Lesson 4.2: Cost Functions

Mathematical Intuition · Module 4 — Optimization Regularization

Node 4.2

Overview

Understanding cost functions in VQE as energy expectation values and how to design and measure them on quantum hardware.

Learning Objectives

- See cost functions as expectation values of Hamiltonians
- Understand how to decompose Hamiltonians into measurable terms
- Recognize the variational principle and energy bounds
- Build intuition for cost function landscapes

Core Concepts

Energy Expectation Value

Definition

- $\mathbf{E(\theta) = \langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle}$: energy of state $|\psi(\theta)\rangle$
- $\mathbf{\hat{H}}$: Hamiltonian (energy operator)
- **Goal**: minimize $E(\theta)$ to find ground state
- **Variational principle**: $E(\theta) \geq E_0$ (ground state energy)

Why Energy?

- Ground state has minimum energy
- Energy is a Hermitian observable (real-valued)
- Variational principle guarantees bound
- Physical meaning: total energy of quantum system

Hamiltonian Structure

Pauli Decomposition

- $\mathbf{\hat{H} = \Sigma_i\ h_i P_i}$: sum of Pauli strings
- $\mathbf{P}_i$: tensor product of Pauli operators (I, X, Y, Z)
- $\mathbf{h}_i$: real coefficients
- **Example**: $\hat{H} = 0.5 \cdot Z_0Z_1 + 0.3 \cdot X_0 - 0.2 \cdot Y_1$

Measuring Pauli Strings

- $\mathbf{\langle P_i\rangle = \langle\psi|P_i|\psi\rangle}$: expectation of Pauli string
- Measure in eigenbasis of P_i
- Eigenvalues: ±1 for Pauli operators
- Estimate: average over many measurements

Total Energy

- $\mathbf{E(\theta) = \Sigma_i\ h_i \langle P_i \rangle}$: sum of weighted expectations
- Each term measured separately
- Total measurements: O(number of terms)

Variational Principle

Upper Bound

- $\mathbf{E(\theta)} \geq \mathbf{E}_0$ for all θ
- Any trial state gives upper bound on ground energy
- Minimizing $E(\theta)$ approaches E_0

Excited States

- Can target excited states with constraints
- Orthogonalize to lower states
- Penalty terms for overlap

Cost Function Design

Standard VQE

- $\mathbf{C(\theta) = \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle}$: just the energy
- Simple, direct
- May have many local minima

With Constraints

- $\mathbf{C(\theta) = E(\theta) + \lambda \cdot penalty(\theta)}$: energy + constraint
- Penalty enforces symmetries or other requirements
- Example: particle number conservation

Subspace VQE

- $\mathbf{C(\theta) = \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle}$ in subspace
- Reduces problem size
- Exploits symmetries

Measurement Strategies

Individual Pauli Measurements

- Measure each Pauli string separately
- Rotate basis: apply gates before measurement
- Estimate expectation from measurement outcomes

Grouping Commuting Terms

- $\mathbf{[P_i, P_j] = 0}$: can measure simultaneously
- Group commuting Pauli strings
- Reduces total measurements

Shadow Tomography

- Estimate many observables from few measurements
- Classical post-processing
- Efficient for large Hamiltonians

Examples in Context

Quantum Chemistry

- **Hamiltonian**: molecular electronic structure
- $\hat{\mathbf{H}} = \Sigma_{ij}\ \mathbf{h}_{ij}\hat{\mathbf{a}}_i\dagger\hat{\mathbf{a}}_j + \Sigma_{ijkl}\ \mathbf{h}_{ijkl}\hat{\mathbf{a}}_i\dagger\hat{\mathbf{a}}_j\dagger\hat{\mathbf{a}}_k\hat{\mathbf{a}}_l$
- Map to qubits: Jordan-Wigner, Bravyi-Kitaev
- Measure energy in Pauli basis

Combinatorial Optimization

- **Hamiltonian**: encodes optimization problem
- $\hat{\mathbf{H}} = \Sigma_{ij}\ \mathbf{J}_{ij}\sigma_i\sigma_j + \Sigma_i\ \mathbf{h}_i\sigma_i$ (Ising model)
- Ground state = optimal solution
- Measure cost function value

Quantum Simulation

- **Hamiltonian**: physical system to simulate
- **Ĥ = Ĥ_kinetic + Ĥ_potential + Ĥ_interaction**
- Find ground state or dynamics
- Measure observables of interest

Cost Function Landscape

Local Minima

- Cost function may have many local minima
- Optimization can get stuck
- Strategies: multiple initializations, simulated annealing

Barren Plateaus

- Gradients vanish in large regions
- Exponentially hard to escape
- Related to ansatz design (see Lesson 4.1)

Noise Effects

- Measurement noise adds variance
- Coherent errors bias energy estimates
- Regularization can help (see Lesson 4.4)

Practical Considerations

Shot Budget

- **N_shots**: number of measurements per Pauli string
- More shots → better estimate, but more time
- Trade-off: accuracy vs runtime

Error Mitigation

- Zero-noise extrapolation
- Probabilistic error cancellation
- Symmetry verification

Adaptive Measurements

- Allocate shots based on term importance
- More shots for large coefficients h_i
- Reduces total measurement cost

Practice Problems

1. If $\hat{H} = 2 \cdot Z_0Z_1 + 3 \cdot X_0X_1$, how many measurement bases do you need?
2. Why does the variational principle guarantee $E(\theta) \geq E_0$?
3. How does measurement noise affect the cost function estimate?

Key Takeaways

- Cost function is energy expectation value $E(\theta) = \langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle$
- Hamiltonians decompose into measurable Pauli strings
- Variational principle: any trial state gives upper bound on ground energy
- Measurement strategies: individual, grouped, or shadow tomography
- Cost landscape has local minima and barren plateaus

Next Steps

Next, we'll explore gradients—how to compute derivatives of the cost function using parameter-shift rules.

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Concepts: cost-function, expectation-value, variational-principle, eigenvalue-decomposition

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