Research Proposal for IGP(A) Program at Tokyo Institute of Technology

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Abstract

The research proposal focuses on development 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, the research expects to expand the application of Quantum Fourier Transform in signal processing field. The encoding in quantum computing will also be included as supplementary study.

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.

Quantum Computing was postulated in the early 1980s as way to perform computations that would not be tractable with a classical computer. Currently, at Noisy Intermediate-Scale Quantum (NISQ) era, 50 to hundreds of qubits are available for algorithm designs [1]. So far, companies like D-wave implemented quantum computers specialized quantum annealing and Xanadu implemented Photonic Quantum Computers with 216 qubits available. Many quantum algorithms have already been developed with the aim at exploiting the capacity of the hardware for machine learning and signal processing application. An interesting question is whether there are efficient quantum machine learning algorithms could approach or outperform the existing machine learning algorithms. The Variational Quantum Circuits (VQC) are demonstrated to approximate the Deep Reinforcement Learning for decision-making and policy-selection [2]. Within decades of research, a universal fault-tolerant quantum computer that can solve efficiently problems such as integer factorization and unstructured database search using millions of qubits are expected to be developed [3].

Notations:
1. Hilbert space: in quantum mechanics, the state of a physical system is represented by a vector in a *Hilbert space*: a complex vector space with an inner product.
2. *Dirac notation* is used to represent the vectors in the Hilbert space, denoted by $|v\rangle$, called ket, where v is some symbol which identifies the vector. One could equally well use something like $\vec{v}$ or $\mathbf{v}$. A multiple of a vector by a complex number c is written as $c\,|v\rangle \implies$ think of it as analogous to $c\,\vec{v}$ or $c\mathbf{v}$.
3. In Dirac notation the inner product of the vectors $|v\rangle$ with $|w\rangle$ is written as $\langle v|w\rangle$. This resembles the ordinary dot product $\vec{v} \cdot \vec{w}$, thus think of $\vec{v}^{\,*} \cdot \vec{w}$.

1.1 Prior Literature and Current Development on Quantum Computing Algorithms

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. Recent years, the robust development of quantum computing has also brought people 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.
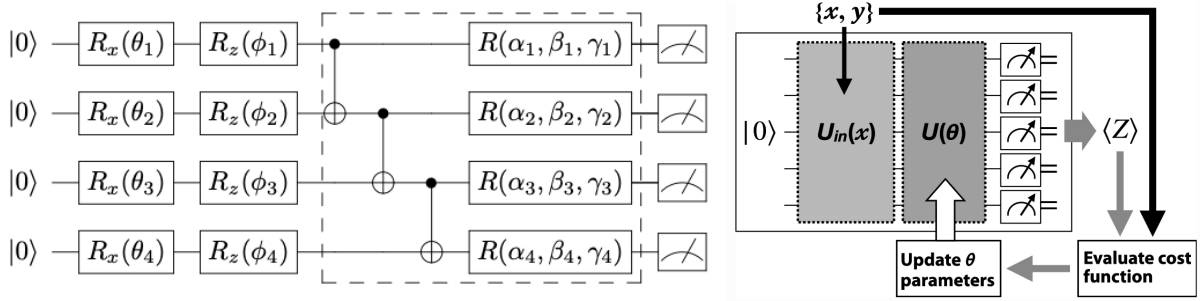

Figure 1: The generic variational quantum circuit architecture and procedure for optimization. The inputs go through encoding, the unitary matrices, measurement, lost function evelution and then update parameters.

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.

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

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j \omega_N^{jk} \tag{1}$$

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:

$$|j\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \omega_N^{jk} |k\rangle \tag{2}$$

Or the unitary matrix:

$$U_{QFT} = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \omega_N^{jk} |k\rangle \langle j| \tag{3}$$

There are already well published paper and books for quantum Fourier transform [4].
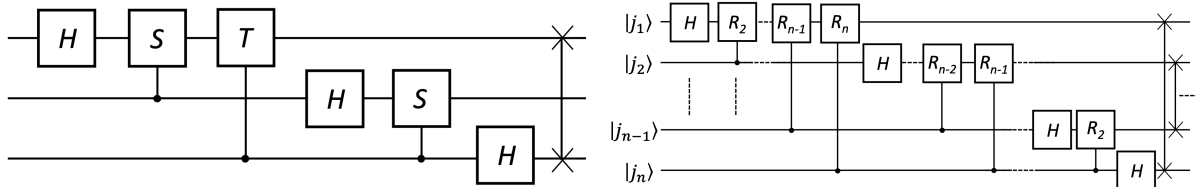

Figure 2: The quantum Fourier Transform Circuit for 3 qubits only and n different qubits

1.2 Motivation for working on Quantum Machine Learning and Quantum Signal Processing

Quantum Machine Learning: Before the robust development of machine learning, people question about what to do with machine learning. Now it turns similar question to quantum machine learning. What is the advantages of quantum version of machine learning over the classical machine learnign? What is the benefit if one just translate the classical algorithm? If current quantum algorithms could solve some problems, is there any quantum algorithm that have better performance? One interesting answer is 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. [5] [6] [7]

Quantum Signal Processing: Moreover, with quantum Fourier transform, could we benefit from formation of Hilbert space in quantum computer and bring it to signal processing field and more? Could we actually prove the universal advantages of quantum computing algorithms over the classical algorithms in machine learning and signal processing?

1. **QFT ready Original Signal State** One important question is: *Can we use the quantum Fourier transform to speed up the computation of the Fast Fourier Transform or Discrete Fourier Transform?* In Issac Chuang's book, he considered the amplitude in a quantum computer cannot be directly accessed by measurement. Moreover, Chuang thinks there is no way of determining the Fourier transformed amplitudes of the original states. However, in image processing field, different Quantum Image Representation were proposed and some quantum analog representation of classical images is demonstrated. Such progress in recent year motivates me to rethink about the possible application of QFT in signal processing.

2. **Efficiency Improvement** 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 $O((logN)^3)$. 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)

2.1 Research Objectives

The ultimate target is to develop breakthrough algorithms in quantum machine learning and quantum signal processing. Developing quantum machine learning algorithms, I hope to find the one outperforms current classical machine learning algorithms. Moreover, in quantum signal processing part, I expect to develop algorithms to complete tasks considered not possible in the past.

A Quantum Machine Learning: Quantum Machine Learning

B Quantum Signal Processing: Quantum Fourier Transform

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.

2.2 Reseaerch Method

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

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. [8]

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 Machine Learning: Quantum Kernel Method and its application on Riemannian Manifold In practice,
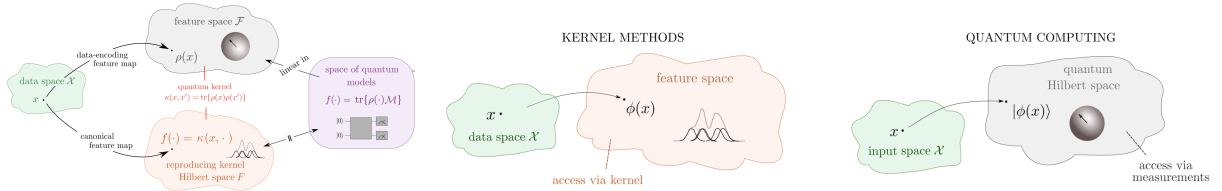

Figure 3: Overview of the link between quantum models and kernel methods.

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(,):

$$K(x_i, x_j) = \phi(x_j)^T \phi(x_i) \tag{4}$$

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

$$y_{\text{pred}} = \text{sign}(< w, x > + b) \tag{5}$$

Also, separation by mapping them into a feature space is another solution, where $y_{pred} = sign(< w', \phi(x) > + b')$ and $w' = \sum_i \alpha_i \phi(x_i)$. with Lagrangian multipliers α_i. Then, under constraints $\alpha_i \leq 0$ and $\sum_i y_i \alpha_i = 0$, we can compute the optimal α_i^*, thus the optimal hyperplane by maximizing:

$$\sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \phi(x_j)^T \phi(x_i) \tag{6}$$

From the equation above, we only need the inner product of feature vectors $\phi(x_j)^T \phi(x_i) = K(x_i, x_j)$, which is the above mentioned kernel function. With such idea, y_{pred} is:

$$y_{\text{pred}} = \text{sign}(\sum_i \alpha_i^* K(x, x') + b') \tag{7}$$

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:

$$U(x)\left|0^N\right\rangle = |\phi(x)\rangle \tag{8}$$

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

$$K_{ij}^Q = |\langle\phi(x_j)|\phi(x_i)\rangle|^2 = |\left\langle 0^{\otimes N}\right|U^\dagger(x_j)U(x_i)\left|0^{\otimes N}\right\rangle|^2 \tag{9}$$

This kind of kernel manipulation could then feed into the common variational quantum circuit learning method and then go through the training as the circuit below. One consideration is the number of qubit and the Hilbert space's
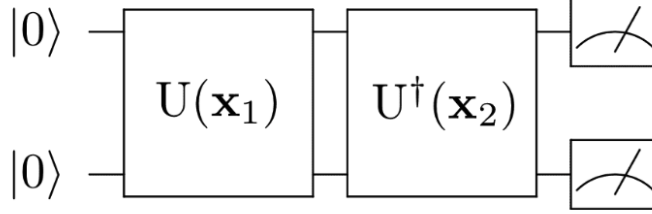

Figure 4: Simple demo for quantum circuit in kernel method

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:

$$K^P(x_i, x_j) = exp(-\gamma \sum_k \sum_{p\in M}(Tr(P\rho(x_i)_k) - Tr(P\rho(x_j)_k))^2) \tag{10}$$

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 $K_v^{(l)}[t] = \phi_v^{(l)}\bigotimes_H \phi_v^{(l)}$ 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 and Image Processing
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 particularlly 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.

Image Processing: The quantum-analog representation of classical images, the pixel value of ith row and the jth 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) exists:

$$|I(\theta)\rangle = \frac{1}{2^n} \sum_{i=0}^{2n-1} (sin(\theta_i)|0\rangle + cos(\theta_i)|1\rangle)|i\rangle \tag{11}$$

it actually maps each pixel's grayscale value to the amplitude as well as captures the corresponding positions in an image and integrate them into a quantum state. Where θ encodes pixel value of the corresponding position $|i\rangle$. The FRQI representation maintains a normalized state and the representation space decreases exponentially compared to the classical image due to the quantum states' superposition effect. Moreover, image representation like **Novel Enhanced Quantum Representation** (NEQR) exists:

$$|I\rangle = \frac{1}{2^n} \sum_{y=0}^{2^{2n}-1} \sum_{x=0}^{2^{2n}-1} |f(y,x)\rangle |yx\rangle \tag{12}$$

Such method uses the basis state of a qubit sequence to store the grayscale value of every pixel instead of probability amplitude encoded in a qubit in FRQI. These representations for images provide possible application on quantum Fourier transform. There are already some study using quantum kernel method to work on classification. If properly organized, edge detection, filtering and more could be realized in thoroughly different method from today. The data for testing the new algorithm could use public dataset like **MNIST** dataset or **CIFAR-10** dataset. If the overall new algorithm works with exceptional performance, the dataset with fMRI could be used.

More importantly, the Quntum Convolutional Neural Network (QCNN) exists for classification and image processing [9]. Parameterized QCNN was benchmarked for classical data classification with high accuracy and the best case being about 99% for MNIST and about 94% for Fashion MNIST [10] [11]. With combination of QCNN, quantum Fourier Transform, and Quantum Representation of Images. Setup of Quantum Fourier Convolutional Neural Network (Q-FCNN) is possible. The big picture for such algorithm is:

1. Classical Image Data Encoding to Quantum Image Representation

    (a) build up kernels for images then convert each kernel to Quantum Representation

    (b) Directly take input images to Quantum Representation

2. Using Quantum Fourier Transform take Image Representaions to Fourier Space

3. MERA QCNN take QFT transfered data

4. Inverse Quantum Fourier Transform

Here is just one possibility for new quantum algorithm in field of signal processing. Other simpler models using previously mentioned VQC is also an option.

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	Learn basics
	Seminars on Quantum Machine Learning	work with Labmates
	Simple Research on Application Oriented Studies	Local Conference Talks
2024 - 2025	Algebraic Geometry and Quantum Computing Theory Courses	Learn basics
	Seminars on QML and Quantum Signal Processing	work with Labmates
	Summarize First two years of study	Journal/Conf Publication
		Master Thesis
2025 - 2026	Research on Quantum Fourier Transform	Journal/Conf Publication
2026 - 2027	Research on QFT and Related Encoding Theory	Journal/Conf Publication
	Research on Quantum Image Processing	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. [3] 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.

3 Present Field of Study

The pixel hit information plays vital rule for the charge particle track reconstructions, especially for flavor tagging such as c-, b-quark jets or hadronic tau identifications, where they form as a colimated spray of the charged particles. The track reconstruction software has been developed to identify such particles in the dense environment of the very narrow space using the neural network technique. Meanwhile, the pixel detector has been experienced significant radiation damage that degradates the performance. The pixel hits will be lost at most 50% of efficiency in b-layer in the end of RUN3, in turn lost the performance for the cluster classification to split or merge the associated cluster in the dense track reconstruction. The evaluation of the radiation damage of the pixel detector and modeling of the pixel cluster classification in the simulation is thus critical to improve the systematic uncertainties through RUN3. The task devotes to monitor the pixel cluster classification performance using the $Z \to \tau\tau$ events. The hadronic tau with 3-prong decay mode is a clean source for the dense tracking. The task first constructs clean dataset of the $Z \to \tau\tau$ with 3-prong final state, then the pixel clustering is compared with the simulation in a various view in term of the radiation damage. The produced dataset would be useful for many area for the tracking aspect as further optimization of the neural network training.

References

[1] Kishor Bharti, Alba Cervera-Lierta, Thi Ha Kyaw, Tobias Haug, Sumner Alperin-Lea, Abhinav Anand, Matthias Degroote, Hermanni Heimonen, Jakob S. Kottmann, Tim Menke, Wai-Keong Mok, Sukin Sim, Leong-Chuan Kwek, and Alán Aspuru-Guzik. Noisy intermediate-scale quantum algorithms. *Rev. Mod. Phys.*, 94:015004, Feb 2022.

[2] Samuel Yen-Chi Chen, Chao-Han Huck Yang, Jun Qi, Pin-Yu Chen, Xiaoli Ma, and Hsi-Sheng Goan. Variational quantum circuits for deep reinforcement learning. *IEEE Access*, 8:141007–141024, 2020.

[3] Wen Guan, Gabriel Perdue, Arthur Pesah, Maria Schuld, Koji Terashi, Sofia Vallecorsa, and Jean-Roch Vlimant. Quantum machine learning in high energy physics. *Machine Learning: Science and Technology*, 2(1):011003, mar 2021.

[4] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, 2011.

[5] Maria Schuld. Supervised quantum machine learning models are kernel methods, 2021.

[6] Vojtěch Havlíček, Antonio D. Córcoles, Kristan Temme, Aram W. Harrow, Abhinav Kandala, Jerry M. Chow, and Jay M. Gambetta. Supervised learning with quantum-enhanced feature spaces. *Nature*, 567(7747):209–212, mar 2019.

[7] Yunchao Liu, Srinivasan Arunachalam, and Kristan Temme. A rigorous and robust quantum speed-up in supervised machine learning. *Nature Physics*, 17(9):1013–1017, jul 2021.

[8] Maria Schuld and Nathan Killoran. Quantum machine learning in feature hilbert spaces. *Physical Review Letters*, 122(4), feb 2019.

[9] Iris Cong, Soonwon Choi, and Mikhail D. Lukin. Quantum convolutional neural networks. *Nature Physics*, 15(12):1273–1278, aug 2019.

[10] Tak Hur, Leeseok Kim, and Daniel K. Park. Quantum convolutional neural network for classical data classification. *Quantum Machine Intelligence*, 4(1), feb 2022.

[11] Edward Grant, Marcello Benedetti, Shuxiang Cao, Andrew Hallam, Joshua Lockhart, Vid Stojevic, Andrew G. Green, and Simone Severini. Hierarchical quantum classifiers. *npj Quantum Information*, 4(1), dec 2018.

References on Riemannian Manifold related research:

1. Slavakis Lab: Fast Sequential Clustering in Riemannian Manifolds for Dynamic and Time-Series-Annotated Multilayer Networks
2. Slavakis Lab: Kernel Regression Imputation in Manifolds Via Bi-Linear Modeling: The Dynamic-MRI Case

References on Quantum Machine Learning: Quantum Kernel Methods

1. Maria Schuld: Supervised quantum machine learning models are kernel methods
2. IBM T.J. Watson Research Center: Supervised learning with quantum enhanced feature spaces
3. Yunchao Liu, IBM Quantum: A rigorous and robust quantum speed-up in supervised machine learning
4. Maria Schuld: Quantum machine learning in feature Hilbert spaces
5. Thomas Hubregtsen: Training Quantum Embedding Kernels on Near-Term Quantum Computers
6. Online Python Lib: Qiskit Link
7. Online Python Lib: Pennylane

References on Quantum Machine Learning Application

1. Wen Guan et al: Quantum machine learning in high energy physics
2. Wonho Jang et al: Quantum Gate Pattern Recognition and Circuit Optimization for Scientific Applications
3. Koji Terashi et al:Event Classification with Quantum Machine Learning in High-Energy Physics

References on Quantum Signal Processing: Quantum Fourier Transform

1. Nielson and Chuang: Quantum Computation and Quantum Information
2. Peter Shor: Lecture on Quantum Computing and quantum Fourier transforms
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
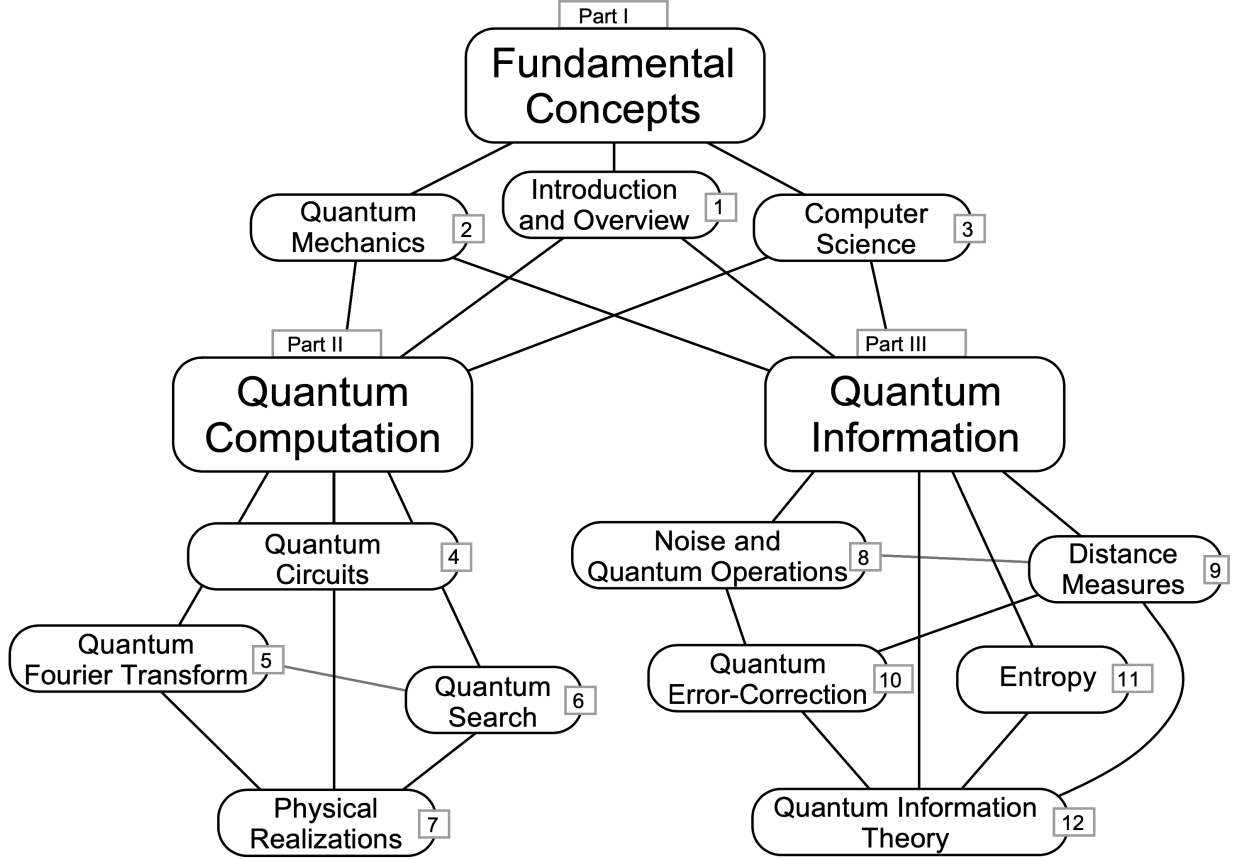
Figure 5: A big picture for the quantum computation and quantum information field in Issac Chuang's book. The proposal here focuses more on quantum circuits and quantum fourier transform study.

Back Up

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

Quantum Gates, Quantum Circuit, and Quantum Computation

Clasical 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:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{13}$$

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

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}, T = \begin{bmatrix} 1 & 0 \\ 0 & exp(i\pi/4) \end{bmatrix} \tag{14}$$

Hadamard gate turns $|0\rangle$ into $(|0\rangle + |1\rangle)/\sqrt{2}$, and $|1\rangle$ into $(|0\rangle - |1\rangle)/\sqrt{2}$, phase gate S and $\pi/8$ gate T have some algebraic relation with H that $H = (X + Z)/\sqrt{2}$ and $S = T^2$. For rotation matrix around X, Y, Z, rotates around x, y, z axes, they are defined by equation:

$$R_\eta(\theta) = e^{-i\theta\eta/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}\eta, \quad \eta \in \{X, Y, Z\}$$

Some important theorem likes Z-Y decomposition for a single qubit exits. Suppose U is a unitary operation on a single qubit. Then there exist real numbers $\alpha, \beta, \gamma, \delta$ such that

$$U = e^{i\alpha} R_z(\beta) R_y(\gamma) R_z(\delta) \tag{15}$$

Controlled Operations

Here are some controlled openeration with CNOT gate. The core idea for controlled operation is "If A is true, then do B". On single qubit, in terms of the computational basis, the action of the CNOT is given by $|c\rangle |t\rangle \rightarrow |c\rangle |t \oplus c\rangle$, which means that the control qubit is set to $|1\rangle$ then the target qubit is flipped, otherwise the target qubit is left alone. Thus, in the computational basis $|control, target\rangle$ the matrix representation of CNOT is:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{16}$$

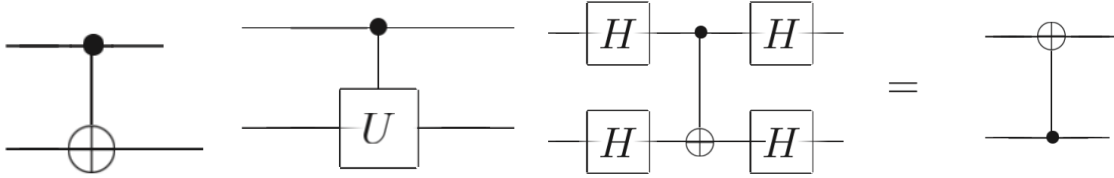which could also replace by *controlled-U* operation.

Figure 6: Some circuit representation of control operation

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 $n = [log_2(N)]$ and $|x\rangle = \sum_i^N x_i |i\rangle$ and $|i\rangle$ is the computational basisi 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:

$$|x\rangle = \bigotimes_i^n R(x_i) |0^n\rangle \tag{17}$$

R can be one of the rotation gate R_x, R_y, and R_z. Usually, the number of qubits used for enoding 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 $|x\rangle = Ry(\pi)|0\rangle \, Ry(\pi)|0\rangle \, Ry(\pi)|0\rangle$, which indicates the result is $|111\rangle$.

IQP Style Encoding

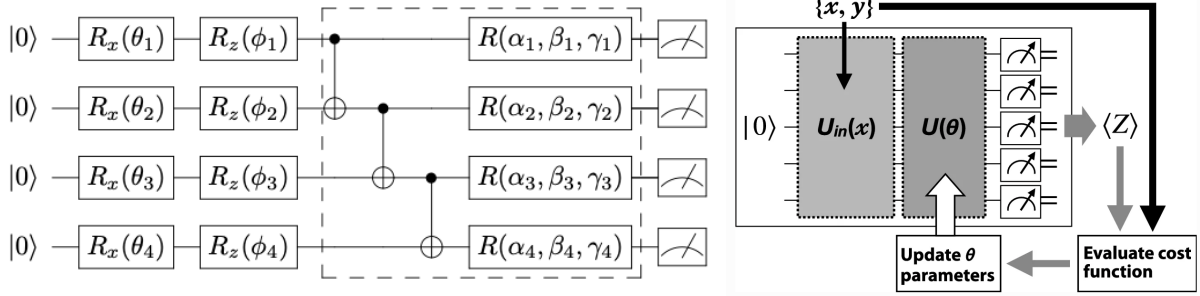**Hamiltonian Evolution Ansatz Encoding**

Quantum Classifier

Figure 7: The generic variational quantum circuit architecture and procedure for optimization. The inputs go through encoding, the unitary matrices, measurement, lost function evelution and then update parameters.

The lost function could be the simplest one:

$$L(\theta) = \sum_{k=1}^{N} \frac{1}{N} |\tilde{y}^k - y^k|^2 \tag{18}$$

Quantum Fourier Transform Phase Estimation

Suppose a unitary operator U has an eigenvalue $|u\rangle$ with eigenvalue $e^{2\pi i \varphi}$, where the value of φ is unknown. The goal of the phase estimation algorithm is to estimate φ.
Inputs: (1) A black box which performs a controlled-U^j operation, for integer j. (2) an eigenstate $|u\rangle$ of U with eigenvalue $e^{2\pi i \varphi}$, and (3) $t = n + [log(2 + \frac{1}{2\epsilon})]$ qubits initialized to $|0\rangle$
Outputs: An n-bit approximation $\tilde{\varphi}_u$ to φ_u
Runtime: $O(t^2)$ operations and one call to controlled-U^j black box. Succeeds with probability at least $1 - \epsilon$.
Procedure:

1. $|0\rangle |u\rangle$ initial state
2. $\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle |u\rangle$ create superposition
3. $\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle U^j |u\rangle$ apply black box
4. $= \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} e^{2\pi i j \varphi_u} |j\rangle |u\rangle$ result of black box
5. $\rightarrow |\tilde{\varphi}_u\rangle |u\rangle$
6. $\rightarrow \tilde{\varphi}_u$

Quantum Fourier Transform Shor's Algorithm

References

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