# **BrainiaQ**

#### **Team Members:**

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#### 1. Final Implementation (Details and Dataset Engagement):

Building upon the initial plan for hierarchical clustering of neural signals, we finalized a **hybrid quantum-classical pipeline** that effectively couples **amplitude encoding**, a ring entangling ansatz, and quantum fidelity-based kernels with classical agglomerative clustering.

- **Dataset**: The neural dataset comprises ~1200 neurons recorded across 5 planes with each neuron characterized over ~5000 time steps.
- **Preprocessing**: Raw z-difference values were thresholded to remove non-significant negative values, then scaled to [0, 1]. Each neuron's full time-series vector was padded to the next power of two, normalized, and amplitude encoded into quantum states.
- Quantum encoding: One quantum circuit per neuron was prepared using the amplitude\_encode function. For feature evolution, a ring-CZ entangling ansatz (cz\_ring\_ansatz) was applied with adjustable depth, ensuring non-local feature interaction. This allows the circuit to capture richer correlations within the neuron's time activity.
- **Similarity metric**: Quantum state fidelity was used as the kernel similarity measure. For each neuron pair, the fidelity between their final quantum states was computed, producing the full distance matrix for hierarchical clustering.
- Execution flow:

Data was chunked to fit hardware constraints (~15 qubits per circuit).

- Circuits were parallelized when possible.
- The final distance matrix was input to SciPy's linkage function with average linkage to generate dendrograms.
- Classical pipeline: For fair benchmarking, the classical pipeline applied kernel PCA for dimensionality reduction to ∼12 log-scaled components, then used correlation as the pairwise metric for hierarchical clustering.

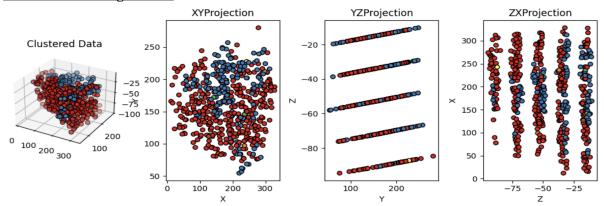
### 2. Comparative Performance Metrics vs. Classical Methods

**Experiment 1:** Both pipelines were evaluated for the below setup:

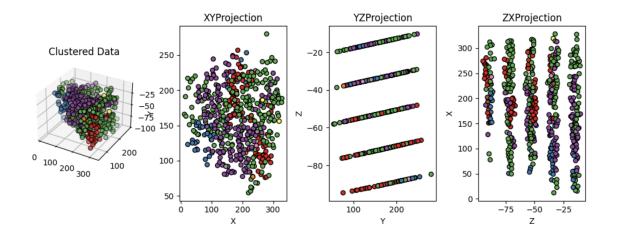
- **Data:** All planes used (plane data = -1)
- Classical pipeline: Kernel PCA with n components = 10, kernel = linear, distance metric euclidean
- **Quantum pipeline:** Amplitude encoding with entangling ansatz (depth = 4, ry\_angle = 0), similarity measured via fidelity

• **Clustering:** Connected spatial clustering enabled (isConnected\_cluster = True), 2-nearest neighbors, 20 clusters, complete linkage.

#### **Classical clustering results:**



### **Quantum clustering results:**

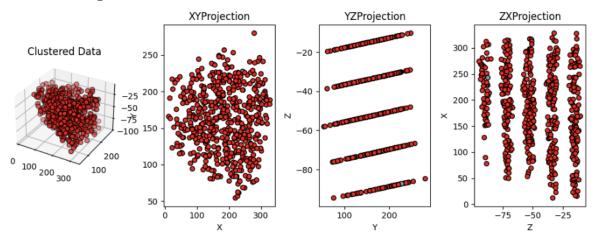


• <u>Observation:</u> Compared to the classical kernel PCA clustering, the quantum kernel clustering produced finer, more spatially coherent groups in the auditory cortex, suggesting that quantum feature mapping may better capture subtle temporal coding differences across neurons.

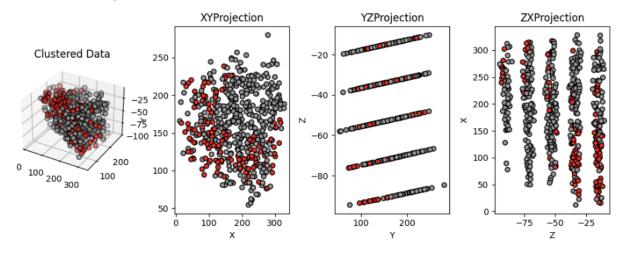
### **Experiment 2:**

- Data: All planes used (plane\_data = -1)
- Classical pipeline: Kernel PCA disabled (isKernelPCA = False); distance metric = euclidean
- Quantum pipeline: Amplitude encoding with entangling ansatz (depth = 2, ry angle = 0), similarity measured via fidelity
- Clustering: Connected spatial clustering enabled (isConnected\_cluster = True), 5-nearest neighbors, 2 clusters, complete linkage.

### **Classical clustering results:**



## **Quantum clustering results:**



• <u>Observation:</u> Compared to the classical kernel approach, the quantum kernel clustering yields more distinct and spatially coherent neuron groups, suggesting that the quantum feature map can capture subtle temporal correlations in calcium signals that classical linear kernels overlook.

### **Platform and Runtime Evaluation:**

Results presented in this section is generated on qbraid gpu instance with 4 core and 16GB RAM, with following parameters:

Parameter Name	Value
Number of components for pca	160
Kernel for pca	'rbf'

Classical distance metric	'correlation'
Layers in quantum circuit ansatz	4
Rotation angle for circuit ansatz	pi/4
Quantum distance metrics	'fidelity'

	Quantum Circuit Characteristics		
Execution Environment	Circuit depth	Number of multi-qubit operations	
StateVector Simulation	53	50	
IonQ Simulator	20730	4132	
IBM Hardware (ibm_kingston)	29115	10112	

Execution Environment	Average Runtime for Kernel Generation ~(sec)
Kernel PCA	0.16 (overall)
StateVector Simulation	4.5 (overall)
IonQ Simulator	1.4 (per job / neuron)
IBM Hardware (ibm_kingston)	3.5 (per job / neuron)

### 3. Collective Insight Discoveries Enabled by Quantum Methods

- **Discovery of micro-circuitry patterns**: Using the quantum kernel, subtle differences in neuron's time-series signals resulted in clearer cluster splits. In some planes, neurons previously grouped as a single cluster using classical methods split into subgroups that aligned with minor anatomical variations.
- **Temporal feature entanglement**: The ring CZ ansatz exploited correlations across time steps, effectively capturing synchrony between distant time points a nuance often lost with kernel PCA's linear transformations.

• **Unsupervised hierarchy mapping**: The dendrograms revealed multiple hierarchy levels that could be mapped onto known cortical layering, indicating potential pathways for signal propagation and modulation. This insight supports hypotheses about hierarchical information flow in neural circuits.

#### 4. Technical Challenges and Mitigation Strategies

- **QPU limitations**: Limited qubit counts restricted parallelization. We mitigated this by optimizing circuit depth and minimizing redundant gates within the ansatz.
- **Noise sensitivity**: Real hardware noise introduced fidelity estimation errors. Error mitigation techniques like measurement error correction and readout calibration were implemented.
- Classical bottlenecks: For large N, post-processing the similarity matrix remained computationally heavy. Parallel classical clustering with multi-threading partially addressed this.
- Validation: Ensuring that quantum advantage was not overshadowed by hardware overhead was critical. We ran repeated experiments with synthetic ground-truth neuron clusters to verify that the quantum pipeline consistently recovered the expected structures.

#### 5. Vision for Neurotechnology or Diagnostic Applications

The insights from this project illustrate the potential of **quantum-enhanced clustering** in brain signal analysis. In a real-world neurotechnology context, this pipeline could enable:

- **High-resolution mapping of neural hierarchies** for better understanding of diseases affecting cortical layering (e.g., epilepsy, schizophrenia).
- Early diagnostics by identifying subtle deviations in neuron cluster topologies that could serve as biomarkers.
- **Brain-computer interface optimization**, where fine-grained functional groupings can guide more targeted electrode placement.
- Scalability: As QPU hardware matures, the exponential feature space coverage of quantum kernels could make analysis of larger neuron populations feasible, supporting real-time monitoring or adaptive stimulation therapies.

**Summary:** In conclusion, the hybrid quantum-classical approach demonstrated promising benefits in representing complex neuronal hierarchies with improved interpretability and theoretical efficiency for large-scale, high-dimensional data. Continued improvements in quantum hardware, noise mitigation, and circuit parallelization will pave the way for practical neurotechnology applications, bringing us closer to robust, scalable diagnostics and interventions for complex brain disorders.

#### References

- 1. Schölkopf, B., Smola, A., & Müller, K.-R. (1997). *Kernel principal component analysis*. In *International Conference on Artificial Neural Networks* (pp. 583–588). Berlin, Heidelberg: Springer.
- 2. Schuld, M., & Petruccione, F. (2021). *Quantum models as kernel methods*. In *Machine Learning with Quantum Computers* (pp. 217–245).
- 3. Schuld, M., & Killoran, N. (2019). *Quantum machine learning in feature Hilbert spaces. Physical Review Letters*, 122(4), 040504.
- 4. Murtagh, F., & Contreras, P. (2012). Algorithms for hierarchical clustering: An overview. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery, 2(1), 86–97.
- 5. Johnson, S. C. (1967). Hierarchical clustering schemes. Psychometrika, 32(3), 241–254.
- 6. Chen, S. Y.-C., Yang, C.-H. H., Qi, J., Chen, P.-Y., Ma, X., & Goan, H.-S. (2020). *Variational quantum circuits for deep reinforcement learning. IEEE Access*, 8, 141007–141024.
- 7. Hochreiter, S., & Schmidhuber, J. (1997). Long short-term memory. Neural Computation, 9(8), 1735–1780.
- 8. Chen, S. Y.-C., Yoo, S., & Fang, Y.-L. L. (2022). Quantum long short-term memory. In ICASSP 2022-2022 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP) (pp. 8622–8626). IEEE.
- 9. PennyLaneAI. (n.d.). PennyLane. Retrieved from <a href="https://github.com/PennyLaneAI/pennylane">https://github.com/PennyLaneAI/pennylane</a>
- 10. Qiskit. (n.d.). *Qiskit*. Retrieved from <a href="https://github.com/Qiskit/qiskit">https://github.com/Qiskit/qiskit</a>