Lesson 6.3: VQE (Variational Quantum Eigensolver)

Mathematical Intuition · Module 6 — Capstone

Node 6.3

Overview

Complete decoding of VQE—the variational quantum eigensolver for finding ground states and energies of quantum systems.

The Core Equations

Energy Expectation

$E(\theta) = \langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle$

Variational Principle

$E(\theta) \geq E_0$ (ground state energy)

Optimization Goal

$\theta* = \text{argmin}_\theta\ E(\theta)$

Symbol-by-Symbol Breakdown

Parameterized State: $|\psi(\theta)\rangle$

$|\psi(\theta)\rangle$ (trial state) - **Form**: $|\psi(\theta)\rangle = U(\theta)|0\rangle\hat{}\otimes n$ - **$U(\theta)$**: Parameterized quantum circuit (ansatz) - θ: Classical parameters $\theta = (\theta_1, \theta_2, \ldots, \theta_p)$ - **Purpose**: Explore Hilbert space to find ground state

Ansatz $U(\theta)$ - **Structure**: Product of parameterized gates - **Example**: $U(\theta) = \prod_k\ e\hat{}(-i\theta_k\ P_k)$ (Pauli rotations) - **Design**: Hardware-efficient or problem-inspired - **Trade-off**: Expressibility vs depth (noise)

Hamiltonian: $\hat{H}$

$\hat{H}$ (Hamiltonian operator) - **Meaning**: Energy operator of quantum system - **Hermitian**: $\hat{H}\dagger = \hat{H}$ (real eigenvalues) - **Eigenvalues**: $\{E_0, E_1, E_2, \ldots\}$ (energy levels) - **Ground state**: $|\psi_0\rangle$ with lowest eigenvalue E_0

Pauli Decomposition:

$\hat{H} = \Sigma_i\ h_i\ P_i$

- $\mathbf{P}_i$: Pauli strings (tensor products of I, X, Y, Z)
- $\mathbf{h}_i$: Real coefficients
- **Example**: $\hat{H} = 0.5 \cdot Z_0Z_1 + 0.3 \cdot X_0$ - $0.2 \cdot Y_1$

Energy Expectation: $\langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle$

$\langle\psi(\theta)|$ (bra) - **Definition**: Dual vector (conjugate transpose of $|\psi(\theta)\rangle$) - **Purpose**: Forms inner product

$\hat{\mathbf{H}}|\psi(\theta)\rangle$ (Hamiltonian acting on state) - **Operation**: Linear transformation - **Result**: Another quantum state - **Meaning**: "Energy operator applied to trial state"

$\langle\psi(\theta)|\hat{\mathbf{H}}|\psi(\theta)\rangle$ (expectation value) - **Definition**: $\langle\hat{H}\rangle = \Sigma_i\ h_i\langle P_i\rangle$ - **Meaning**: Average energy if we measured many times - **Real-valued**: Because $\hat{H}$ is Hermitian - **Units**: Energy (Joules, eV, Hartree, etc.)

Measurement of Expectation Value

For each Pauli string $\mathbf{P}_i$:

$\langle P_i\rangle = \langle\psi(\theta)|P_i|\psi(\theta)\rangle$

Measurement process: 1. Prepare state $|\psi(\theta)\rangle$ 2. Rotate to eigenbasis of P_i 3. Measure in computational basis 4. Outcome: ±1 (eigenvalues of Pauli operators) 5. Repeat N times, estimate: $\langle P_i\rangle \approx (n_+ - n_-)/N$

Total energy:

$E(\theta) = \Sigma_i\ h_i\langle P_i\rangle$

- Sum of weighted expectation values
- Each term measured separately (or grouped if commuting)

Variational Principle: $E(\theta) \geq E_0$

Statement: Any trial state gives upper bound on ground energy

Proof sketch: - Expand: $|\psi(\theta)\rangle = \Sigma_n\ c_n|n\rangle$ (eigenbasis of $\hat{H}$) - Energy: $E(\theta) = \Sigma_n\ |c_n|^2 E_n$ - Since $E_n \geq E_0$ and $\Sigma_n|c_n|^2 = 1$: - $E(\theta) = \Sigma_n|c_n|^2 E_n \geq \Sigma_n|c_n|^2 E_0 = E_0$

Consequence: Minimizing $E(\theta)$ approaches E_0

Equality: $E(\theta) = E_0$ iff $|\psi(\theta)\rangle = |\psi_0\rangle$ (ground state)

Optimization: $\theta* = \text{argmin}_\theta\ E(\theta)$

Goal: Find parameters that minimize energy

Gradient-based optimization:

$\theta_new = \theta_old - \alpha\cdot\nabla E(\theta_old)$

- α: Learning rate
- $\nabla\mathbf{E}$: Gradient (vector of partial derivatives)

Gradient computation (parameter-shift rule):

$\partial E/\partial\theta_i = [E(\theta + \pi/2\cdot e_i) - E(\theta - \pi/2\cdot e_i)]/2$

- $\mathbf{e}_i$: Unit vector in direction i
- **Exact**: For Pauli generators
- **Cost**: 2p circuit evaluations (p parameters)

Complete VQE Workflow

Step 1: Problem Setup

- **Define Hamiltonian**: $\hat{H}$ for system of interest
- **Example**: Molecular Hamiltonian for H_2, LiH, etc.
- **Decompose**: $\hat{H} = \Sigma_i h_i\ P_i$ (Pauli strings)

Step 2: Ansatz Design

- **Choose structure**: UCC, hardware-efficient, etc.
- **Determine depth**: Balance expressibility and noise
- **Initialize** θ: Random, classical guess, or heuristic

Step 3: Energy Evaluation

For given θ: 1. Prepare $|\psi(\theta)\rangle$ on quantum computer 2. Measure each $\langle P_i \rangle$ (with shots) 3. Compute $E(\theta) = \Sigma_i h_i \langle P_i \rangle$

Step 4: Gradient Computation

For each parameter θ_i: 1. Evaluate $E(\theta + \pi/2 \cdot e_i)$ 2. Evaluate $E(\theta - \pi/2 \cdot e_i)$ 3. Compute $\partial E/\partial\theta_i = [E(+) - E(-)]/2$

Step 5: Parameter Update

$\theta \leftarrow \theta - \alpha \cdot \nabla E(\theta)$

- Classical optimization step
- Various optimizers: GD, Adam, BFGS, etc.

Step 6: Convergence Check

- **Criterion**: $|E_{new} - E_{old}| < \varepsilon$
- **Or**: $||\nabla E|| < \varepsilon$ (gradient vanishes)
- **Or**: Maximum iterations reached

Step 7: Solution Extraction

- **Optimal parameters**: θ^*
- **Ground state**: $|\psi(\theta^*)\rangle$
- **Ground energy**: $E(\theta^*) \approx E_0$

Example: H_2 Molecule

Hamiltonian (STO-3G basis, 0.74 Å)

$$\hat{H} = -1.0523 \cdot I + 0.3979 \cdot Z_0 - 0.3979 \cdot Z_1 - 0.0112 \cdot Z_0Z_1 + 0.1809 \cdot X_0X_1 + 0.1809 \cdot Y_0Y_1$$

Terms: - **$-1.0523 \cdot I$**: Constant energy shift - **$0.3979 \cdot Z_0$, $-0.3979 \cdot Z_1$**: One-body terms - **$-0.0112 \cdot Z_0Z_1$**: Coulomb interaction - **$0.1809 \cdot X_0X_1$, $0.1809 \cdot Y_0Y_1$**: Exchange interaction

Ansatz (UCC Singles and Doubles)

$$U(\theta) = e^{-i\theta(X_0Y_1 - Y_0X_1)/2}$$

- **Single parameter**: θ (excitation amplitude)
- **Operator**: $X_0Y_1 - Y_0X_1$ (single excitation)
- **Initial state**: $|01\rangle$ (Hartree-Fock)

Circuit Implementation

1. **Prepare $|01\rangle$**: X gate on qubit 1
2. **Apply $U(\theta)$**:
   - $R_\gamma(\theta)$ on qubit 0
   - CNOT ($0 \to 1$)

- $R_\gamma(-\theta)$ on qubit 1
- CNOT ($0 \to 1$)

Energy Landscape

- **E(θ)**: Smooth function of θ
- **Minimum**: $\theta^* \approx 0.2$ radians
- **Ground energy**: E(θ^*) $\approx$ -1.137 Ha
- **Exact**: -1.137 Ha (chemical accuracy achieved!)

Optimization Trace

```
Iteration 0: θ = 0.0,    E = -1.116 Ha
Iteration 1: θ = 0.05,   E = -1.130 Ha
Iteration 2: θ = 0.10,   E = -1.135 Ha
...
Iteration 20: θ = 0.20,  E = -1.137 Ha (converged)
```

Advanced Topics

Excited States

- **Orthogonality constraint**: $\langle\psi(\theta)|\psi_0\rangle = 0$
- **Penalty method**: E(θ) + $\lambda|\langle\psi(\theta)|\psi_0\rangle|^2$
- **Subspace search**: Find multiple eigenstates

Adaptive VQE

- **Grow ansatz**: Add layers when needed
- **Prune parameters**: Remove unimportant ones
- **Balance**: Expressibility vs circuit depth

Quantum Natural Gradient

- **Metric**: Fisher information matrix F
- **Update**: $\theta \leftarrow \theta$ - $\alpha \cdot \mathrm{F}^{-1}\nabla\mathrm{E}$
- **Benefit**: Accounts for parameter space geometry
- **Faster convergence** than standard gradient descent

Error Mitigation

- **Zero-noise extrapolation**: Extrapolate to zero noise
- **Probabilistic error cancellation**: Invert noise channel
- **Symmetry verification**: Check physical constraints

Challenges and Solutions

Challenge 1: Barren Plateaus

- **Problem**: Gradients vanish exponentially
- **Solution**: Problem-inspired ansätze, local cost functions

Challenge 2: Local Minima

- **Problem**: Optimizer gets stuck
- **Solution**: Multiple initializations, simulated annealing

Challenge 3: Measurement Noise

- **Problem**: Finite shots → noisy gradients
- **Solution**: Adaptive shot allocation, more shots

Challenge 4: Hardware Noise

- **Problem**: Gate errors, decoherence
- **Solution**: Error mitigation, shorter circuits

Practice Problems

1. **Variational principle**: Prove $\mathrm{E}(\theta) \geq \mathrm{E}_0$ for any normalized $|\psi(\theta)\rangle$.
2. **Gradient formula**: Derive the parameter-shift rule for $\partial \mathrm{E}/\partial\theta$.
3. **H_2 energy**: Compute $\mathrm{E}(\theta{=}0)$ for the H_2 Hamiltonian above with $|\psi(0)\rangle = |01\rangle$.
4. **Measurement**: How many shots needed to estimate $\langle \mathrm{P}_i \rangle$ to precision ε?
5. **Ansatz expressibility**: Can a single-parameter ansatz reach all 2-qubit states?

Key Takeaways

- VQE finds ground states via variational principle
- Energy expectation $\mathrm{E}(\theta) = \langle\psi(\theta)|\hat{\mathrm{H}}|\psi(\theta)\rangle$ is cost function
- Variational principle: $\mathrm{E}(\theta) \geq \mathrm{E}_0$ (upper bound)
- Parameter-shift rule computes exact gradients
- Hybrid quantum-classical: quantum state prep, classical optimization
- Applications: quantum chemistry, materials science, condensed matter

Historical Note

VQE introduced by Peruzzo et al. (2014) - First demonstrated on photonic system - Calculated H_2 ground state energy - Pioneered variational quantum algorithms - Foundation for NISQ-era quantum computing

Next Steps

Next, we'll decode Maxwell's equations—the fundamental equations of classical electromagnetism.

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Concepts: variational-principle, expectation-value, parameterized-circuits, cost-function, gradient-descent, eigenvalue-decomposition

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