State-Averaged Subspace-Aligned Variational Quantum PCA

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Background and Motivation

- Principal component analysis (PCA) is a fundamental method for dimensionality reduction and feature extraction
- Quantum PCA promises compact representations in high-dimensional or implicit feature spaces, potentially beyond classical limits.
- Canonical density-matrix exponentiation method for QPCA is impractical on near-term devices.
- Usual Near-Term Variational QPCA methods are unstable for computing multiple PCs:
  - Deflation: Subtracting found principal components accumulates noise.
  - Penalty Terms: $Cost+\lambda|\langle\psi_0|\psi_1\rangle|^2$ often creates local minima.
  - Barren Plateaus: Deep ansatzes fail to train.

Idea

We propose state-averaged, variational subspace-learning framework that learns all principal components simultaneously.

Our approach, inspired by the SA-OO method in chemistry, is based on three principles:

- **Shared variational circuit**: A single parametrized unitary that generates all components from orthogonal reference states
- **State-averaged objective:** All components are optimized together, enforcing orthogonality by construction
- **Representation alignmen**t: A classical or shallow quantum rotation aligns the basis with the learned subspace, reducing circuit depth and improving stability

Method

We adopted a two loop architecture to decouple the problem and reduce the constraints on the anzat :

- Loop 1 (Alignment): Rotates the basis to match the data
- Loop 2 (Correlation): Learns the principal subspace within that basis

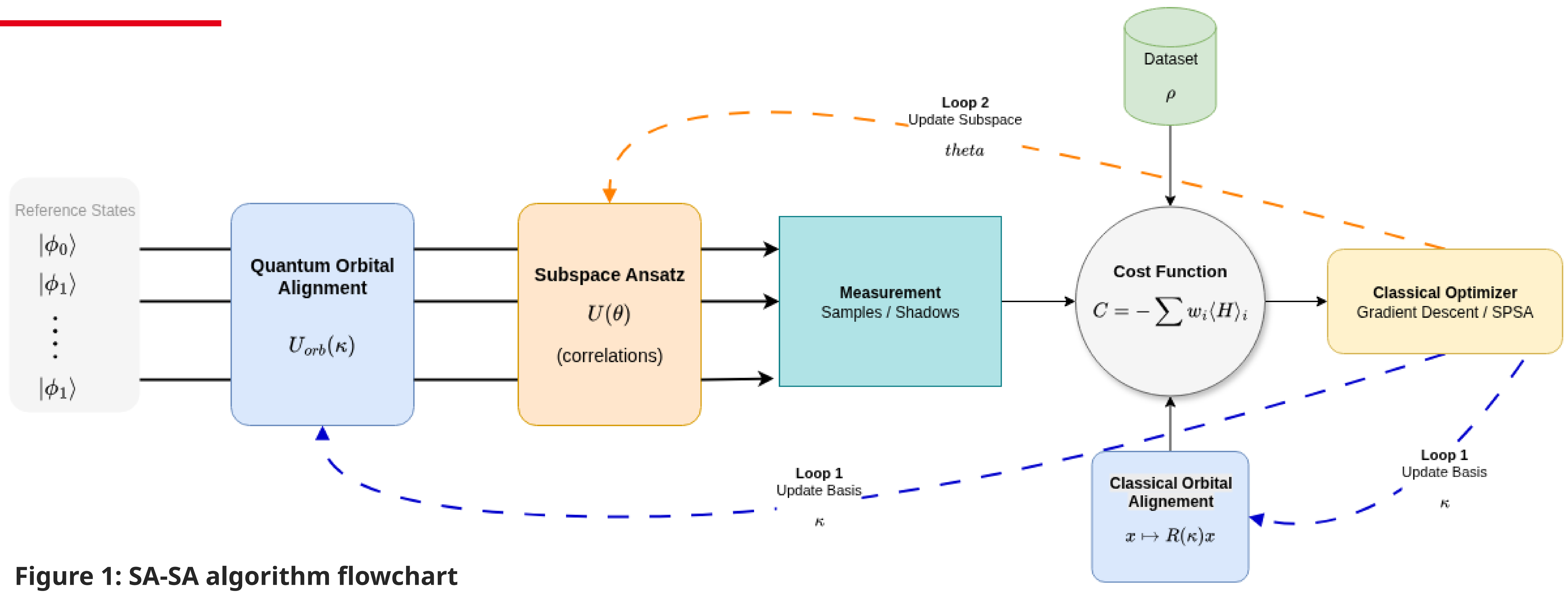

Figure 1: SA-SA algorithm flowchart

Variational Subspace Learning

- We encode the dataset into a covariance operator: $\rho=\frac{1}{N}\sum_i \langle x_i|x_i\rangle$
- We select k orthonormal reference states $|\phi_i\rangle$ and apply a shared variational circuit $U(\theta)$:

  $|\psi_i\rangle=U(\theta)|\phi_i\rangle$
- All components are learned simultaneously by minimizing a state-averaged objective:

$$L(\theta)=-\sum_{i=0}^{k-1} w_i\langle\psi_i|\rho|\psi_i\rangle, w_0>...>w_{k-1}$$

Subspace alignment

To reduce circuit depth and improve optimization, we adapt the basis representation using either:

- Classical alignment: a rotation R∈SO(D) is applied to the input features
- Quantum alignment: a shallow, data-independent unitary U_{orb}

These alignment layers are shared across all components and updated using gradients from the quantum objective

Alignment simplifies the learning task and improves stability and convergence.

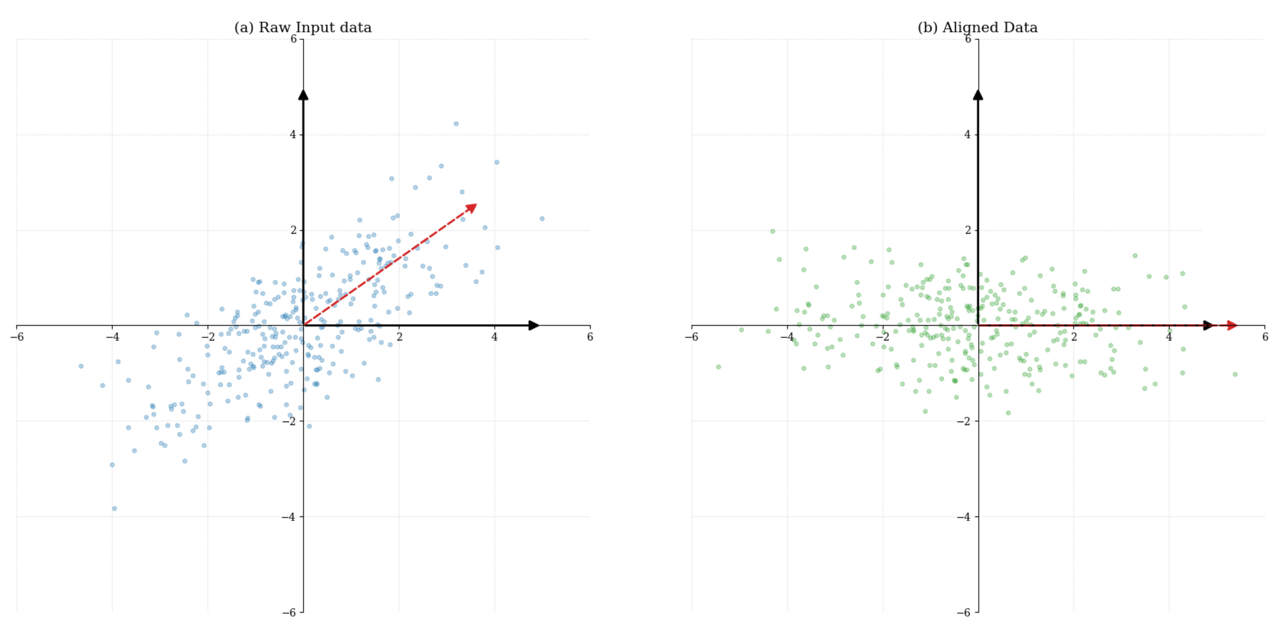

Figure 2: Illustration of the subspace alignment

Preliminary results

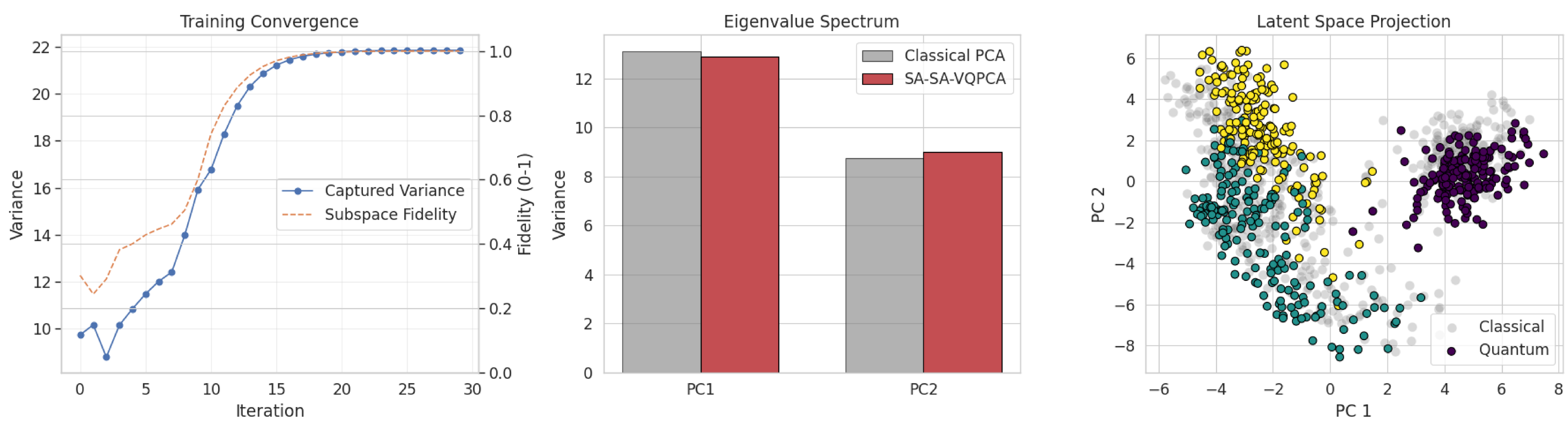

Figure 3: Cost convergence, eigenvalue matching and projection of the test data for the wine dataset

Experiments on Iris, Wine, and MNIST-Digit subsets (4–64 features) using a two-layer hardware-efficient ansatz:

- stable convergence across all datasets,
- automatic orthogonality without deflation,
- improved learning speed when including classical or quantum orbital optimization,
- kernel variant capturing nonlinear structure unavailable to linear PCA

A classifier built on the kernel variant achieves 73% accuracy on PneumoniaMNIST using four qubits,

Extensions and applications

- Kernel PCA via quantum feature maps
- Sparse or structured PCA through constrained generators
- Quantum autoencoders via subspace-based compression
- General variational eigensubspace learning
- Representation learning for quantum machine learning
- Dimensionality reduction in implicit or kernel feature spaces
- Noise-robust subspace extraction on NISQ devices
- Preprocessing for downstream tasks (classification, clustering, or anomaly detection)

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