
RESEARCH PROPOSAL FOR IGP(A) PROGRAM AT TOKYO INSTITUTE OF TECHNOLOGY

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ABSTRACT

The research proposal mainly focuses on implementation of state-of-art Quantum Computing Algorithms for Machine Learning and Signal Processing. The more detailed studies lie in field of quantum machine learning algorithms, with combination of Data Analysis Techniques in Riemannian Manifolds. Meanwhile, it also digs into the fundamentals, like the discrete Fourier transform, and expects to expand the Quantum Fourier Transform (QFT) to larger framework. If possible, the encoding in quantum computing will also be included as supplementary study. The first section discusses the motivation and current progress on quantum machine learning, quantum signal processing and data analysis in Riemannian Manifolds. The second section contains the research objective and research method at both Master and PhD level and more. The last section works more on my current research background and on-going projects. This draft serves as the backbone for IGP(A) application at Tokyo Institute of Technology.

Keywords Quantum Signal Processing · Quantum Fourier Transform · Quantum Machine Learning · Variational Quantum Circuit · Variational Shadow Quantum Learning · Quantum Kernel Method · Quantum Block Encoding

*The citation is not precisely managed.

1 Your research topic in Japan: Describe articulately the research you wish to carry out in Japan.

Research theme: Quantum Computing Algorithms for Machine Learning and Signal Processing

1.1 Prior Literature and Current Development

Quantum Machine Learning Machine learning has been used in various fields for a long time, with algorithms like deep neural network (DNN), binary decision tree (BDT), convolutional neural network (CNN), Generative adversarial network (GAN) and etc. Quantum computing was postulated in the early 1980s as way to perform computations that would not be tractable with a classical computer. With the advent of noisy intermediate-scale quantum computing devices, more quantum algorithms are being developed with the aim at exploiting the capacity of the hardware for machine learning applications. Recent years, the robust development of quantum computing has also brought people Variational Quantum Circuit Learning (VQC), Quantum Kernel Methods, Variational Shadow Quantum Learning (VSQL), and Quantum Generative Adversarial Network (Quantum-GAN). These new approaches solve the clustering, classification, discrimination problems in Quantum Computing. Most of them take advantages of exponential improvement in computational speed of quantum computer and are expected to have better performance than its classical version of algorithms.

Quantum Kernel Method Among all the Quantum Machine learning algorithms, Quantum Kernel Method plays an important role for classification problem using large dimension of quantum Hilbert space. Traditionally, kernel methods

for machine learning are ubiquitous for pattern recognition, with support vector machines (SVMs) being the most well-known method for classification problems. In kernel methods, the access to the feature space is facilitated through kernels or inner products of feature vectors. In quantum computing, access to the Hilbert space of quantum states is given by measurements, which can also be expressed by inner products of quantum states.

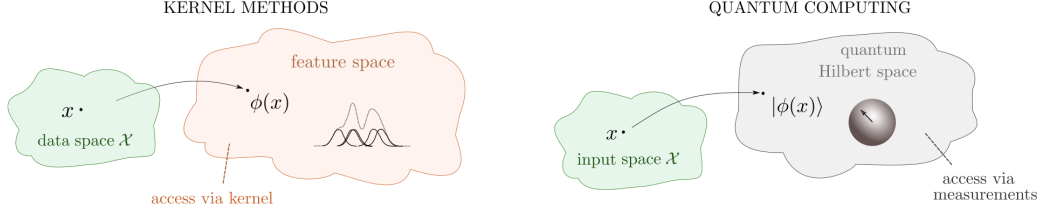


Figure 1: Quantum computing and kernel methods are based on a similar principle.

There are limitations to the successful solution to such problems when the feature space becomes large, and the kernel functions become computationally expensive to estimate. Then, people start to think of computational speed-ups afforded by quantum algorithms. The exploitation of an exponentially large quantum state space through controllable entanglement and interference could resolve current limitations.

Clustering Problems in Riemannian Manifolds Currently in Machine Learning and Signal Processing field, people study the learning from data/features which Numerous well-known features in signal processing and machine learning belong to Riemannian manifolds, like correlation matrices, orthogonal matrices, fixed rank linear subspaces and etc.

Many learning tasks could be studied with forming feature space and Riemannian Manifold. The state clustering, connectivity among network nodes that stays fixed over a time interval. The community detection, subgroup detection of nodes within a single state/layer. Subnetwork-sequence clustering, sequence of subgroups of nodes with changing state. The algorithms study benefits understanding of the brain networks and its relation with Alzheimer disease, autism, depression and more.

Quantum Signal Processing The Fourier transform occurs in many different classical computing fields, especially signal processing. The decompose of wave from silicon detectors, image processing from CMOS detector, the noise filtering and more all require use of Fourier Transform. The quantum Fourier transform is the quantum implementation of the discrete Fourier transform over the amplitudes of a wavefunction. It is part of many quantum algorithms, most notably Shor's factoring algorithm and quantum phase estimation.

1.2 Motivation

Quantum Machine Learning: One interesting question is whether there are methods to combine quantum machine learning algorithms with clustering algorithms using Riemannian Manifold, and benefit from advantages in both algorithms. In Riemannian Manifold, reproducing Kernel Hilbert space(RKHS) plays important role in extracting the features. Also in quantum kernel method, RKHS is also form before input to the quantum circuit for further learning, with additional encoding required for quantum circuit processing. The shared procedure provides idea to improve the existing algorithms using Riemannian Manifold and combine it to quantum kernel method, either deriving the completely new algorithm or improving the existing clustering algorithms would be interesting.

Quantum Signal Processing: The Shor's algorithm is a quantum computer algorithm for finding the prime factors of an integer. Shor's algorithm runs polynomial time and allows us to find prime decomposition of very big numbers in $O((\log N)^3)$. One of the important factors such algorithm is so efficient is due to the efficiency of quantum Fourier transform. The discrete Fourier transform on 2^n amplitudes can be implemented as quantum circuit consisting of only $O(n^2)$ Hadamard gates and controlled phase shift gates using n qubits. Compared with discrete Fourier transform, which takes $O(n2^n)$ bits in classical computer. Such exponentially improvement efficiency using quantum Fourier transform, motivates me to think how to apply this to imaging processing, noise filtering and more. With more detailed study on classical algorithms in signal processing, the exploration of quantum Fourier transforms and formation of quantum signal processing framework based on this idea would be really interesting.

2 Study program in Japan: (Describe in detail and with specifics - particularly concerning the ultimate goal(s) of your research in Japan)

Ultimately, I wish to develop the fundamental method or algorithm in exploring today's hard question in natural science. I hope my research mentioned could have similar breakthrough as Machine Learning today and reach "Ubiquitous quantum signal processing or quantum machine learning in natural science and more". Not only in biomedical science, neurological science, fMRI, but also in gravitational wave detection, precise measurement of Higgs particles, general data analysis method for searching new physics phenomena and more.

Nevertheless, my goals could definitely not be achieved by imagination, logically organized research and efforts are necessary. Therefore, the research objectives, research method and originality are demonstrated in this section. Hopefully, my research at Tokyo Institute of Technology could possibly **expand the field of machine learning and signal processing**.

2.1 Research Objectives

The ultimate target is to develop research in quantum machine learning and quantum signal processing. The goal set up for quantum machine learning mainly focuses on improvement, with possibility build up new algorithms. The goal for quantum signal processing is more closely related with original work. Moving the classical theory one step forward to quantum realm, two topics have been introduced in previous section, with one topic as supplementary but necessary to these two research:

A Quantum Machine Learning: Quantum Kernel Method and Clustering in the Riemannian Manifold

B Quantum Signal Processing: Quantum Fourier Transform and Discrete Fourier Transform

C Quantum Signal Processing: Encoding Theory

A. The existing Kernel or Reproducing Kernel Hilbert space in the Riemann Manifold Method will be enhanced or improved models for data analysis using Quantum Kernel Method. Combination of these two algorithms could possibly solve the clustering problems in Riemannian Manifold and improve the time and space exponentially.

B. In imaging analysis, Fourier transform is definitely an unavoidable technique. In analog signal processing, we could apply the quantum Fourier transform and the classical discrete Fourier transform. Then compare their differences and how quantum Fourier transform could possibly enhance the classical result to get started. Later, several goals for working on Quantum Fourier Transform:

1. Forming algorithms could possibly enhance or replace the classical discrete Fourier transform. Such replacement may improve classical algorithms to achieve better performance in feature extraction, like noise filtering, image processing and etc.
2. By the theory of Big-O, the quantum Fourier transform is exponentially faster than classical discrete Fourier transform. Verification the efficiency improvement would also be a nice work to implement and get started.

C. Encoding is essential for quantum computing. Before precossing data into the variational quantum circuit, or any type of quantum circuit, encoding of data using angle encoding or amplitude encoding are mandatory. The efficient encoding algorithm is considered as side product of research in quantum machine learning and the quantum signal processing.

2.2 Research Method and Originality

With motivation in last section, the method to achieve research objective A B C will be explained in more details.

Quantum Machine Learning: Quantum Kernel Method and its application on Riemannian Manifold In practice, the feature space's demensionality sometimes can be extremely large. While not tackling these feature vectors directly, we implicitly analyze the feature vectors by only accessing their inner products in the feature space, which gives the classical kernel functions $K(\cdot, \cdot)$:

$$K(x_i, x_j) = \phi(x_j)^T \phi(x_i) \quad (1)$$

With support vector machine (SVM), a given dataset $T = \{(x_1, y_1), \dots, (x_m, y_m)\}$ in Z_2 , and a hyperplane (w, b) , a SVM can assign labels through signs of the decision function, as:

$$y_{pred} = \text{sign}(\langle w, x \rangle + b) \quad (2)$$

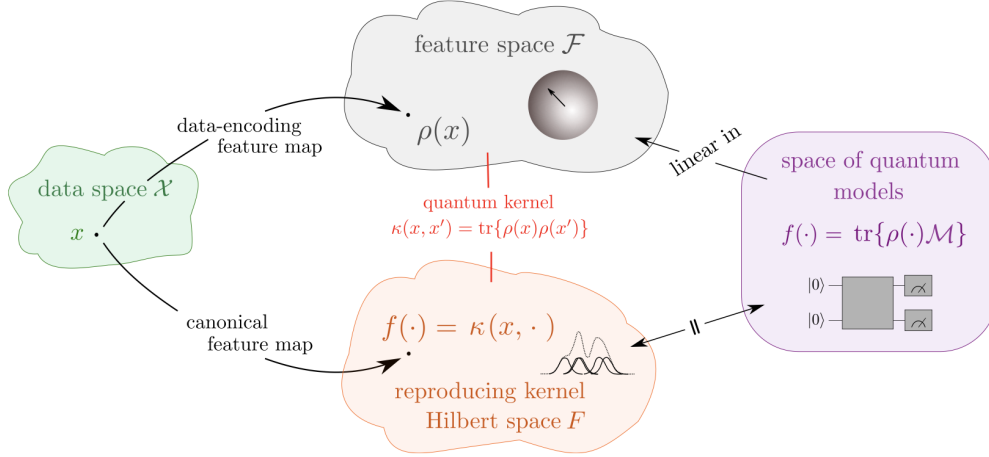


Figure 2: Overview of the link between quantum models and kernel methods.

Also, separation by mapping them into a feature space is another solution, where $y_{pred} = \text{sign}(\langle w', \phi(x) \rangle + b')$ and $w' = \sum_i \alpha_i \phi(x_i)$.

With the idea of classical methods, the essentials of quantum kernel methods are the same, if we map a classical data vector x into quantum state $|\phi(x)\rangle$ by encoding circuit $U(x)$ as follows:

$$U(x) |0^N\rangle = |\phi(x)\rangle \quad (3)$$

The quantum kernel function is the inner products of two quantum feature vectors in the Hilbert space:

$$K_{ij}^Q = |\langle \phi(x_j) | \phi(x_i) \rangle|^2 \quad (4)$$

This kind of kernel manipulation could then feed into the common variational quantum circuit learning method and then go through the training.

One consideration is the number of qubit and the Hilbert space's dimensionality. The Hilbert space's dimensionality grows exponentially with the number of qubits, nearly all quantum states will be perpendicular to each other when we have a large number of qubits. The kernel matrix will converge to identity matrix $K_{ij} = K(x_j, x_i) I$, and the kernel methods fail. One solution here is to extract the "features" from Hilbert space and then construct the kernel function with these extracted features. The projected quantum kernel is therefore proposed:

$$K^P(x_i, x_j) = \exp(-\gamma \sum_k \sum_{p \in M} (Tr(P\rho(x_i)_k) - Tr(P\rho(x_j)_k))^2) \quad (5)$$

where $\rho(x_i)_k$ the reduce density matrix of qubits k , M a set of measurements on the reduce density matrix. Then, the idea for combination of the Quantum Kernel Method in RKHS with the Fast Sequential Clustering in Riemannian Manifolds will be illustrated.

Combine with Clustering Problem on Riemannian Manifold

In paper Fast Sequential Clustering in Riemannian manifolds for Dynamic and Time-series-Annotated Multilayer Networks. This work focus on building a sequential-clustering framework able to address a wide variety of clustering tasks in dynamic multilayer (brain) networks via the information extracted from their nodal time-series. I consider two essential algorithms are here:

1. feature extraction from time-series
2. Riemannian Manifolds

This work claims that the rich geometry of (not necessarily embedded in Euclidean spaces) Riemannian manifolds allows latent feature patterns to unfold to the benefit of all of the aforementioned network-clustering tasks.

The Grassmanian $Gr(\rho, M)$ is defined as the collection of all linear subspaces fo R^M with rank equal to ρ . Motivated by the success of kernel methods in capturing non-linearities in data, user could define RKHS H with its associated

reproducing kernel function $\kappa(*, *)$ and the mapping could extract features from the Grassmanian $Gr(\rho, M)$. In such algorithm, Kernel correlations $K_v^{(l)}[t] = \phi_v^{(l)} \otimes_H \phi_v^{(l)}$ itself as a feature in Riemannian manifold of $P(S)D(T_w)$ of positive-(semi)definite matrices, of dimension $T_w(T_w + 1)/2$, to take advantages of the rich Riemannian Geometry of $P(S)D(T_w)$

With proper study of the quantum kernel method, the kernel relation here could be possibly replace with $K^P(x_i, x_j) = \exp(-\gamma \sum_k \sum_{p \in M} (Tr(P\rho(x_i)_k) - Tr(P\rho(x_j)_k))^2)$ then process through the quantum computer. Based on processing result through quantum kernel method, the features could be well discovered through time interval or more. It could expect that in the future, applications facing large-scale networks and data, e.g., very long nodal time-series, if the quantum kernel method is computationally efficient clustering framework. Quantum kernel method could operates together on data and features and carries through all of the network clustering tasks in Riemannian manifolds.

Quantum Signal Processing: Quantum Fourier Transform Approach

The structure for the development of Quantum Signal Processing starts from measurement. The wave break down by using Fourier transform's quantum analog part, Quantum Fourier Transform (QFT). The Quantum Fourier transform could particularly decompose into a product of simpler unitary matrices. With Simple decomposition, the discrete Fourier transform on 2^n amplitudes can be implemented as a quantum circuit consisting of $O(n^2)$ Hadamard gates and controlled phase shift gates.

Borrowed from Qiskit's notation, the classical discrete Fourier Transforms act on vector $x = (x_0, x_1, \dots, x_n)$ and its mapping to vector $y = (y_0, y_1, \dots, y_n)$ according to formula:

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j \omega_N^{jk} \quad (6)$$

Where $\omega_N^{jk} = e^{2\pi i \frac{jk}{N}}$. The quantum state $|X\rangle = \sum_{j=0}^{N-1} x_j |j\rangle$ and mapped to $|Y\rangle = \sum_{k=0}^{N-1} y_k |k\rangle$ and the map could therefore be expressed as:

$$|j\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \omega_N^{jk} |k\rangle \quad (7)$$

Or the unitary matrix:

$$U_{QFT} = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \omega_N^{jk} |k\rangle \langle j| \quad (8)$$

There are already well published paper for quantum Fourier transform. Moreover, the quantum-analog representation of classical images, the pixel value of i^{th} row and the j^{th} column can be stored as: $|pixel_{i,j}\rangle = \cos\left(\frac{\theta_{i,j}}{2}\right) |0\rangle + \sin\left(\frac{\theta_{i,j}}{2}\right) |1\rangle$ as formed in **Qubit Lattice** model. Other image representations like **Flexible Representation of Quantum Images** (FRQI) and **Novel Enhanced Quantum Representation** (NEQR) also provide new type of representation for images that could be proceed by quantum Fourier transform. If properly organized, edge detection, filtering and more could be realized in thoroughly different method from today.

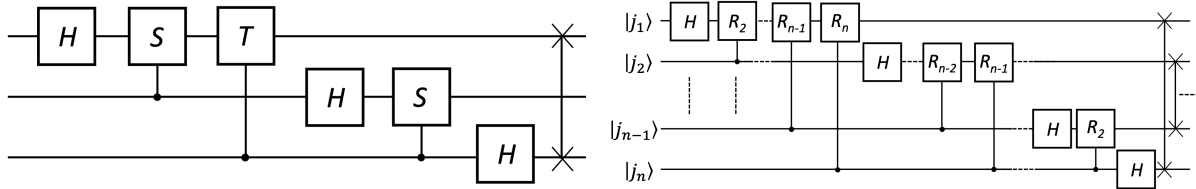


Figure 3: The quantum Fourier Transform Circuit for 3 qubits only and n different qubits

2.3 Tentative Plan/Timetable

The first two years are filled with more details and later three years would be planned at later stage.

Year	Content	Outcome
2023 - 2024	Signal Processing and Differential Geometry Theory Courses Seminars on Quantum Machine Learning Simple Research on Application Oriented Studies	Learn basics work with Labmates Local Conference Talks
2024 - 2025	Algebraic Geometry and Quantum Computing Theory Courses Seminars on QML and Quantum Signal Processing Summarize First two years of study	Learn basics work with Labmates Journal Publication Master Thesis
2025 - 2026	Research on Quantum Fourier Transform	Journal Publication
2026 - 2027	Research on QFT and Encoding Theory Research on Quantum Image Processing	Journal Publication International Conference Talks
2027 - 2028	Summarize Five years of study	PhD Thesis and Graduation

Research Originality: Quantum computing and quantum information science became a hot topics in recent years. Once there is breakthrough on Noise intermediate Scale quantum era NISQ. All the research could take the data analysis, machine learning, signal processing to next level. As Tokyo Insitute of Technology has quite strong bond with IBM and development of quantum computer, I expect the new methods I provide would not only run on the emulators on super computer, but also on latest real quantum computers.

Moreover, with connection globally, not only using the fMRI data in brain locally at Tokyo Institute of Technology, collaboration with people from international institute like MIT, University of Chicago, University of Hong Kong, CERN, KEK and more are all possible. The clustering algorithms anti-kt is already the default on clustering analysis for jets in colliders and there are so many possibilities my research could create a new methodology for all types of study in natural science and broader human society.

References on Riemannian Manifold related research:

1. Slavakis Lab: Fast Sequential Clustering in Riemannian Manifolds for Dynamic and Time-Series-Annotated Multilayer Networks
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References on Quantum Signal Processing: Quantum Fourier Transform

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3. Shor's Algorithm wiki IBM quantum composer
4. Leandro Aolita et. al: Fourier-based quantum signal processing
5. Alok Anand et. al: Quantum Image Processing
6. Qiskit: Quantum Image Processing

References on Quantum Signal Processing: Encoding Theory

1. Marcello Benedetti et. al: Parameterized quantum circuits as machine learning models

3 Present Field of Study

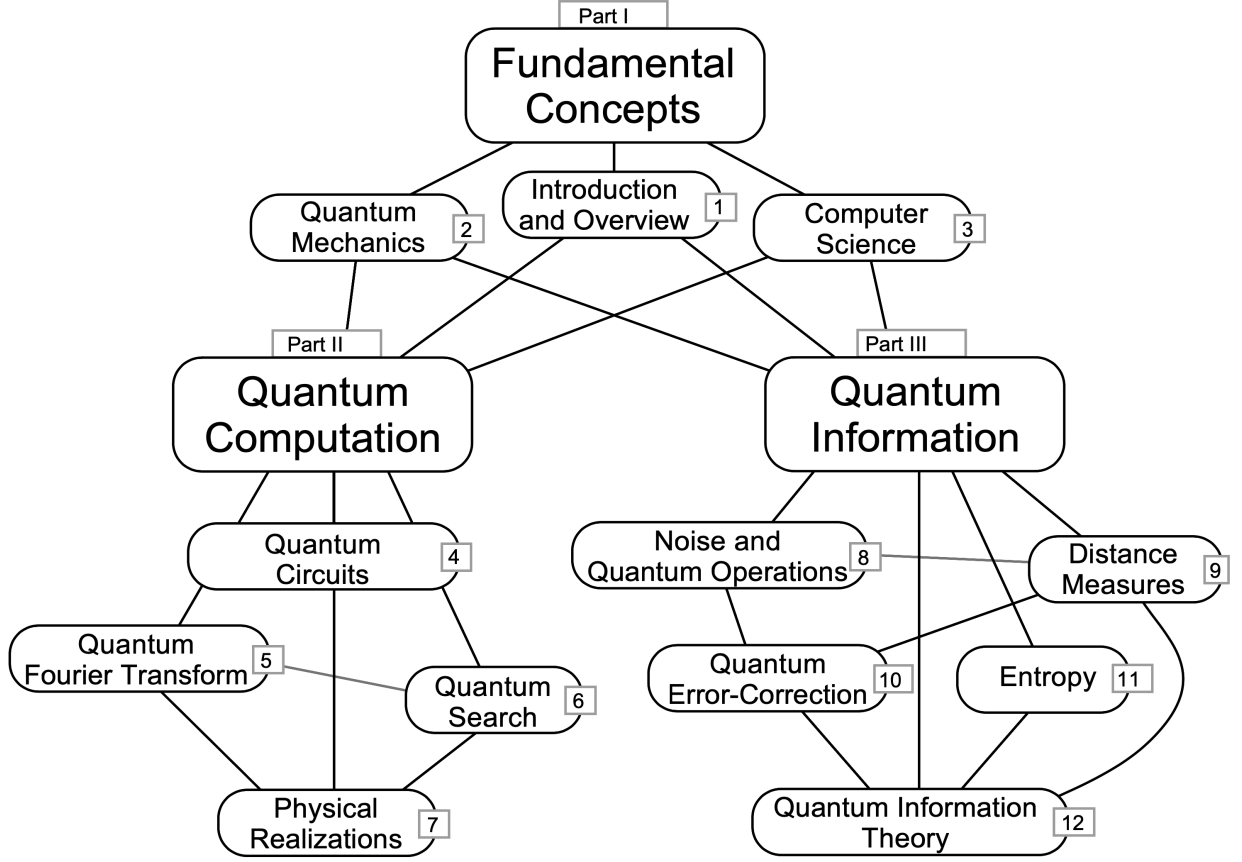


Figure 4: A big picture for the quantum computation and quantum information field in Issac Chuang's book. The proposal here focuses more on quantum circuits and quantum fourier transform study.

Back Up

Some notes and materials to help people understand the basics. Hope this section could explain bit more on how we construct a Variational Quantum Circuit and how to use or understand each gate, and the position of my research.

Quantum Gates and quantum computation

Classical computer consists of wires and logic gates. Similarly, the quantum computer takes quantum version and logic gates and act on each qubit. The most famous Pauli Matrices, X are used as NOT gates:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (9)$$

Z gate flips the sign of $|1\rangle$ to give $-|1\rangle$ and *Hadamard* gate,

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad (10)$$

Hadamard gate turns $|0\rangle$ into $(|0\rangle + |1\rangle)/\sqrt{2}$, and $|1\rangle$ into $(|0\rangle - |1\rangle)/\sqrt{2}$

Controlled Operations

Here are some controlled operation with CNOT gate.

Encoding Classical Data into Quantum States

Quantum Encoding is a process to transform classical information into quantum states. In order to use quantum algorithms to solve classical problems, such encoding is unavoidable. The simple concept is quantum circuit acts on $|0^n\rangle$ state, where n is the number of qubits. Based on different requirements, the style of requirement is different. The first three are most basic ones and the last two require more depth.

Basis Encoding

Conceptually the simplest one, encodes an n -bit binary string to an n -qubit quantum state $|x\rangle = |i_x\rangle$, where $|i_x\rangle$ is a computational basis state. Concrete example: $x = 1011$ maps to $|1011\rangle$

Amplitude Encoding

Vector x of length N into amplitudes of an n -qubit quantum state with $n = \lceil \log_2(N) \rceil$ and $|x\rangle = \sum_i^N x_i |i\rangle$ and $|i\rangle$ is the computational basis for the Hilbert space. Since the classical information forms the amplitudes of a

quantum state, the input needs to satisfy the normalization condition. For instance, $x1 = \begin{bmatrix} 1/2 \\ 1/2 \\ -1/2 \\ -1/2 \end{bmatrix}$, the quantum

state will be written as: $|x1\rangle = \frac{1}{2} |00\rangle + \frac{1}{2} |01\rangle - \frac{1}{2} |10\rangle - \frac{1}{2} |11\rangle$ similarly, for $x2 = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ -1/\sqrt{3} \end{bmatrix}$ the state would be:

$$|x2\rangle = \frac{1}{\sqrt{3}} |00\rangle + \frac{1}{\sqrt{3}} |01\rangle - \frac{1}{\sqrt{3}} |10\rangle$$

Angle Encoding

Angle encoding uses rotation gates to encode the classical information x . The classical information determines angles of rotation gates:

$$|x\rangle = \bigotimes_i^n R(x_i) |0^n\rangle \quad (11)$$

R can be one of the rotation gate R_x , R_y , and R_z . Usually, the number of qubits used for encoding is equal to the dimension of vector. For example, if $x = \begin{bmatrix} \pi \\ \pi \\ \pi \end{bmatrix}$, angle encoding rotates every qubit around Y-axis (if we choose R_y) for degree π , the corresponding quantum state is then $|x\rangle = R_y(\pi) |0\rangle R_y(\pi) |0\rangle R_y(\pi) |0\rangle$, which indicates the result is $|111\rangle$.

IQP Style Encoding

Hamiltonian Evolution Ansatz Encoding

Quantum Classifier

References

1. Hamiltonian Evolution Ansatz Encoding: Strategies for solving the Fermi-Hubbard model on near-term quantum computers