Regularization and Generalization Bounds

Variational Quantum Algorithms · Module 5 — Regularization

Node 5.4

Position in Knowledge Graph

System: Variational Quantum Algorithms **Structural Domain:** Regularization **Node:** 5.4

The fourth standard regularization technique. Asks: *given* the optimizer succeeds in reducing the training cost, what does the regularizer guarantee about the cost on **unseen** problem instances?

For VQE specifically, "unseen instances" means: different shots, different noise realizations, or different molecular geometries.

Formal Definition

Let $\mathcal{D}$ be a distribution over problem instances and let $\hat{C}(\boldsymbol{\theta})$ be the empirical cost on a finite training set. A **generalization bound** is an inequality of the form

$$\mathbb{E}_{x\sim\mathcal{D}}[C(\boldsymbol{\theta};x)] \leq \hat{C}(\boldsymbol{\theta}) + \mathcal{B}(\mathcal{H}, n, \delta)$$

with probability at least $1-\delta$ over training set draws, where $\mathcal{B}$ is a complexity term that depends on the hypothesis class $\mathcal{H}$ (the ansatz family) and the training-set size n.

A **regularizer reduces** $\mathcal{B}$ by restricting the effective complexity of $\mathcal{H}$.

Intuition

Generalization is the answer to: "My circuit got the right answer on the data I trained it on. Will it get the right answer on new data?"

Without regularization, an overparameterized ansatz can perfectly fit any training set — including the noise — and fail catastrophically on new instances. A regularizer says: "Don't fit the noise. Restrict yourself to a smaller class of functions, where overfitting is impossible."

The bound $\mathcal{B}$ is the price you pay in worst-case error for the freedom to choose any $\boldsymbol{\theta}$ in the unrestricted class. Regularization shrinks the class, which shrinks the price.

Structural Role

This is the most theoretical of the four standard regularization nodes. It is the lens that lets you state, with formal probability guarantees, *why* L2 / spectral / geometric regularization should work.

But it is also the lens that **fails most cleanly in the VQA setting**, which is why it sets up the polemic in node 5.5. The standard generalization story assumes (a) you have a well-defined data distribution, (b) you reach a fixed steady-state solution, (c) your optimizer is essentially noise-free. None of these hold for VQA. See 5.5 for the full critique.

Relations to Other Concepts

- **Rademacher complexity** — the complexity term $\mathcal{B}$ for many concrete hypothesis classes.
- **PAC-Bayes** — generalization bounds that incorporate a Bayesian prior over $\boldsymbol{\theta}$, making the connection to node 5.1 explicit.
- **Stability-based bounds** — generalization through algorithmic stability rather than hypothesis-class size.
- **VC dimension** — the combinatorial measure of capacity for binary classifiers.

Worked Derivations

A schematic Rademacher bound

For a hypothesis class $\mathcal{H}$ with Rademacher complexity $\mathfrak{R}_n(\mathcal{H})$ on samples of size n, the standard bound gives

$$\mathbb{E}[C] \leq \hat{C} + 2\,\mathfrak{R}_n(\mathcal{H}) + 3\sqrt{\frac{\log(2/\delta)}{2n}}$$

with probability $1-\delta$.

Spectral regularization (node 5.3) bounds $\|U(\boldsymbol{\theta})\|_{\mathrm{Lip}}$, which in turn bounds $\mathfrak{R}_n(\mathcal{H})$, tightening the inequality.

What goes wrong for VQA

The bound assumes $\hat{C}$ is the *minimum* of the empirical objective. In VQA, $\hat{C}$ is whatever the optimizer happened to converge to — typically a stochastic transient, not a minimum. The bound still holds in principle, but it ceases to be informative because the optimizer's actual behavior is governed by *dynamics*, not by the geometry of the loss surface. This is the gap that node 5.5 fills.

Visualization

Pending. Diagram: the bound as an envelope around the empirical-cost curve, shrinking as a regularizer is applied.

Exercises

1. Compute the Rademacher complexity of a linear classifier with bounded L2 weight norm.
2. Sketch why a depth-L hardware-efficient ansatz has Rademacher complexity at least exponential in L without regularization.
3. (Conceptual) Argue why "training cost" and "test cost" are not the right concepts in VQE — and what should replace them.

Research Extensions

- **Quantum PAC-Bayes** — recent work extending PAC-Bayes bounds to variational quantum models.
- **Implicit-bias generalization** — explaining generalization without explicit regularization, by analyzing the bias of the optimizer itself. This is a direct neighbor of node 5.5.
- **Distribution-free bounds** — generalization that does not depend on a fixed training distribution.

Cross-links to Other Courses

- **Statistics Module 10** — Model Selection (cross-validation, AIC/BIC, structural risk minimization).
- **Statistics Module 7** — Asymptotic Theory (uniform convergence, empirical processes).

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Concepts: regularization, bias-variance-tradeoff, concentration-of-measure
Prerequisites: 5.1, 5.3
Enables: 5.5

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