Quantum Computing: Recent Advances

Three Research Papers on Quantum GANs and Protein Folding

Presentation

Ngày 18 tháng 11 năm 2025

Nội dung trình bày

Paper 1: Tổng quan

Tiêu đề: Quantum Generative Adversarial Networks in a Silicon Photonic Chip with Maximum Expressibility

Tác giả: Haoran Ma, Liao Ye, Fanjie Ruan, et al. (Zhejiang University)

Nguồn: arXiv:2404.05921v1

Lĩnh vực: Quantum Machine Learning, Silicon Photonics, GANs

Động lực nghiên cứu

Vấn đề:

- Quantum GANs có tiềm năng lợi thế hàm mũ so với classical GANs
- Cần nền tảng phần cứng có khả năng biểu diễn cao (high expressibility)
- Các chip photonic trước đây bị giới hạn về khả năng tạo trạng thái lượng tử

Giải pháp:

- Thiết kế chip silicon photonic 2-qubit có thể tạo **bất kỳ trạng thái thuần 2-qubit nào**
- Thực thi các phép toán Controlled-Unitary (CU) tùy ý
- Kết hợp AMZI (Asymmetrical MZI) và frequency post-selection

Kiến trúc chip

Thành phần chính:

1. **Nguồn photon:** 2 spiral waveguides tạo photon pairs qua SFWM
2. **AMZI:** Điều chỉnh biên độ entangled states
3. **Controlled-Unitary operations:** Tạo trạng thái 2-qubit tùy ý
4. **Single-qubit gates:** State tomography và tính toán

Đặc điểm kỹ thuật:

- Kích thước: $3mm \times 0.8mm$
- 14 phase shifters (PS) điều khiển nhiệt-quang
- Bước sóng: Signal 1555.75nm, Idler 1546.12nm
- Coupling loss: ~ 4.5 dB

AMZI với Frequency Post-selection

Nguyên lý hoạt động:
Ma trận truyền AMZI:

$$U_{AMZI} = e^{j(\beta_{s,i}\Delta l+\phi)} \begin{bmatrix} \sin((\beta_{s,i}\Delta l+\phi)/2) & \cos((\beta_{s,i}\Delta l+\phi)/2) \\ \cos((\beta_{s,i}\Delta l+\phi)/2) & -\sin((\beta_{s,i}\Delta l+\phi)/2) \end{bmatrix}$$

Coincidence rate:

$$C(\phi) \propto C_{max} \sin^4(\phi/2)$$

Trạng thái tạo ra:

$$|\psi_0\rangle = e^{i\theta_s} \frac{\sqrt{C_1(\phi_1)}|0_s\rangle|0_i\rangle + \sqrt{C_2(\phi_2)}|1_s\rangle|1_i\rangle}{A}$$

với góc quay: $\tan(\phi) = \sqrt{C_2(\phi_2)/C_1(\phi_1)}$

Khả năng tạo trạng thái tùy ý

Quantum circuit tương đương:
Kết hợp $R_y(\phi)$ gate và 2 unitary $\hat{U}$ và $\hat{V}$ có thể tạo bất kỳ trạng thái 2-qubit nào:

$$|\psi_2\rangle = \sqrt{p_0}|00\rangle + \sqrt{p_1}|01\rangle + \sqrt{p_2}|10\rangle + \sqrt{p_3}|11\rangle$$

với $p_0 + p_1 + p_2 + p_3 = 1$

Ý nghĩa:

- Hệ số trước mỗi basis state hoàn toàn tùy ý
- Maximum expressibility cho quantum GANs
- Vượt trội so với các công trình trước [32-36]

Thí nghiệm 1: Học trạng thái Single-qubit

Mô hình PQ-GAN (Pure Quantum GAN):

- Generator G: Tạo trạng thái lượng tử $\rho(\theta_g)$
- Discriminator D: Đo quantum measurement $M(\theta_d)$

Hàm tối ưu:

$$\min_{\theta_g} \max_{\theta_d} \text{tr}[M(\theta_d)\rho(\theta_g)] - \text{tr}[\sigma M] = 0$$

Kết quả:

- **Pure state:** Fidelity **99.41%** (trạng thái mục tiêu: $(|0\rangle + |1\rangle)/\sqrt{2}$)
- **Mixed state:** Fidelity **98.39%** (trạng thái: $0.7|0\rangle\langle 0| + 0.3|1\rangle\langle 1|$)
- Huấn luyện: 200 epochs, D:G ratio = 3:1
- Learning rates: $\eta_G = 0.02$, $\eta_D = 0.1$

Thí nghiệm 2: Load Classical Distribution

Kiến trúc HQC-GAN (Hybrid Quantum-Classical):

- Quantum Generator: PQC với 3 tham số trainable
- Classical Critic: Fully-connected NN (4-5-3-1)
- Loss function: Wasserstein distance với gradient penalty

Hàm tối ưu (WGAN-GP):

$$\min_{\theta_g} \max_{\theta_c} D_{p_\theta}(G(\theta_g)) - D_{p_\theta}(\hat{x}) + \lambda \mathbb{E}_{p_\theta}[||\nabla_\theta D_{p_\theta}(\hat{x})||_2 - 1]^2$$

Distributions được học:

1. Normal: $X \sim N(\mu = 1.5, \sigma = 1)$
2. Log-normal: $X \sim LN(\mu = 0.5, \sigma = 0.5)$
3. Bimodal: Superposition của 2 Gaussians

Kết quả Load Distribution

Hiệu suất:

- KLD (Kullback-Leibler Divergence) < 0.05 cho cả 3 distributions
- Huấn luyện: 500 epochs, 5 rounds với initialization khác nhau
- Critic:Generator ratio = 3:1
- Learning rates: $\eta_G = 0.08$, $\eta_C = 0.1$

Ưu điểm:

- WGAN-GP khắc phục mode collapse và vanishing gradients
- Quantum circuit depth thấp (chỉ 3 tham số)
- Data encoding vào basis state probabilities: $\vec{p} = [p_0, p_1, p_2, p_3]^T$

Thí nghiệm 3: Tạo ảnh MNIST nén

Hybrid Generator mới:

- Classical NN (2×2 với Leaky ReLU) + Quantum PQC
- Mục đích: Đưa nonlinearity vào quantum GANs
- Input: Noise vector $z \sim U[0, 1]$
- Output: MNIST digits 2×2 sau PCA

Preprocessing:

- MNIST $28 \times 28 \rightarrow$ PCA $\rightarrow$ 3 dimensions
- Augment: $\vec{x}' = [\vec{x}^T, 0.5]$
- Map: $p_i = x'_i / \sum_{j=0}^{3} x'_j$

Gradient computation:

$$\frac{\partial \theta_g}{\partial t} = \frac{L(\theta_g + \epsilon) - L(\theta_g - \epsilon)}{2\epsilon}$$

(Finite difference method với $\epsilon = 0.02$)

Kết quả MNIST Generation

Thành công:

- Tạo được hình ảnh cho tất cả 10 digits (0-9)
- KLD và critic loss hội tụ về 0
- Batch size: 5, 200 epochs
- Learning rates: $\eta_{NN} = 0.02$, $\eta_{PQC} = 0.08$, $\eta_C = 0.02$

Đổi mới:

- **Lần đầu tiên** quantum photonic chip học mixed states
- **Lần đầu tiên** tạo compressed images với silicon photonic
- Hybrid generator khác với cách tiếp cận hiện có: giữ info trong quantum state thay vì classical post-processing
- Có thể tích hợp vào quantum circuits phức tạp hơn

Paper 1: Đóng góp và Hạn chế

Đóng góp chính:

1. Chip silicon photonic có maximum expressibility (tạo mọi trạng thái 2-qubit)
2. 3 ứng dụng quantum GANs thành công trên phần cứng thực
3. Hybrid generator với classical NN để thêm nonlinearity
4. Kết quả SOTA cho quantum photonic GANs

Hạn chế:

- Chỉ 4 dimensions (2 qubits) - giới hạn ứng dụng
- Success rate bị ảnh hưởng bởi post-selection
- Requires cryogenic cooling cho SNSPDs

Triển vọng:

- Mở rộng lên high-dimensional encoding
- Kết hợp với patched GAN cho large-scale data
- Ứng dụng trong quantum state distribution loading

Paper 2: Tổng quan

Tiêu đề: Protein folding with an all-to-all trapped-ion quantum computer

Tác giả: Sebastián V. Romero, et al. (Kipu Quantum & IonQ Inc.)

Nguồn: arXiv:2506.07866v2

Lĩnh vực: Quantum Optimization, Protein Folding, Trapped-Ion Computing

Bài toán Protein Folding

Tầm quan trọng:

- Cấu trúc 3D protein quyết định chức năng sinh học
- Hiểu folding $\rightarrow$ drug design, disease treatment
- Thuật toán cổ điển: AlphaFold2 (AI-based) rất thành công

Tiếp cận lượng tử:

- Map protein folding $\rightarrow$ ground-state search
- Higher-Order Unconstrained Binary Optimization (HUBO)
- Lattice model: Tetrahedral lattice (4 directions/residue)

Challenges:

- Exponential growth của search space
- Dense coupling giữa các amino acids
- Hardware noise và limited connectivity

BF-DCQO Algorithm

Bias-Field Digitized Counterdiabatic Quantum Optimization:

Ưu điểm:

- Non-variational $\rightarrow$ tránh barren plateaus
- Phù hợp với dense HUBO problems
- Tận dụng all-to-all connectivity của trapped-ion

Hamiltonian:

$$H_{total} = \lambda_c H_c + \lambda_g H_g + \lambda_d H_d + \lambda_i H_i$$

- H_c: Chirality constraints
- H_g: Geometric constraints
- H_d: Steric/distance constraints
- H_i: Miyazawa-Jernigan interactions

Two-Stage Architecture

Tại sao cần 2 stages?

- Hardware noise ảnh hưởng đến measurement accuracy
- Tách energy estimation và structural decoding

Stage 1: Energy Estimation

- Chạy BF-DCQO để tìm ground state
- Đo năng lượng quantum system
- Output: Optimal parameters

Stage 2: Structural Decoding

- Fix parameters từ Stage 1
- Chạy với shots cao hơn để decode cấu trúc
- Map bitstring $\rightarrow$ 3D coordinates

Hardware: IonQ Trapped-Ion

Đặc điểm:

- All-to-all connectivity (fully connected graph)
- 36 qubits available
- High fidelity 2-qubit gates
- Longer coherence times so với superconducting

Circuit Pruning Strategies:

1. Soft Pruning:

- Chọn 1000 DCQO solutions ngẫu nhiên
- Đánh giá bằng local search
- Giữ top-5 solutions

2. Hard Pruning (better):

- Giới hạn entangling gates ở hàng trăm
- Giảm circuit depth và noise
- Consistently outperforms soft pruning

Kết quả: Protein Sequences

Tested proteins:

1. `GYDPETGTWG` (10 amino acids)
2. `QPPGGSKVILF` (11 amino acids)
3. `WTFGQGTKVEIK` (12 amino acids - **33 qubits**)

Achievements:

- **Optimal solutions** cho cả 3 sequences
- **Largest quantum protein folding** implementation to date
- Energy correlation với conformational energy rất tốt

Energy scaling:

- 5 residues $\rightarrow$ 14 residues: Minimum energy tăng **230,000%**
- Thể hiện exponential growth của energy landscape

Kết quả: MAX 4-SAT

Testing robustness với combinatorial optimization:

Setup:

- MAX 4-SAT instances at computational phase transition
- Clause-to-variable ratio ~ 9.7
- Kích thước: 24-36 qubits

Results:

- **Optimal solutions achieved** cho tất cả instances
- Consistent performance across different problem sizes
- Validates algorithm effectiveness beyond protein folding

Kết quả: Spin-Glass Problems

Fully connected spin-glass (36 qubits):

Test cases:

- 3 random instances với all-to-all coupling
- Dense interaction graph

Performance:

- **2 out of 3** instances: Exact ground state found
- 1 instance: Near-optimal solution
- Demonstrates synergy between:
  - Non-variational optimization
  - All-to-all connectivity hardware

Paper 2: So sánh và Triển vọng

So với Classical/AI approaches:

- AlphaFold2: Data-driven, cần large training set
- Quantum: Physics-based energy minimization
- Quantum có thể complement AI methods

Pathway to Quantum Advantage:

1. Trapped-ion scalability đang được cải thiện
2. BF-DCQO tránh được barren plateau problem
3. Dense HUBO problems với industrial relevance

Future directions:

- Longer protein sequences (>15 residues)
- Improved lattice models (off-lattice)
- Integration với experimental validation
- Drug discovery applications

Paper 3: Tổng quan

Tiêu đề: Prediction of Protein Three-dimensional Structures via a Hardware-Executable Quantum Computing Framework

Tác giả: Yuqi Zhang, et al. (Kent State, Cleveland Clinic, Harvard)

Nguồn: arXiv:2506.22677

Lĩnh vực: Quantum Computing, Structural Biology, Drug Discovery

Động lực: Beyond AlphaFold

AlphaFold3 limitations:

- Data-driven approach
- "Information trap"cho short peptides
- Limited capacity với fragments < 10 residues
- Không trực tiếp optimize physical energy

Quantum advantage hypothesis:

- Physics-based: Trực tiếp minimize Hamiltonian
- Higher theoretical reliability cho peptide fragments
- Better cho active site prediction (drug binding)

Goal:

- End-to-end executable pipeline trên utility-level quantum hardware
- Validation với therapeutic proteins
- Benchmarking vs AlphaFold3

Framework Architecture

Complete Pipeline:

1. **Problem Formulation**
   - Tetrahedral lattice encoding
   - Hamiltonian construction: $H_t = \lambda_c H_c + \lambda_g H_g + \lambda_d H_d + \lambda_i H_i$
2. **VQE Optimization**
   - EfficientSU2 ansatz
   - COBYLA optimizer
   - 2,000 shots, $\geq$ 200 iterations
3. **Two-Stage Execution**
   - Stage 1: Energy estimation
   - Stage 2: Fixed-parameter measurement (20,000 shots)
4. **Post-processing**
   - Atom completion
   - Charge neutralization
   - PDB file generation

Hardware: IBM Quantum

Platform:

- IBM-Cleveland Clinic 127-qubit processor
- Eagle r3 architecture
- Heavy-hex topology (limited connectivity)

Encoding scheme:

- Sparse Pauli operators
- Amino acid connectivity trong tetrahedral lattice
- Constraints: Chirality, geometry, distance, interactions

Computational efficiency:

- Average: $\sim$ 10 seconds/iteration
- 73.53% time trên quantum end
- Rest: Classical optimization overhead

Evaluation: Metrics

Geometric accuracy:

$$\text{RMSD} = \sqrt{\frac{1}{N}\sum_{i=1}^{N} ||r_i^{pred} - r_i^{ref}||^2}$$

Functional consistency:

- Molecular docking với AutoDock Vina
- Binding affinity (kcal/mol)
- Lower is better (stronger binding)

Test set:

- 23 protein fragments từ PDB
- Lengths: 5-10 residues
- 7 với therapeutic potential

Kết quả: vs AlphaFold3

Overall performance (23 fragments):

Metric	Quantum Method	AlphaFold3
Average RMSD (Å)	**3.33**	3.87
Average Binding Affinity (kcal/mol)	**-4.38**	-4.00

Superiority rates:

- RMSD: **18 out of 23** cases lower
- Binding affinity: **21 out of 23** cases better

Statistical significance:

- Clear advantage cho short peptides
- Especially good for active site regions

Kết quả: Therapeutic Proteins

Validation với 7 therapeutic targets:

1. **6mu3** - Anti-HIV-1 Fab 2G12
2. **3ans** - Human soluble epoxide hydrolase
3. **1a9m** - HIV-1 protease G48H
4. **1qin** - Lactoylglutathione lyase
5. **3b26** - HSP 90-alpha
6. **1fkn** - Beta-Secretase BACE1 (Alzheimer's)
7. **2xxx** - Glutamate receptor GluK2

Success:

- All structures predicted successfully
- Suitable for molecular docking
- Demonstrates feasibility cho drug discovery

Energy-Structure Correlation

Key finding:

- Positive correlation giữa quantum system energy và docking affinity
- Lower quantum energy $\rightarrow$ Better binding affinity
- Validates physics-based approach

Implications:

- Quantum method captures relevant molecular interactions
- Energy minimization meaningful cho structural biology
- Not just mathematical optimization - physically grounded

Advantage over AI:

- AI learns patterns, quantum solves physics
- More reliable cho novel sequences
- Less dependent on training data distribution

Scalability: Sliding Window

Challenge:

- Long proteins > 10 residues
- Exponential qubit requirements

Solution - Sliding Window approach:

- Window size: 7 residues
- Stride: 1 residue
- Overlap và merge fragments

Demonstration:

- Full-length Aβ42 (Alzheimer's peptide)
- Successfully predicted từ overlapping windows
- Enables handling arbitrary length sequences

Future improvement:

- Better merging algorithms
- Adaptive window sizes

Paper 3: Đóng góp chính

Scientific contributions:

1. **First** complete hardware-executable pipeline cho protein structure
2. **First** validation trên utility-level quantum processors
3. **Outperforms** AlphaFold3 cho short peptides
4. Direct application to drug discovery

Technical innovations:

- Two-stage architecture for noise mitigation
- Sliding-window scalability
- Post-processing for docking compatibility
- Comprehensive benchmarking methodology

Practical impact:

- Blueprint cho domain-specific quantum applications
- Demonstrates utility-level quantum computing feasibility
- Real-world therapeutic protein validation

So sánh 3 Papers

Aspect	Paper 1	Paper 2	Paper 3
Hardware	Silicon Photonic	Trapped-Ion (IonQ)	Superconducting (IBM)
Qubits	2 qubits	Up to 36 qubits	Up to 127 qubits
Algorithm	Quantum GANs	BF-DCQO	VQE
Application	Machine Learning	Protein Folding	Structure Prediction
Key Strength	Max expressibility	All-to-all connectivity	End-to-end pipeline
Main Result	99.41% fidelity	12 AA folded	Beats AlphaFold3

Common themes:

- Demonstrating quantum utility on real hardware
- Addressing NISQ-era challenges (noise, limited qubits)
- Application-driven research

Hardware Platforms Comparison

Silicon Photonic (Paper 1):

+ Room temperature operation
+ Low noise, high precision
+ Naturally suited for quantum communication
- Limited scalability (currently 2 qubits)
- Post-selection reduces success rate

Trapped-Ion (Paper 2):

+ All-to-all connectivity
+ High gate fidelities
+ Long coherence times
- Slower gates
- Moderate scalability challenges

Superconducting (Paper 3):

+ Most scalable (100+ qubits)
+ Fast gates

Quantum GANs vs Protein Folding

Different approaches to quantum advantage:

Quantum GANs (Paper 1):

- Exploit quantum superposition và expressibility
- Generator tạo quantum states
- Hybrid quantum-classical learning
- Focus: Machine learning applications

Protein Folding (Papers 2 & 3):

- Ground-state energy minimization
- Map biological problem $\rightarrow$ Hamiltonian
- Physics-based approach
- Focus: Scientific computing applications

Complementary directions:

- GANs: Generative models, creative tasks
- Folding: Optimization, structure discovery

Challenges và Limitations

Common challenges across all papers:

1. **Hardware noise**
   - Mitigation: Two-stage architectures, error mitigation
   - Still limits problem sizes
2. **Limited qubit counts**
   - Workarounds: Circuit pruning, sliding windows
   - Fundamental scaling needed
3. **Classical-Quantum interface**
   - Measurement overhead
   - Parameter optimization loops
   - Data encoding/decoding
4. **Validation**
   - How to verify quantum advantage?
   - Need better benchmarks
   - Classical baselines improving rapidly

Future Directions

Near-term (1-3 years):

- Scale to 50-100 logical qubits với error correction
- Better hybrid classical-quantum algorithms
- Application-specific quantum processors
- Improved noise mitigation techniques

Medium-term (3-7 years):

- Fault-tolerant quantum computing
- Quantum advantage cho practical problems
- Integration với AI/ML pipelines
- Commercial quantum applications

Long-term (7+ years):

- Universal quantum computers
- Drug discovery revolution
- Materials design

Ý nghĩa thực tiễn

Drug Discovery (Papers 2 & 3):

- Faster protein structure prediction
- Better binding affinity predictions
- Novel therapeutic target discovery
- Personalized medicine

Machine Learning (Paper 1):

- Quantum-enhanced generative models
- Distribution learning cho finance, physics
- Quantum data encoding
- Hybrid classical-quantum AI

Scientific Computing:

- Materials science simulations
- Chemical reaction modeling
- Optimization problems

Kết luận chung

Key takeaways:

1. **Quantum utility is emerging**
   - Real hardware demonstrations
   - Competitive with/surpassing classical methods
   - Application-specific advantages
2. **Multiple hardware platforms viable**
   - Photonic: Precision, low noise
   - Trapped-ion: Connectivity, fidelity
   - Superconducting: Scale, speed
3. **Hybrid approaches essential**
   - Classical-quantum co-design
   - Noise mitigation strategies
   - Domain-specific optimizations
4. **Path to quantum advantage**
   - Focus on specific applications
   - Leverage quantum strengths
   - Continuous hardware improvement

Tài liệu tham khảo

Papers discussed:

1. Haoran Ma, et al. "Quantum Generative Adversarial Networks in a Silicon Photonic Chip with Maximum Expressibility."arXiv:2404.05921v1, 2024.
2. Sebastián V. Romero, et al. "Protein folding with an all-to-all trapped-ion quantum computer."arXiv:2506.07866v2, 2025.
3. Yuqi Zhang, et al. "Prediction of Protein Three-dimensional Structures via a Hardware-Executable Quantum Computing Framework."arXiv:2506.22677, 2025.

Additional resources:

- IBM Quantum: `https://quantum-computing.ibm.com`
- IonQ Platform: `https://ionq.com`
- Xanadu Photonics: `https://xanadu.ai`

Cảm ơn!

Questions?