🧠 Variational Quantum Eigensolver (VQE) for Ising Model

A Comparative Analysis of Classical and Quantum Optimization Methods

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📘 Abstract

This study investigates the **Variational Quantum Eigensolver (VQE)** applied to the **Transverse Ising Model (TIM)** as a benchmark problem.
A new **hybrid optimization algorithm**, **QN-SPSA+PSR**, is proposed — combining the approximate computation of the **Fubini–Study metric** (from Quantum Natural Gradient) with the **exact gradient evaluation** via the **Parameter-Shift Rule (PSR)**.

This method achieves **faster convergence**, **better numerical stability**, and **low computational cost**, demonstrating promise for **Noisy Intermediate-Scale Quantum (NISQ)** devices.

⚛ 1. Introduction

Quantum computers leverage **superposition, probabilistics, and entanglement** to surpass classical computation.
However, due to current **noise and hardware limitations**, algorithms like **Variational Quantum Algorithms (VQAs)** — notably **VQE** and **QAOA** — are suitable for NISQ devices.

The **VQE** is a hybrid quantum-classical routine used to estimate ground-state energies via the variational principle:

$$ E_g \leq E[\Psi(\theta)] = \frac{\langle \Psi(\theta) | \hat{H} | \Psi(\theta) \rangle}{\langle \Psi(\theta) | \Psi(\theta) \rangle} $$

where the ansatz $|\Psi(\theta)\rangle = \hat{U}(\theta)|\Psi_0\rangle$ is optimized to minimize energy.

⚙ 2. Variational Quantum Eigensolver Workflow

The VQE process involves four main steps:

1. **Hamiltonian Construction** – Encode the problem into a measurable Hamiltonian $\hat{H}$.
2. **Ansatz Preparation** – Build a parametrized quantum circuit $\hat{U}(\theta)$.
3. **Measurement Strategy** – Measure expectation values $\langle \hat{H} \rangle$.
4. **Optimization Loop** – Update θ via classical or quantum optimization.

The hybrid structure ensures: $$ \text{Quantum: State preparation & measurement} \quad \leftrightarrow \quad \text{Classical: Optimization} $$

🔬 3. Transverse Ising Model (TIM)

Hamiltonian for the 1D TIM ring:

$$ \hat{H}_{TIM} = -J \sum_{n=1}^{N} \sigma_z^{n-1}\sigma_z^{n} - h \sum_{n=0}^{N-1}\sigma_x^{n} $$

- Exhibits **Z_2 spin-flip symmetry** and **real-valued representation**.
- Two regimes:
  - $ h < 1 $: Ferromagnetic phase
  - $ h > 1 $: Paramagnetic phase
- Critical point at $ h = 1 $.

🧱 4. Ansatz Construction

✦ Symmetry-based design:

- Real coefficients $ C_n \in \mathbb{R} $
- Local spin interaction
- Global spin-flip symmetry $ (\sigma_x)^{\otimes N} $

✦ Selected ansatz types:

- **RealAmplitudes** — simple, real-valued rotations $ R_Y(\theta) $, linear entanglement.
- **EfficientSU2** — complex structure with $ R_X, R_Y, R_Z $ and full entanglement.

Number of variational parameters:

$$ p = N(L + 1), \quad L \geq \frac{2^{N-1} - 1}{N} - 1 $$

🧮 5. Optimization Methods

Type	Method	Description
Classical	COBYLA	Derivative-free, stable, low accuracy
	Finite Difference (FD)	Numerical gradient approximation
	SPSA	Stochastic gradient with only 2 evaluations
Quantum	PSR	Exact gradient using shifted parameters
	QN-BDA	Quantum natural gradient (block-diagonal approx.)
	QN-SPSA	Approximates Fubini–Study metric via SPSA
Hybrid (proposed)	**QN-SPSA+PSR**	Combines QN-SPSA metric + PSR gradient for stability & efficiency

Computational cost summary:

$$ \text{Gradient: } \begin{cases} \text{PSR: } 2p \\ \text{FD: } 2p \\ \text{SPSA: } 2 \end{cases} \quad \text{Metric: } \begin{cases} \text{QN-BDA: } L \\ \text{QN-SPSA: } 4 \end{cases} $$

📊 6. Simulation Results

- Tested on **12-spin TIM** using **RealAmplitudes** and **EfficientSU2** ansätze.
- **QN-SPSA+PSR** achieved:
  - **Faster convergence** than SPSA, FD, and COBYLA.
  - **Comparable accuracy** to **QN-BDA+PSR** but with **lower cost**.
- Linear entanglement performed nearly identical to full entanglement.

Estimated ground-state energy vs. field strength $ h $ and qubit number $ N $ matches the exact analytical solution.

🧾 7. Conclusion

- The **QN-SPSA+PSR** algorithm demonstrates a **quantum advantage** in optimization:
  - Fast convergence
  - Stable dynamics
  - Low computational overhead
- Well-suited for **NISQ** devices and extensible to **Quantum Machine Learning**.

🔑 Keywords

`Ising Model`, `VQE`, `Quantum Optimization`, `Ansatz Construction`, `Gradient Estimation`

```
flowchart TD
  %% ===== KHỞI TẠO =====
  subgraph INIT [Khởi tạo]
    A1[Chọn Hamiltonian H_TIM] --> A2[Chọn ansatz: RealAmplitudes hoặc
EfficientSU2]
    A2 --> A3[Khởi tạo tham số θ₀]
    A3 --> A4[Đặt siêu tham số: η₀, s₀, β, số vòng lặp tối đa]
  end

  %% ===== VQE MAIN LOOP =====
  subgraph LOOP [Vòng lặp VQE: k = 0..K]
    direction TB
    B1["Chuẩn bị trạng thái lượng tử |ψ(θₖ)⟩ = U(θₖ)|0⟩"]
    B1 --> QMEAS[Đo lường lượng tử: chia 2 nhánh PSR và QN-SPSA]

    %% --- PSR GRADIENT ---
    subgraph PSR [PSR: Tính gradient chính xác]
      direction TB
      P1[Cho mỗi tham số i]
      P1 --> P2[Đo năng lượng tại θₖ + Δᵢ]
      P2 --> P3[Đo năng lượng tại θₖ - Δᵢ]
      P3 --> P4["Tính gradient gᵢ = s * (f(θ+Δᵢ) - f(θ-Δᵢ))"]
    end

    %% --- QN-SPSA METRIC ---
    subgraph QN [QN-SPSA: Ước lượng metric Fubini–Study]
```

```
      direction TB
      S1["Tạo hai vector ngẫu nhiên Δ¹, Δ² ∈ {±1}ᵖ"]
      S1 --> S2[Đo 4 trạng thái để tính 2-SPSA metric]
      S2 --> S3[Tạo estimator H̄ₖ từ 4 phép đo]
      S3 --> S4["Làm mượt: H̃ₖ = (k/(k+1))·H̃ₖ₋₁ + (1/(k+1))·H̄ₖ"]
      S4 --> S5["Tạo metric nghịch đảo ổn định Mₖ = sqrt(H̃ₖ² + βI)"]
    end

    QMEAS --> PSR
    QMEAS --> QN

    %% --- CLASSICAL UPDATE ---
    subgraph CLASSICAL [Cập nhật tham số cổ điển]
      direction TB
      C1[Tính gradient gₖ từ PSR]
      C1 --> C2["Tính Mₖ⁺ (pseudo-inverse metric từ QN-SPSA)"]
      C2 --> C3[Cập nhật θₖ₊₁ = θₖ - ηₖ·Mₖ⁺·gₖ]
      C3 --> C4["Kiểm tra điều kiện dừng: |θₖ₊₁ - θₖ| < ε hoặc max_iter"]
    end

    PSR --> CLASSICAL
    QN --> CLASSICAL

    CLASSICAL -->|Nếu chưa hội tụ| B1
    CLASSICAL -->|Nếu hội tụ| END[Trả về θ*, năng lượng E*]
  end
```