQAs reveal challenges in modeling hybrid quantum-classical workflows.

Types of Errors

- Improvisation error: use unsupported namespaces/OpenQASM 3.0 features.
- Counting error: fail to identify ‘1’ bits in the secret string *(e.g., Bernstein-Vazirani)*.
- Data contamination: strong at generic Qiskit/Cirq, weak at gate-level QASM synthesis.

Fine-tuning Results

- LoRA-based fine-tuning on LLaMA3-8B.
- Improves scores, especially better at counting '1' bits *(Bernstein-Vazirani)*.
- Scores drop on random circuits, indicating challenge of encoding quantum state vectors within a language model and overfitting on tasks with high output diversity.

Table 2: Fine-tuning oracle construction scores.

Score	Model	Setting	Bernstein-Vazirani	Deutsch-Jozsa	Grover	Simon	Clifford	Universal	Avg
BLEU	gpt4o	few-shot(5)	95.6388 (±0.3062)	91.0564 (±0.6650)	92.0620 (±0.6288)	80.3390 (±2.0900)	39.5469 (±3.6983)	33.3673 (±3.1007)	72.0017
	Llama3	few-shot(5)	53.5574 (±5.2499)	69.8996 (±5.7812)	61.3102 (±5.4671)	26.3083 (±2.0048)	13.0729 (±0.9907)	13.4185 (±1.2299)	39.5945
	Llama3	finetune	76.0480 (±7.9255)	71.8378 (±2.4179)	67.7892 (±7.8900)	43.8469 (±3.2998)	10.8978 (±0.6169)	7.1854 (±0.5009)	46.2675
Verification	gpt4o	few-shot(5)	0.0000 (±0.0246)	0.4300 (±0.0590)	0.0000 (±0.1005)	-0.0200 (±0.0141)	-0.0333 (±0.0401)	-0.1023 (±0.0443)	0.0457
	Llama3	few-shot(5)	-0.2700 (±0.0468)	0.0900 (±0.0668)	-0.5200 (±0.0858)	-0.6600 (±0.0476)	-0.7303 (±0.0473)	-0.5056 (±0.0549)	-0.4327
	Llama3	finetune	-0.1300 (±0.0485)	-0.2000 (±0.0402)	-0.3300 (±0.0900)	-0.7400 (±0.0441)	-0.8741 (±0.0343)	-0.9342 (±0.0262)	-0.5347
PPL	Llama3	few-shot(5)	1.1967 (±0.0028)	1.1174 (±0.0015)	1.1527 (±0.0021)	1.1119 (±0.0017)	1.4486 (±0.0054)	1.4975 (±0.0051)	1.2541
	Llama3	finetune	1.0004 (±0.0002)	1.1090 (±0.0014)	1.0010 (±0.0006)	1.1072 (±0.0011)	1.2944 (±0.0053)	1.3299 (±0.0055)	1.1403

Takeaways

❖ **Novelty**

- First large-scale benchmark for LLM-driven quantum algorithm design.

❖ **Dataset Design**

- A perspective from code generation.
- Modular and extensible structure.
- Automatic verification functions.

❖ **Experiments**

- QCircuitBench poses significant challenges to SOTA LLMs.
- Fine-tuning experiments demonstrate early promise.

Thanks!