Quantum Machine Learning Seminars

Week 5: Quantum Clustering & Classification

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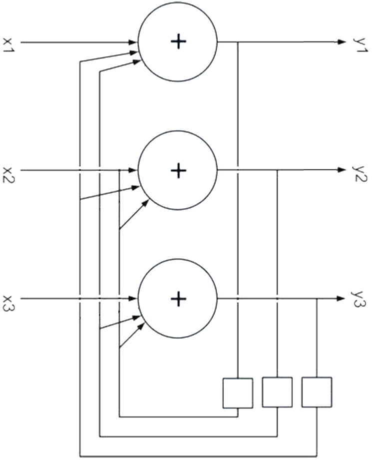
Outline

1. Quantum Pattern Recognition

2. Quantum Clustering

Associative Memory

- RAM is address-oriented, it assigns an address for information to be located upon request.
- QRAM has an "associated" memory that retrieves information using patterns instead.
- Classical RAM can have "associated memory" (Hopfield network) too but it is limited.
- The neurons interactions are defined using the Hebbian learning rule so that a "pattern completion" is realized as a whole memory recall from related partial cues:
  $\mathcal{P} = \{p^{(1)}, p^{(2)}, \cdots, p^{(N)}\},\ N < 2^n$



Quantum Pattern Recognition

Storing/Processing components

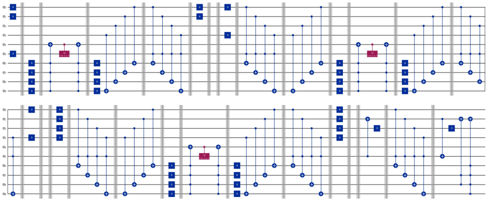
- $\{p^{(k)}\}^n$ is basic encoded $|M\rangle = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} |p^{(k)}\rangle$ (how?)
- Three qubit registers are required:

i. n-qubit "input" register for the patterns.

ii. 2-qubit "utility" register.

iii. n-qubit "memory" register to store the input.

i.e., $|\Psi_0\rangle = |p_1 \cdots p_n\rangle_{in} |01\rangle_u |0 \cdots 0\rangle_m$



A. Wichert, [arXiv:2510.07354]

- Store of $p^{(1)}$ in two steps:

i. $|\Psi_1\rangle = \prod_{j=1}^{n} \texttt{CNOT}_{in_j m_j} |\Psi_0\rangle = |p_1 \cdots p_n\rangle_{in} |01\rangle_u |p_1 \cdots p_n\rangle_m.$

ii. $|\Psi_2\rangle = |p_1 \cdots p_n\rangle_{in} \left[\frac{1}{\sqrt{N}} |00\rangle_u + \sqrt{\frac{N-1}{N}} |01\rangle_u \right] |p_1 \cdots p_n\rangle_m$

Pattern Store

- Reset:

$$\prod_{j=1}^{n} \mathtt{CNOT}_{in_j m_j} |\Psi_2\rangle = \frac{1}{\sqrt{N}} |p^{(1)}\rangle_{in} |00\rangle_u |p^{(1)}\rangle_m + \sqrt{\frac{N-1}{N}} |p^{(1)}\rangle_{in} |01\rangle_u |0\cdots0\rangle_m .$$

- Prepare another $|p\rangle \equiv |q\rangle$ using basic encoding then load it on $|\Phi_0\rangle$ as:

$$|\Phi_0\rangle = \frac{1}{\sqrt{N}} |q\rangle_{in} |00\rangle_u |p\rangle_m + \sqrt{\frac{N-1}{N}} |q\rangle_{in} |01\rangle_u |0\cdots0\rangle_m$$

$$|\Phi_1\rangle = \prod_{j=1}^{n} \mathtt{CNOT}_{in_j u_2 m_j} |\Phi_0\rangle = \frac{1}{\sqrt{N}} |q\rangle_{in} |00\rangle_u |p\rangle_m + \sqrt{\frac{N-1}{N}} |q\rangle_{in} |01\rangle_u |q\rangle_m$$

$$|\Phi_2\rangle = \prod_{j=1}^{n} \mathtt{NOT}_{m_j} \mathtt{CNOT}_{in_j m_j} |\Phi_1\rangle = \frac{1}{\sqrt{N}} |q\rangle_{in} |00\rangle_u |\overline{p \oplus q}\rangle_m + \sqrt{\frac{N-1}{N}} |q\rangle_{in} |01\rangle_u |1\rangle_m$$

$$|\Phi_3\rangle = \mathtt{CNOT}_{m_1\cdots m_n u_1} |\Phi_2\rangle = \frac{1}{\sqrt{N}} |q\rangle_{in} |00\rangle_u |\overline{p \oplus q}\rangle_m + \sqrt{\frac{N-1}{N}} |q\rangle_{in} |11\rangle_u |1\rangle_m$$

Pattern Store

$$
\begin{aligned}
|\Phi_4\rangle &= \mathtt{CS}^{(N-1)}_{u_1u_2}\,|\Phi_3\rangle \\
&= \frac{1}{\sqrt{N}}|q\rangle_{in}|00\rangle_u|\overline{p\oplus q}\rangle_m + \sqrt{\frac{N-1}{N}}\,|q\rangle_{in}|1\rangle_{u_1}\left(\frac{1}{\sqrt{N-1}}|0\rangle_{u_2} + \sqrt{\frac{N-2}{N-1}}|1\rangle_{u_2}\right)|1\rangle_m \\
|\Phi_5\rangle &= \mathtt{CNOT}_{m_1\cdots m_n\,u_1}\,|\Phi_4\rangle \\
&= \frac{1}{\sqrt{N}}|q\rangle_{in}|00\rangle_u|\overline{p\oplus q}\rangle_m + \sqrt{\frac{N-1}{N}}\,|q\rangle_{in}|0\rangle_{u_1}\left(\frac{1}{\sqrt{N-1}}|0\rangle_{u_2} + \sqrt{\frac{N-2}{N-1}}|1\rangle_{u_2}\right)|1\rangle_m \\
|\Phi_6\rangle &= \prod_{j=1}^{n}\mathtt{CNOT}_{in_j\,m_j}\,\mathtt{NOT}_{m_j}\,|\Phi_5\rangle \\
&= \frac{1}{\sqrt{N}}|q\rangle_{in}|00\rangle_u|p\rangle_m + \frac{1}{\sqrt{N}}|q\rangle_{in}|00\rangle_u|q\rangle_m + \sqrt{\frac{N-2}{N}}\,|q\rangle_{in}|01\rangle_u|q\rangle_m \\
&= \frac{1}{\sqrt{N}}|q\rangle_{in}|00\rangle_u\left(|p\rangle_m + |q\rangle_m\right) + \sqrt{\frac{N-2}{N}}\,|q\rangle_{in}|01\rangle_u|q\rangle_m
\end{aligned}
$$

Quantum Pattern Recognition

Pattern Store

- Continue

$$|\Phi_7\rangle = \prod_{j=1}^{n} \mathtt{CNOT}_{in_j\, u_2\, m_j} |\Phi_6\rangle$$
$$= \frac{1}{\sqrt{N}} |q\rangle_{in} |00\rangle_u \big(|p\rangle_m + |q\rangle_m\big) + \sqrt{\frac{N-2}{N}}\, |q\rangle_{in} |01\rangle_u |0\cdots 0\rangle_m \,.$$

- The steps above are repeated for any $p^{(i)}$ to be stored. Gate $\mathtt{CS}^{N+1-i}$ in step 4 processes the pattern $p^{(i)}$. After uploading k patterns, the overall state of the three registers is:

$$\left|\Phi_7^{(k)}\right\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{k} \left|p^{(k)}\right\rangle_{in} |00\rangle_u \left|p^{(i)}\right\rangle_m + \sqrt{\frac{N-k}{N}} \left|p^{(k)}\right\rangle_{in} |01\rangle_u |0\cdots 0\rangle_m \,.$$

- When $k = N$, all the patterns in $\mathcal{P}$ are stored as:

$$\left|\Phi_7^{(N)}\right\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \left|p^{(N)}\right\rangle_{in} |00\rangle_u \left|p^{(i)}\right\rangle_m \,.$$

Retrieval from Quantum Memory

- Once a collection of binary patterns of length n is stored in a quantum memory encoded in the n-qubit state $|M\rangle$, the task is to retrieve information efficiently even when the query is incomplete. A natural idea is to use Grover's algorithm for retrieval.
- Example: The stored pattern collection is $\mathcal{P} = \{0000, 0011, 0110, 1001, 1100, 1111\}$.
- In the basis encoding, patterns are embedded as computational-basis states of a 4-qubit register. The resulting memory state is $|M\rangle = \frac{1}{\sqrt{6}}(1,0,0,1,0,0,1,0,0,1,0,0,1,0,0,1)^T$.

Retrieval from Quantum Memory

- To retrieve the pattern 0110 using standard Grover with initial state $|M\rangle$, the Grover iteration $U_G U_f$ is applied about $\frac{\pi}{2}\sqrt{6}$ times (here taken as two iterations). The intermediate states shown are:
  $U_f|M\rangle = \frac{1}{\sqrt{6}}(1,0,0,1,0,0,-1,0,0,1,0,0,1,0,0,1)^T$,
  $GU_f|M\rangle = \frac{1}{2\sqrt{6}}(-1,1,1,-1,1,1,3,1,1,-1,1,1,-1,1,1,-1)^T$,
  $U_f GU_f|M\rangle = \frac{1}{2\sqrt{6}}(-1,1,1,-1,1,1,-3,1,1,-1,1,1,-1,1,1,-1)^T$,
  $GU_f GU_f|M\rangle = \frac{1}{8\sqrt{6}}(5,-3,-3,5,-3,-3,13,-3,-3,5,-3,-3,5,-3,-3,5)^T$.
- Measuring in the computational basis yields the target with probability $\mathbb{P}(0110) = \left(\frac{13}{8\sqrt{6}}\right)^2 \simeq 44\%$, which is low because the diffusion operator U_G effectively introduces amplitudes (phases) on states that were not part of the original stored set, enlarging the effective search space.

Quantum Pattern Recognition

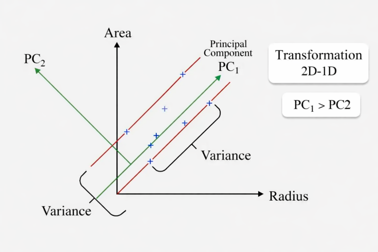
Modified Grover Algorithm

- To fix the phase-structure issue, an additional oracle is introduced to mark stored patterns by a phase flip: $U_{\mathcal{P}}|x\rangle := (-1)^{g(x)}|x\rangle$, where $g : \{0,1\}^n \to \{0,1\}$ is the indicator function $g(x) = \begin{cases} 1, & x \in \mathcal{P}, \\ 0, & x \notin \mathcal{P}. \end{cases}$ so that the amplitude amplification becomes more effective.
- For the same target 0110, the state entering the iterative part of the modified algorithm is $GU_{\mathcal{P}}GU_f|M\rangle = \frac{1}{4\sqrt{6}}(1,1,1,1,1,1,9,1,1,1,1,1,1,1,1,1)^T$. Performing a single iteration yields $GU_{\mathcal{P}}GU_f|M\rangle \xrightarrow{U_f} \frac{1}{4\sqrt{6}}(1,1,1,1,1,1,-9,1,1,1,1,1,1,1,1,1)^T \xrightarrow{G}$ $\frac{1}{16\sqrt{6}}(1,1,1,1,1,1,39,1,1,1,1,1,1,1,1,1)^T$, with success $\boxed{\mathbb{P}(0110) \simeq 99\%}$.

Quantum Clustering

Quantum Principal Component Analysis

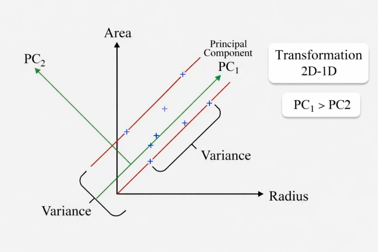
- Let the real feature space be $\mathcal{F} \cong \mathbb{R}^d$ with standard basis $\{e_j\}_{j=1}^d$. The i-th data instance is $x_i = \sum_{j=1}^d x_{ij}\, e_j, \qquad i = 1, \ldots, N.$
- Collect the dataset into matrix $X_{N\times d} := (x_{ij})$, where rows are instances and columns are features, assuming mean-zero features $\mathbb{E}_i(x_{ij}) = 0$.
- Define the "unnormalized" covariance matrix $M_{d\times d} := X^T X$, as a symmetric matrix with diagonal entries as variances and off-diagonal entries as covariances
$m_{kk} = \sum_{i=1}^N x_{ik}^2, \qquad m_{kl} = \sum_{i=1}^N x_{ik} x_{il} \quad (k \neq l).$



Quantum Clustering

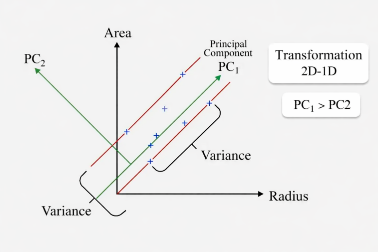
Quantum Principal Component Analysis

- Let W be the eigenvector matrix of M and Λ the diagonal ordered decreasingly eigenvalues matrix, so $M = W\Lambda W^T$. Projecting data onto the eigenvector basis gives the transformed matrix $P := XW$, with $P_{11} > P_{22} > \cdots$, i.e., variance concentrates in leading components, so drop the trailing coordinates of P (low-variance), treat PCA as both feature extraction and feature selection.
- Classical PCA requires $\mathcal{O}(dN^2)$ operations to form M and $\mathcal{O}(d^3)$ for a full eigendecomposition; if only the top k eigenpairs are needed, there are methods achieving about $\mathcal{O}(kdN)$.



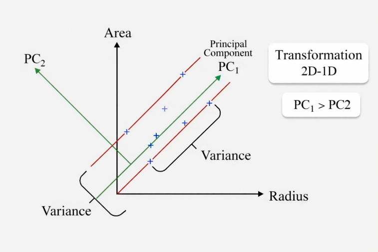
Quantum Principal Component Analysis

- The quantum version encodes a covariance matrix as a density matrix ρ and then applies quantum phase estimation (QPE) to $U = e^{-i\rho t}$, to extract eigenvalues and eigenvectors of ρ (hence principal components).
- Define the normalization constant and normalized covariance
  $C := \sum_{k=1}^{d} \sum_{i=1}^{N} x_{ik}^2 = \sum_i \|x_i\|^2, \qquad M_1 := \frac{1}{C} M.$
  Each datum is amplitude-encoded as
  $|x_i\rangle := \|x_i\|^{-1} \sum_{k=1}^{d} x_{ik} |k\rangle \in \mathcal{H}(\simeq \mathbb{C}^d).$



Quantum Principal Component Analysis

- Using an index basis $\{|i\rangle\}_{i=1}^{N}$ for $\mathbb{C}^N$, the data matrix can be written as $X = \sum_{i=1}^{N} \|x_i\| \, |i\rangle\langle x_i|$.
- Then $M = X^T X = \sum_i \|x_i\|^2 \, |x_i\rangle\langle x_i|$, and with the composite state $|\Psi\rangle := \frac{1}{\sqrt{C}} \sum_{i=1}^{N} \|x_i\| \, |x_i\rangle|i\rangle$, the normalized covariance: $M_1 = \rho = \mathrm{tr}\big(|\Psi\rangle\langle\Psi|\big)$.
- Running QPE yields a spectral decomposition of the form $\sum_i \lambda_i \, |\hat{\lambda}_i\rangle\langle\hat{\lambda}_i| \otimes |\psi_i\rangle\langle\psi_i|$. The claimed QPCA complexity grows logarithmically in Nd (exponential speedup in principle), but it relies on QRAM and QPE and is noted as lacking experimental demonstration.



Thank You!