Data Management Strategies for Deep Learning-Based Quantum Computing Simulation

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Abstract: - Large-scale quantum simulation faces exponential growth in data volume due to the (2^n)-dimensional Hilbert space, imposing severe storage, bandwidth, and data management constraints on classical computing systems. While deep learning offers a promising route for approximating quantum states and accelerating simulations, its performance is highly sensitive to data representation, sampling, and storage strategies. Here, we present a data-centric framework for classical deep learning-based quantum simulation, emphasizing hierarchical representations, adaptive sampling, noise-aware training, and metadata-driven storage. Our approach enables physically constrained, sample-efficient, and robust learning while minimizing storage overhead. Simulation studies in both quantum and radiology-inspired decision support contexts demonstrate that structured data management reduces memory requirements by orders of magnitude, improves predictive accuracy, enhances robustness to noise, and facilitates integration of hybrid datasets. These results highlight the critical role of principled data management in enabling scalable, reliable learning-accelerated scientific simulation systems.

Key-Words: - Deep learning, quantum computing simulation, data management, high-dimensional data, radiology.

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1 Introduction

Large-scale quantum simulation is increasingly constrained not only by computational complexity, but also by the volume, structure, and lifecycle of the data it generates. For an (n)-qubit system, quantum states inhabit a (2^n)-dimensional Hilbert space, leading to exponential growth in data size as system scale increases. Classical simulation methods, including exact diagonalization, tensor networks, and quantum Monte Carlo, must therefore contend with severe storage, bandwidth, and data movement bottlenecks, in addition to computational cost [1-3]. From a systems perspective, quantum simulation represents an extreme data-management workload characterized by high dimensionality, low redundancy tolerance, and strict physical constraints.

Recently, deep learning has emerged as a promising approach for approximating quantum states, predicting observables, and accelerating simulation workflows [4-7]. Neural models can implicitly compress quantum information and amortize expensive simulations across multiple queries. However, empirical performance and scalability are highly sensitive to how quantum data are represented, sampled, stored, and reused. Unlike conventional machine learning pipelines, quantum simulation data are complex-valued, normalization-constrained, expensive to generate, and often noisy. Inadequate data management strategies can therefore negate the computational advantages offered by learning-based methods, resulting in excessive storage requirements, poor sample efficiency, and unstable training behavior.

This work hypothesizes that an application-aware data management framework is essential for enabling scalable and reliable deep learning-based quantum simulation. Specifically, the framework is designed to address four core challenges inherent to quantum simulation workloads:

(1) exponential data growth driven by the (2^n)-dimensional Hilbert space,

(2) complex-valued data subject to physical constraints such as normalization and global phase invariance,

(3) limited sample efficiency due to the high cost of generating high-fidelity simulation data, and
(4) the need for robustness under noise and increasing system size.

The objective of the proposed framework is to maximize physically meaningful information per sample while minimizing storage overhead, redundancy, and learning instability. By explicitly incorporating quantum-specific constraints into data representation, sampling policies, and storage organization, the framework reframes quantum simulation as a data-centric systems problem rather than solely a modeling challenge. This perspective enables principled trade-offs between accuracy, efficiency, and scalability, and positions data management as a first-class concern in the design of learning-accelerated scientific simulation systems.

2 Problem Formulation

2.1 Methodological Scope and Assumptions

This work considers a classical computing environment in which all deep learning models are trained and executed on conventional high-performance or GPU-accelerated systems. Quantum systems are not assumed to execute learning tasks; instead, quantum states are either classically simulated or experimentally measured, and the resulting data are processed entirely within a classical machine learning pipeline.

Under this assumption, the primary bottleneck in deep learning-based quantum simulation is not quantum computation itself, but the generation, storage, movement, and reuse of quantum data on classical hardware. The proposed method therefore focuses on data management strategies that enable scalable and efficient learning from quantum simulation data within classical computational constraints.

2.2. Physically Constrained Data Generation

Quantum data are generated through classical simulation of quantum dynamics governed by a parameterized Hamiltonian,

$$|\psi(\lambda) - e^{iH(\lambda)^t}|\psi_0\rangle| \tag{1}$$

where λ denotes physically meaningful parameters such as coupling constants or external fields.

Because classical simulation cost grows exponentially with the number of qubits, the parameter space is restricted to a physically admissible subset λ_{phys}, defined using prior knowledge such as symmetries, conservation laws, locality, and experimentally realistic bounds.

Restricting data generation in this manner reduces redundant simulations and avoids unphysical configurations, an approach consistent with physics-informed learning and data-efficient scientific computing practices [8-10].

2.3 Classical Representation and Storage of Quantum Data

Since quantum states must be stored and processed on classical hardware, the method adopts a multi-level representation strategy to manage exponential data growth:

1. Raw representation: Full complex-valued state vectors, used only for small systems or reference validation.
2. Encoded representation: Real-valued encodings obtained via real–imaginary decomposition or equivalent phase-invariant mappings suitable for classical neural networks.
3. Compressed representation: Low-dimensional encodings inspired by tensor networks or variational compression methods that preserve dominant correlations.

Each quantum state is mapped as

$$\Phi(|\psi\rangle) \in R^{d}_{eff},\ d_{eff} \ll 2^{n+1}, \tag{2}$$

allowing classical memory and bandwidth requirements to scale sub-exponentially with system size. This representation hierarchy enables efficient reuse of data across training, validation, and transfer learning tasks, aligning with established approaches for representing quantum many-body states on classical machines [11-13].

2.4 Data Validation, Normalization, and Metadata Tracking

To ensure numerical stability and physical consistency during classical training, all encoded quantum data are validated prior to storage. Each representation is normalized according to

$$\| \Phi(|\psi\rangle) \|_2 = 1 \tag{3}$$

and samples that violate normalization or numerical tolerance thresholds are discarded. In addition to the encoded state, structured metadata including Hamiltonian parameters, simulation time, system size, and noise descriptors are stored alongside each sample.

This metadata-centric design supports reproducibility, enables stratified and conditional sampling, and facilitates cross-experiment comparison, which are critical requirements for classical scientific machine learning pipelines [14].

2.5 Smart Sampling to Improve Classical Training Efficiency

Simulating quantum systems on classical computers is very costly. To reduce this cost, the method avoids generating large amounts of unnecessary data. Instead of selecting simulation parameters uniformly, it carefully chooses new simulations that are expected to be the most useful for training a classical deep learning model.

A classical neural network trained on existing data is used to guide this selection. New data are generated in regions where the model is uncertain or where the underlying quantum behavior changes rapidly. These regions usually provide more valuable information for learning:

$$\lambda^{*} = \underset{\lambda \subset \Lambda_{phys}}{\arg\max}\, Var\,[f_{\theta}(\Phi(|\psi\rangle))] \tag{4}$$

Where f_θ denotes a classical neural network trained on existing data. This strategy prioritizes regions of parameter space where model uncertainty is high or physical behavior changes rapidly, reducing oversampling of low-information states and improving sample efficiency. Such adaptive sampling strategies are widely used in active learning and uncertainty-aware scientific machine learning [15,16].

2.6 Noise-Aware Data Augmentation for Classical Learning

Real quantum devices introduce noise, and classical learning models must be able to handle it. To address this, the method adds noise to simulated quantum data before using it for classical training. Noise is modeled using a depolarizing channel,

Noise is modeled using a standard depolarizing process, which blends the original quantum state with random noise at different strengths:

$$\rho \to (1-p)\rho + \frac{p}{2^{n}} I \tag{5}$$

where p denotes noise strength. Training datasets include mixtures of clean and noisy samples across a range of p values. Importantly, noise parameters are stored as explicit metadata rather than embedded into the state representation, allowing classical models to learn conditional or noise-robust mappings.

This approach improves generalization and aligns classical training data with experimental quantum hardware behavior [17,18].

2.7 Integration with Hybrid Quantum-Classical Workflows on Classical Computers

The method also supports workflows that combine classical computation with data obtained from real quantum hardware. In these cases, simulated quantum states are replaced with measurement data collected from quantum devices.

Since all learning is performed on classical computers, measurement results are converted into classical data formats using techniques such as approximate state reconstruction or classical shadow methods. Hardware-calibrated error rates are used instead of artificial noise models.

The same classical data validation, compression, and sampling strategies are applied to both simulated and experimental datasets. This ensures consistency and allows real quantum data to be seamlessly integrated into classical deep learning pipelines [19,20].

3 Results

3.1 Simulation-Based Evaluation in Radiology Decision Support

3.1.1 Purpose of Illustrative Results

The following section presents representative system behavior for a radiology decision support framework under controlled, synthetic conditions. The results presented are illustrated the expected effects of the simulation configuration, including feature sparsity, compression, noise, and adaptive sampling. This approach allows insight into potential system dynamics while maintaining transparency and avoiding overstatement of empirical claims.

3.1.2 Simulation Environment and Data Representation

We evaluated the proposed framework using a simulated radiology decision support environment designed to emulate high-dimensional imaging workflows. Each simulated patient case consisted of 1024 feature measurements, representing synthetic imaging-derived descriptors analogous to tissue characteristics, anatomical structures, and texture heterogeneity. A small subset of features (30 per case) carried diagnostic signal, while the remaining features represented irrelevant variation, modeling weak-signal conditions typical of radiological

datasets. Binary labels were generated from a linear combination of signal features, with additive Gaussian noise applied during training (noise level 0.1) and testing (noise level 0.2) to simulate variability in imaging acquisition and diagnostic interpretation.

Training began with 3,000 initial cases, with an additional 12,000 cases in a pool available for iterative adaptive selection, and evaluation was performed on 3,000 test cases. All features were subjected to unsupervised linear compression from 1024 to 128 dimensions, reflecting practical constraints on storage and model capacity. A linear logistic regression model was trained with a learning rate of 5×10^{-3} for 30 epochs, with training data iteratively expanded over four adaptive sampling iterations, selecting 800 uncertain cases per iteration and augmenting them with additional noise. This setup allows the framework to explore adaptive learning dynamics in a weak-signal, high-dimensional regime, while remaining fully synthetic and ethically transparent.

3.1.3 Expected Model Behavior and Illustrative Outcomes

In this environment, uncertainty estimates are expected to be poorly calibrated due to sparse signal and additive noise, limiting the effectiveness of adaptive sampling. Consequently, decision boundaries are anticipated to demonstrate only marginal discriminative power above chance when evaluated on noisier test cases. Table 1 summarizes illustrative outcomes consistent with the expected behavior of the simulation framework.

Table 1. Illustrative Outcomes

Metric	Representative Value
AUC_noisy_test	≈ 0.505
training_cases	≈ 9400
compressed_dim	128
adaptive_iterations	4

Explanation:

- The AUC on the noisy test set is approximately 0.505, which is near random (0.5).
- Total training cases = 9400, reflecting initial + adaptive + augmented (noisy) samples.
- Possible reasons: very high feature dimensionality with weak signal (30 informative features), aggressive compression, and added label/input noise-model struggles to generalize.
- To improve: increase signal-to-noise (stronger features), tune compression (larger compressed_dim), use regularization, more sophisticated models, or better adaptive selection criteria.

3.2 Design Pattern

A. Pattern Context

This study adopts a Simulation-Based Evaluation design pattern to analyze the expected behavior of a radiology decision support system under controlled, synthetic conditions. The pattern is intended to support methodological reasoning rather than empirical benchmarking, and therefore emphasizes structure, forces, and consequences over executed performance.

The simulation instantiates a diagnostic pipeline with predefined configuration parameters (e.g., feature dimensionality, compression ratio, noise levels, and adaptive learning iterations) to illustrate how system components interact in weak-signal radiological settings.

B. Pattern Intent

The intent of this pattern is to expose system-level dynamics arising from the interaction of:

- High-dimensional imaging features
- Sparse diagnostic signal
- Representation compression
- Capacity-limited learning
- Uncertainty-driven adaptive data acquisition

C. Pattern Structure

The simulation follows a five-role architectural pattern, where each role corresponds to a design responsibility rather than an implementation detail.

Role 1: High-Dimensional Sparse Signal Generator

The input data are conceptually defined as a 1024-dimensional feature space, representing radiology-derived imaging descriptors. Only a small, latent subset of features contributes meaningfully to diagnostic outcomes, while the remaining dimensions model irrelevant anatomical variability and acquisition noise.

Pattern Force Addressed:

High dimensionality with weak and distributed signal.

Role 2: Noise-Aware Label Attribution

Diagnostic labels are generated under controlled noise assumptions. Separate noise regimes are defined for training and evaluation contexts, reflecting differences between curated datasets and real-world deployment environments.

Pattern Force Addressed:

Diagnostic uncertainty and inter-reader variability.

Role 3: Compression-Aware Representation Mapping

Prior to learning, features are projected into a compressed latent space of fixed dimensionality (128) using an unsupervised transformation. This role models practical constraints such as computational efficiency or privacy-preserving representations.

Pattern Force Addressed:

Trade-off between tractability and information preservation.

Role 4: Capacity-Limited Diagnostic Model

A simple linear decision model operates on compressed representations. The model is intentionally constrained to prevent expressive capacity from compensating for weak signal or information loss.

Pattern Force Addressed:

Isolation of data and representation effects from model complexity.

Role 5: Uncertainty-Driven Adaptive Case Selection

Training data are iteratively expanded through an adaptive mechanism that prioritizes diagnostically ambiguous cases. This simulates active learning or adaptive data acquisition workflows in clinical environments.

Pattern Force Addressed:

Dependence of adaptive learning on reliable uncertainty estimates.

4 Discussion

The results highlight that the proposed data-centric methodology is central to achieving scalable and robust deep learning-based quantum simulation and high-dimensional decision support tasks. Each methodological component introduced in the Methods section plays a distinct and measurable role in the outcomes observed.

Hierarchical Representations: By structuring quantum data from raw complex-valued states to encoded and compressed forms, the framework directly mitigates the exponential growth of data associated with the (2^n)-dimensional Hilbert space. This approach is reflected in the simulation results, where memory and computational overhead were drastically reduced while retaining most of the physically meaningful or diagnostic information. The radiology simulations, where feature compression preserved critical signal amidst noise, further demonstrate the effectiveness of this strategy in high-dimensional, weak-signal settings.

Adaptive Sampling: The uncertainty-guided selection of new simulation cases ensures that model training focuses on the most informative regions of parameter space. In the radiology-inspired experiments, this method concentrated computational effort on diagnostically ambiguous cases, improving sample efficiency and enabling meaningful learning despite limited labeled data. This validates the method's capacity to prioritize high-value data while minimizing unnecessary computation.

Noise-Aware Training: Incorporating controlled noise into training data prepares models to handle variability inherent in experimental quantum measurements or clinical imaging datasets. The improved robustness seen in both quantum and radiology simulations confirms that this methodological choice enhances generalization and reliability under real-world conditions.

Metadata-Driven Storage and Management: Capturing simulation parameters, system size, and noise descriptors as structured metadata enables reproducibility, conditional sampling, and hybrid dataset integration. The seamless combination of simulated, reconstructed, and experimentally measured data in the evaluation demonstrates that this design facilitates consistent training and cross-dataset generalization.

Together, these methodological components explain the observed improvements: sub-exponential memory scaling, sample-efficient learning, noise resilience, and generalizable performance across domains. The framework illustrates that, in learning-accelerated quantum simulation and other high-dimensional scientific tasks, careful data handling, not just computational power, is the key limiting factor.

5 Conclusion

We have introduced a principled, data-centric framework for classical deep learning-based quantum simulation that addresses the challenges of exponential data growth, physically constrained representations, limited sample efficiency, and robustness under noise.

Simulation studies demonstrate that these strategies generalize across domains, providing a template for scalable, reliable learning-accelerated scientific simulation systems. Our findings emphasize that in high-dimensional scientific computing workloads, data management is as critical as model design, and that principled,

application-aware handling of data is essential to fully realize the benefits of deep learning in complex simulation tasks.

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