

Frequency-Domain Analysis of Quantum Neural Networks: From Output Approximation to Interpretability Insights

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Outline

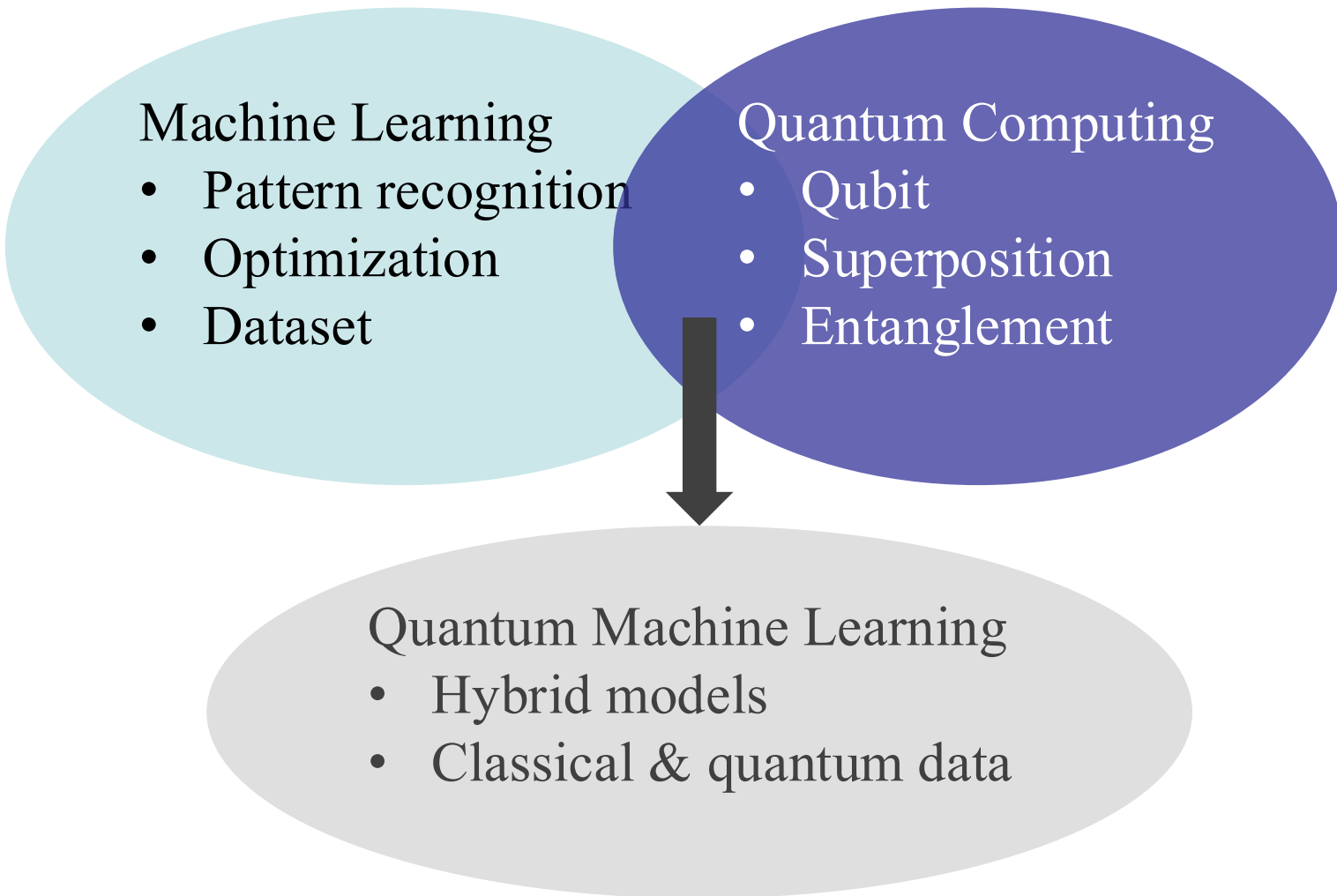
- Background and motivation
- Fourier representation for Quantum Neural Networks
- Recent research and key findings
- Future work

Background & Motivation

Quantum Machine Learning

Quantum Neural Networks and interpretability

Quantum Machine Learning (QML)



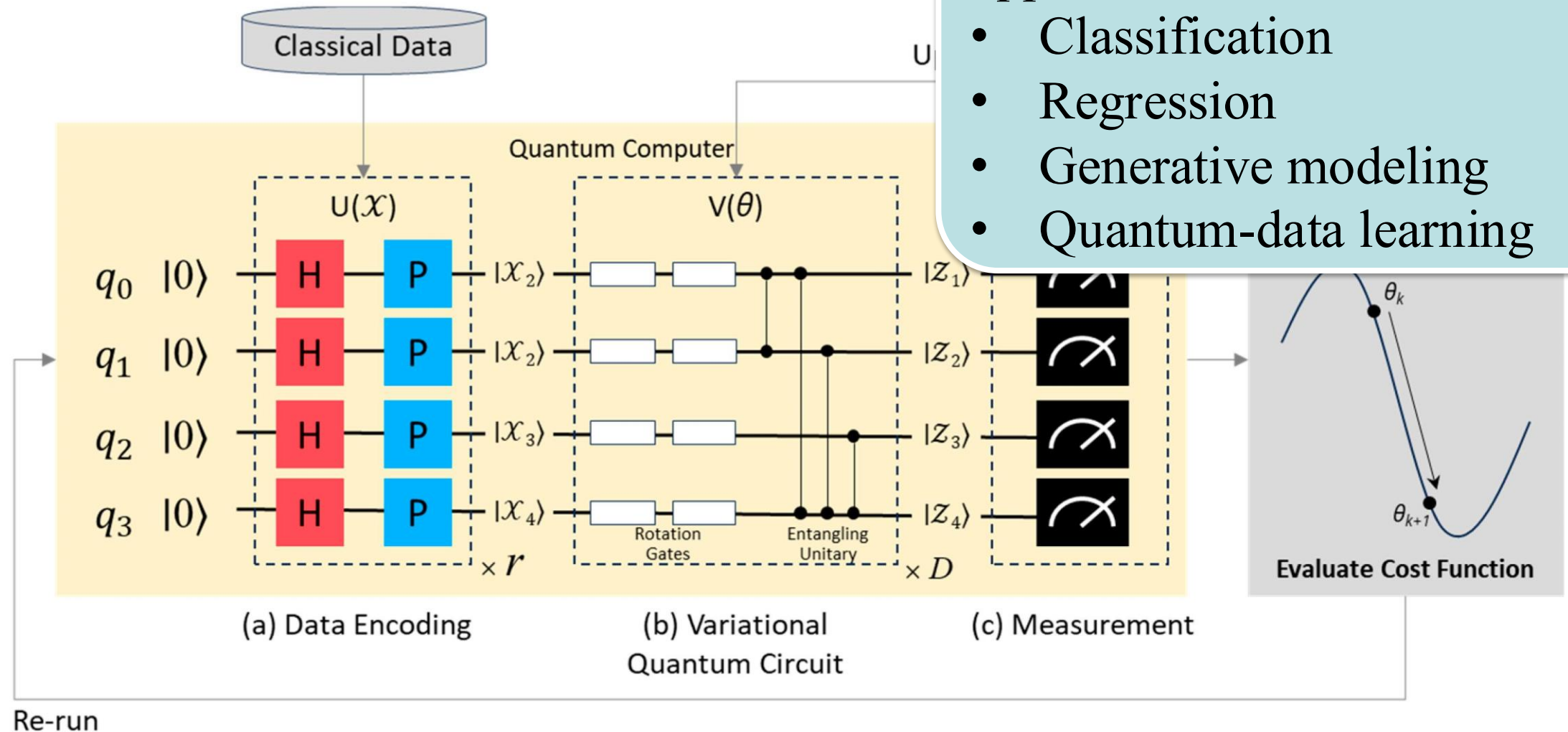
Quantum advantages

- High-dimensional feature space
- Parallel computation
- Quantum-data learning

Proposed algorithms

- Quantum Support Vector Machine
- Quantum Kernel Method
- Quantum Neural Network
- ...

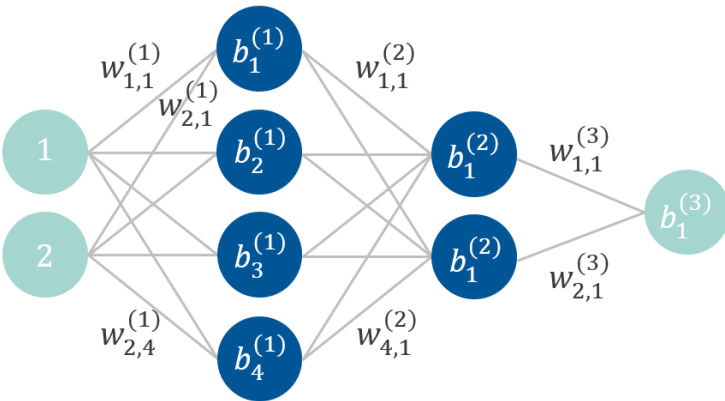
Quantum Neural Network (QNN)



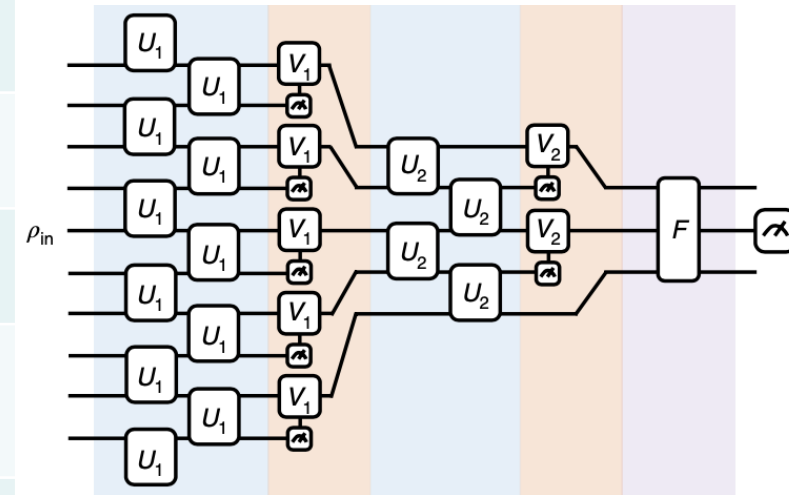
Applications

- Classification
- Regression
- Generative modeling
- Quantum-data learning

QNN vs. DNN



DNN	QNN
Neurons	Qubits
Weights	Gate parameters
Layers	Circuit layers
Forward propagation	State evolution
Network output	Measurement



Directly accessible

- DNN

$$x \rightarrow h^{(1)} \rightarrow h^{(2)} \rightarrow \dots \rightarrow y$$

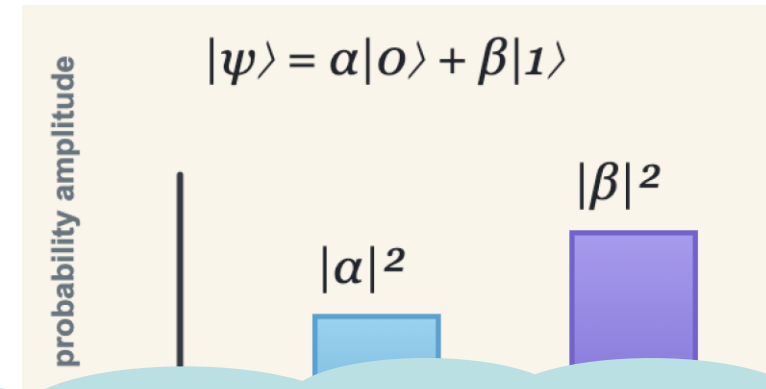
- QNN

$$|0\rangle \rightarrow |\psi_1\rangle \rightarrow \dots \rightarrow |\psi_L\rangle = |\psi(x, \theta)\rangle \xrightarrow{\text{Measurement } O} f_\theta(x)$$

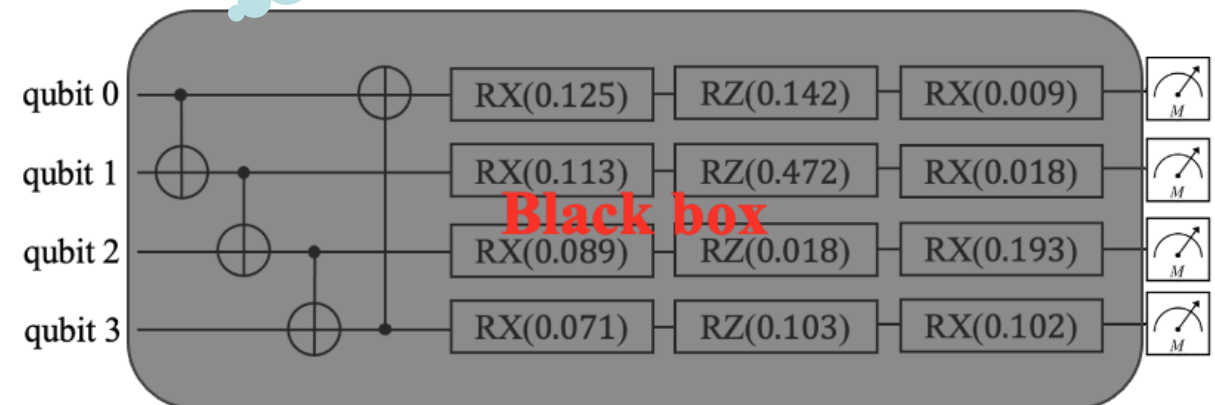
Quantum state collapse
Inaccessible

Challenge: QNN interpretability

- Limited observability
 - Inaccessible quantum states
 - Partial information by measurement
- Complicated quantum nature
 - Superposition
 - Entanglement
- Stochastic factors
 - Finite shots
 - Noise



How can we understand what function a QNN has learned?



Fourier Representation for QNNs

Frequency, spectrum and coefficients

A Possible View: Fourier Representation

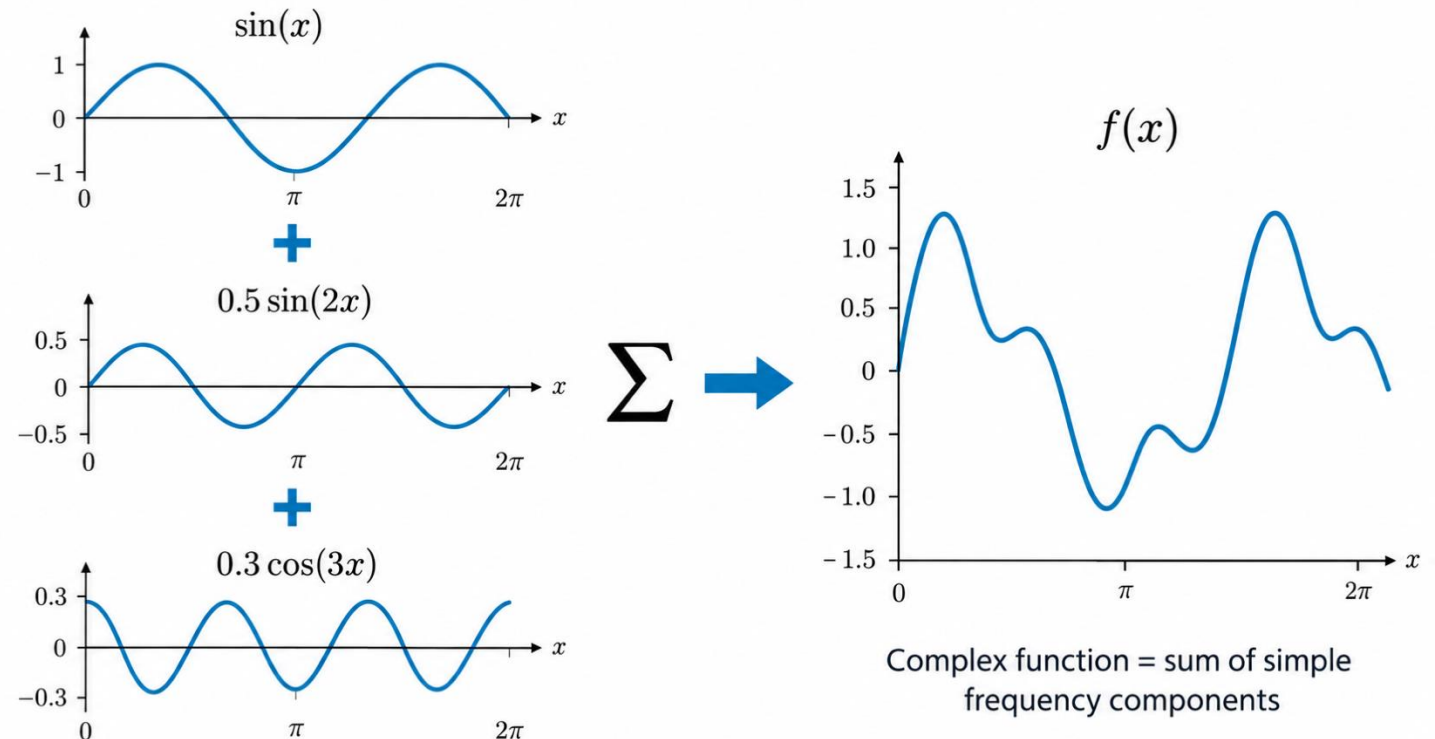
- 1-D Partial Fourier series
 - Trigonometric form

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(nx) + b_n \sin(nx)]$$

Exponential form

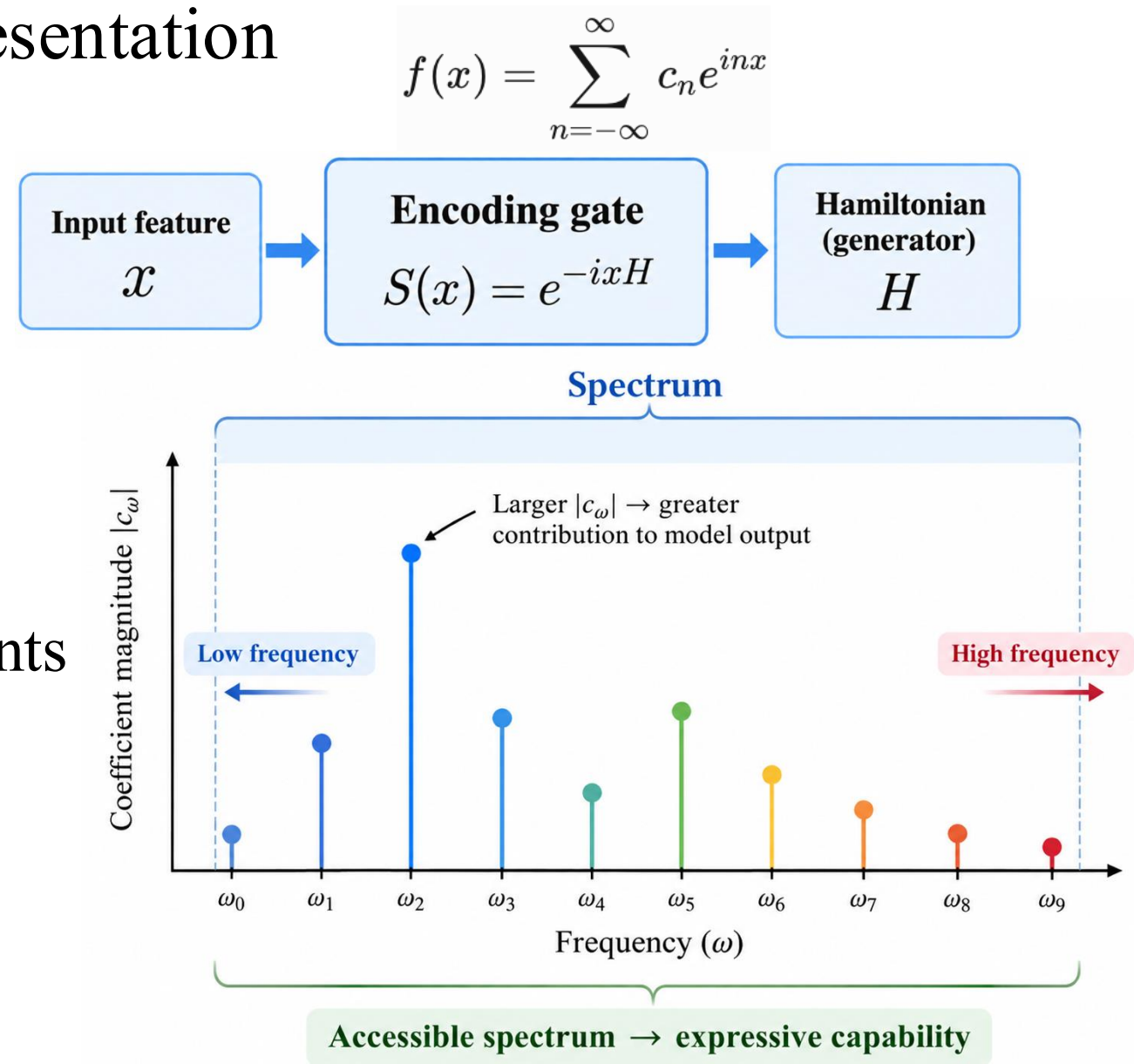
$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx}$$

A complex function: multiple simple frequency components



A Possible View: Fourier Representation

- Motivation
 - Data-encoding gates
 - Hamiltonian evolutions
- Meaning
 - Frequency ω
what pattern the model represents
 - Frequency Spectrum Ω
how rich the function space is
 - Coefficient $c_\omega(\theta)$
contribution to the function



Fourier representation

- Mathematical form for QNNs

$$S(x) = e^{-ixH} = \sum_j e^{-i\lambda_j x} |j\rangle\langle j|$$

$$f_{\theta}(x) = \langle 0|U^{\dagger}(x, \theta)MU(x, \theta)|0\rangle$$

- Frequency

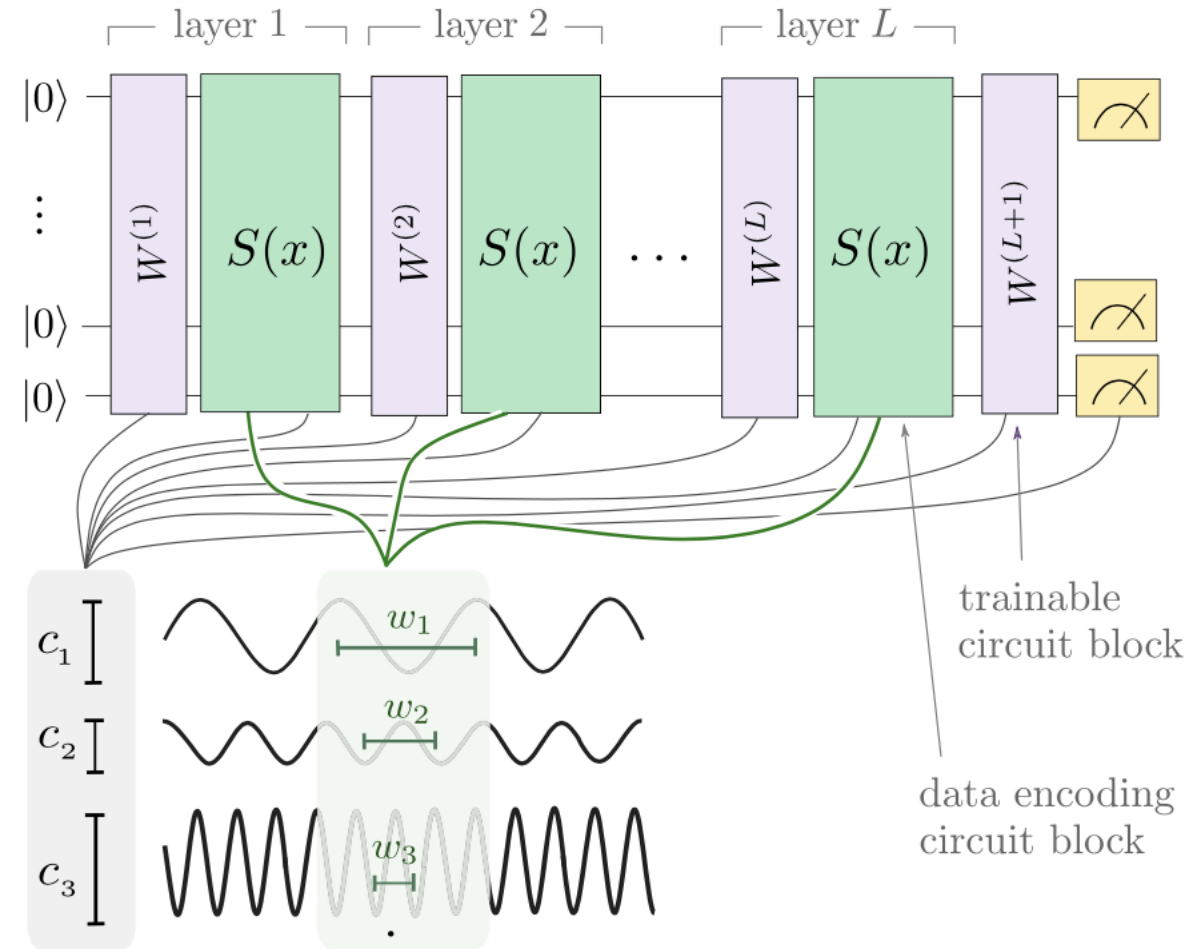
$$\Lambda_j = \lambda_{j_1} + \lambda_{j_2} + \dots + \lambda_{j_L}$$

Measurement process

$$\Omega = \{\Lambda_k - \Lambda_j\}$$

Spectrum comes from encoding. [1]

Data Re-uploading Structure



Fourier representation

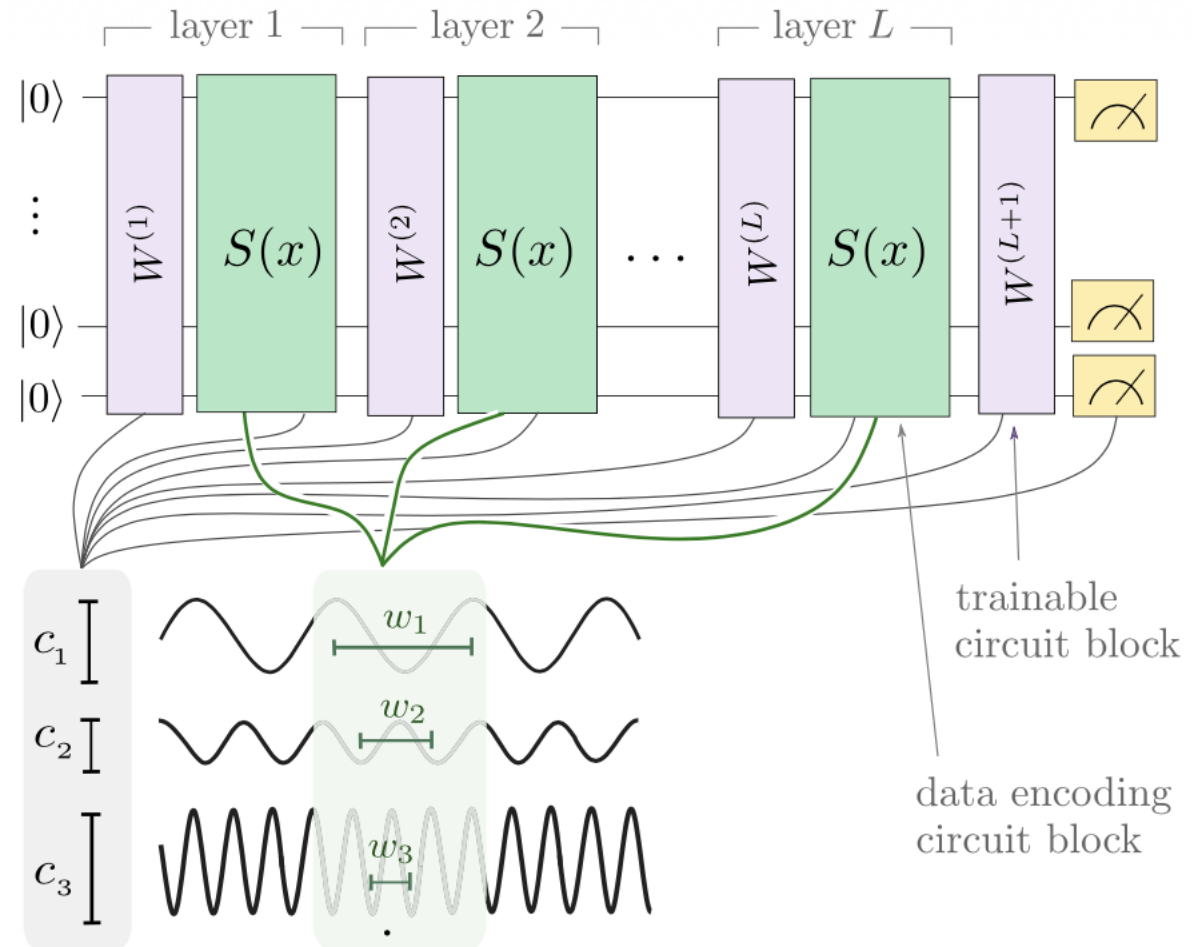
- Coefficients

$$a_{k,j} = \sum_{i,i'} W_{1k_1}^{*(1)} W_{j_1 j_2}^{*(2)} \dots W_{j_L i}^{*(L+1)} M_{i,i'} \\ \times W_{i' j_L}^{(L+1)} \dots W_{j_2 j_1}^{(2)} W_{j_1 1}^{(1)}.$$

- Final function

$$c_\omega = \sum_{\substack{k,j \in [d]^L \\ \Lambda_k - \Lambda_j = \omega}} a_{k,j}.$$

$$f_\theta(x) = \sum_{\omega \in \Omega} c_\omega(\theta) e^{i\omega x}$$



Coefficients come from trainable parts. [1]

Related Research

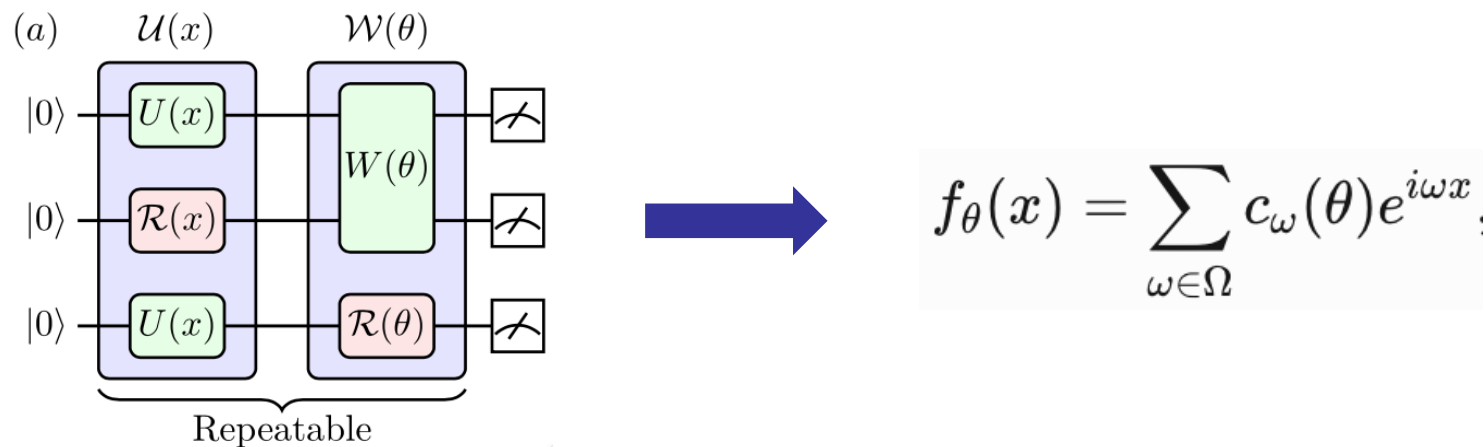
Research focus and key findings

Research Focus of Related Work

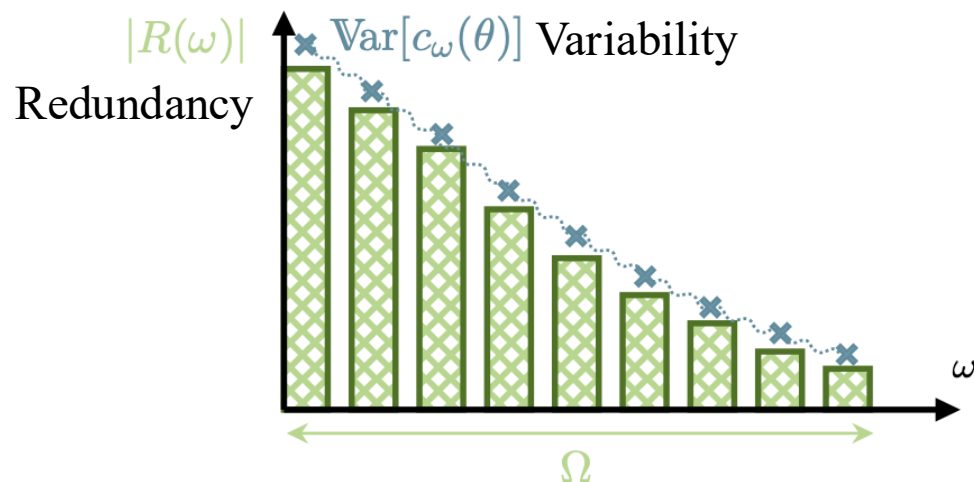
- **Expressivity**
What Fourier series can QNNs represent?
- **Trainability**
Which Fourier components are easier to learn?
- **Dequantization**
Can QNNs be classically approximated?
- **Architecture design**
Can spectral information guide QNN design?

Expressivity: What Fourier Series Can a QNN Represent?

Finding 1: Encoding defines the candidate spectrum



Finding 2: Frequency redundancies constrain coefficients

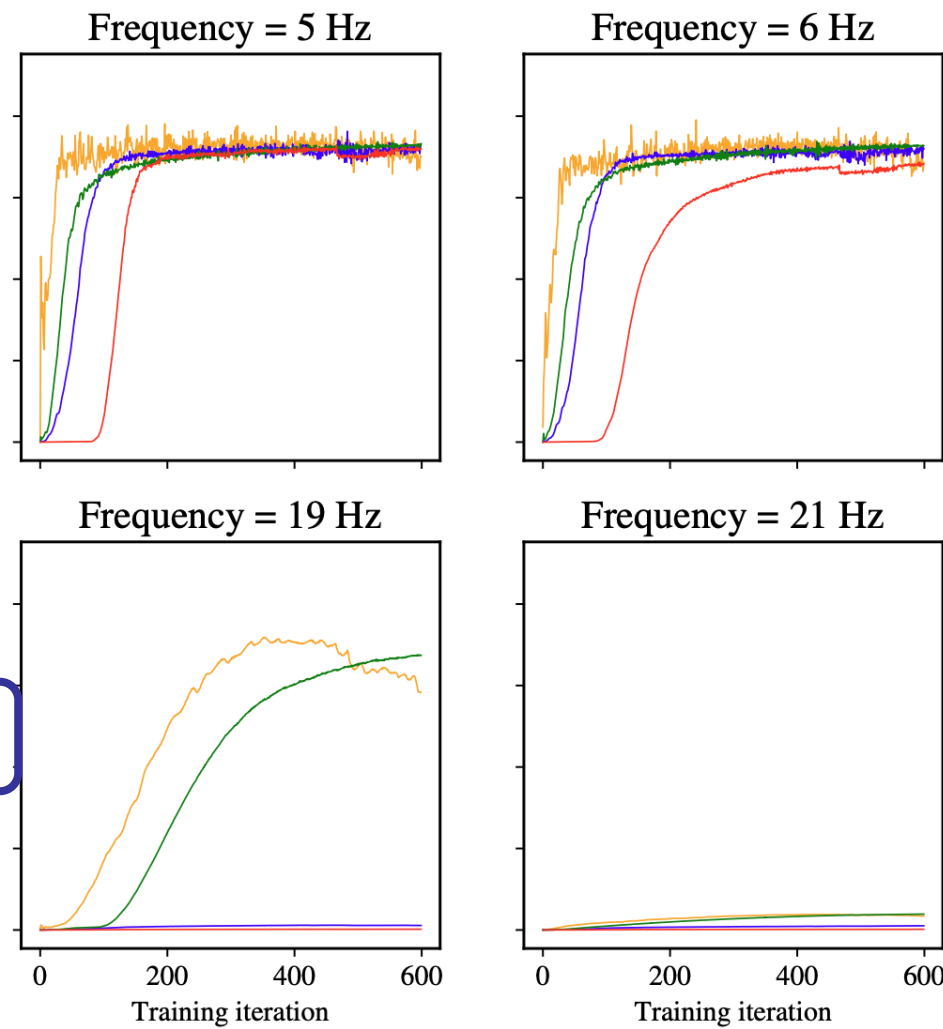


Higher frequency redundancy allows greater coefficient variability.

Expressivity: What Fourier Series Can a QNN Represent?

Finding 3: Frequency order also constrains coefficients

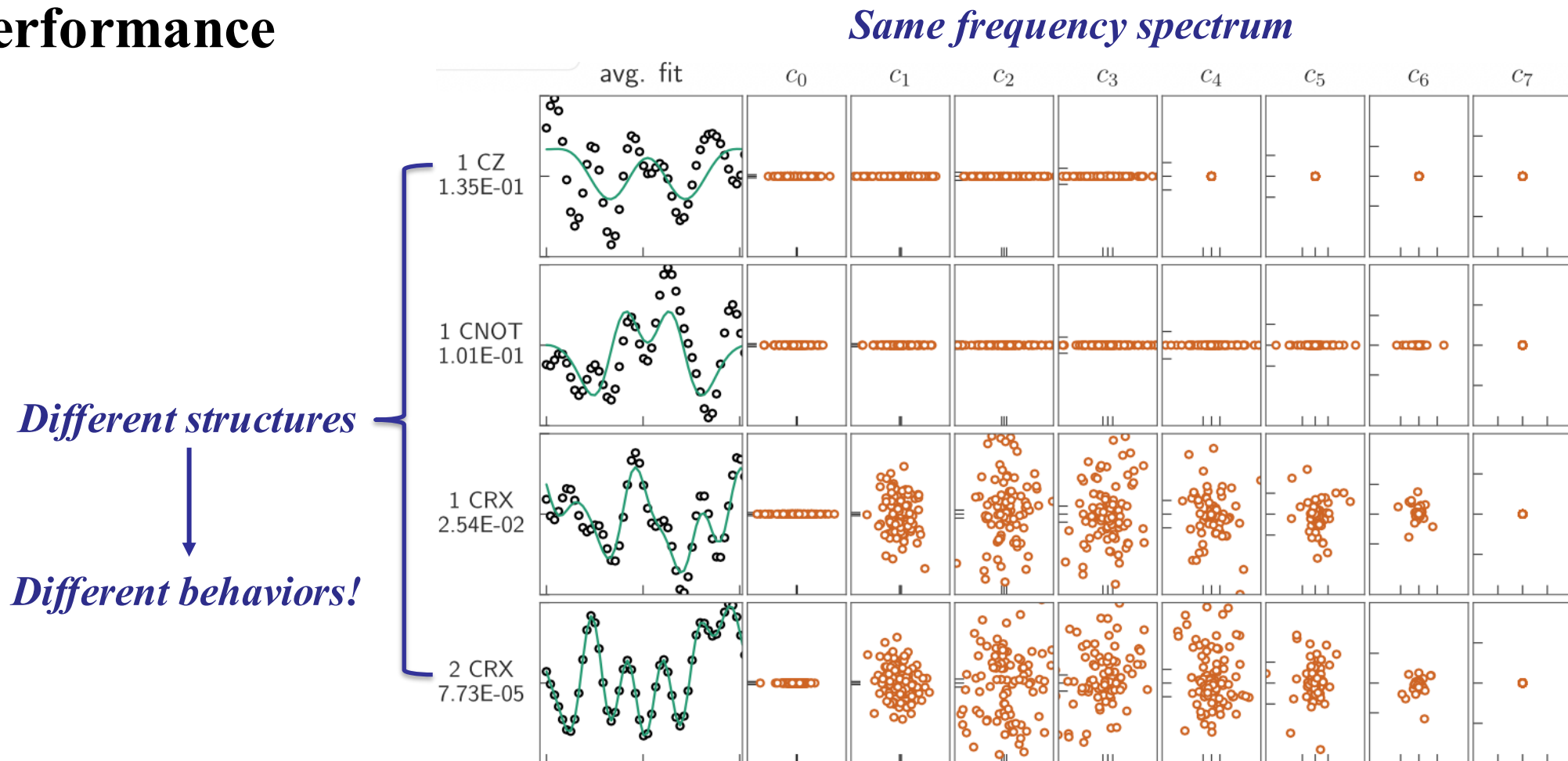
$$\text{Var}_{\theta}(c_{\omega}(\theta)) \leq O\left(\alpha \frac{|\tilde{R}(\omega)|}{2^n}\right) \leq O(\exp(-\|\omega\|_1))$$



Theoretical accessibility $\neq$ Practical accessibility

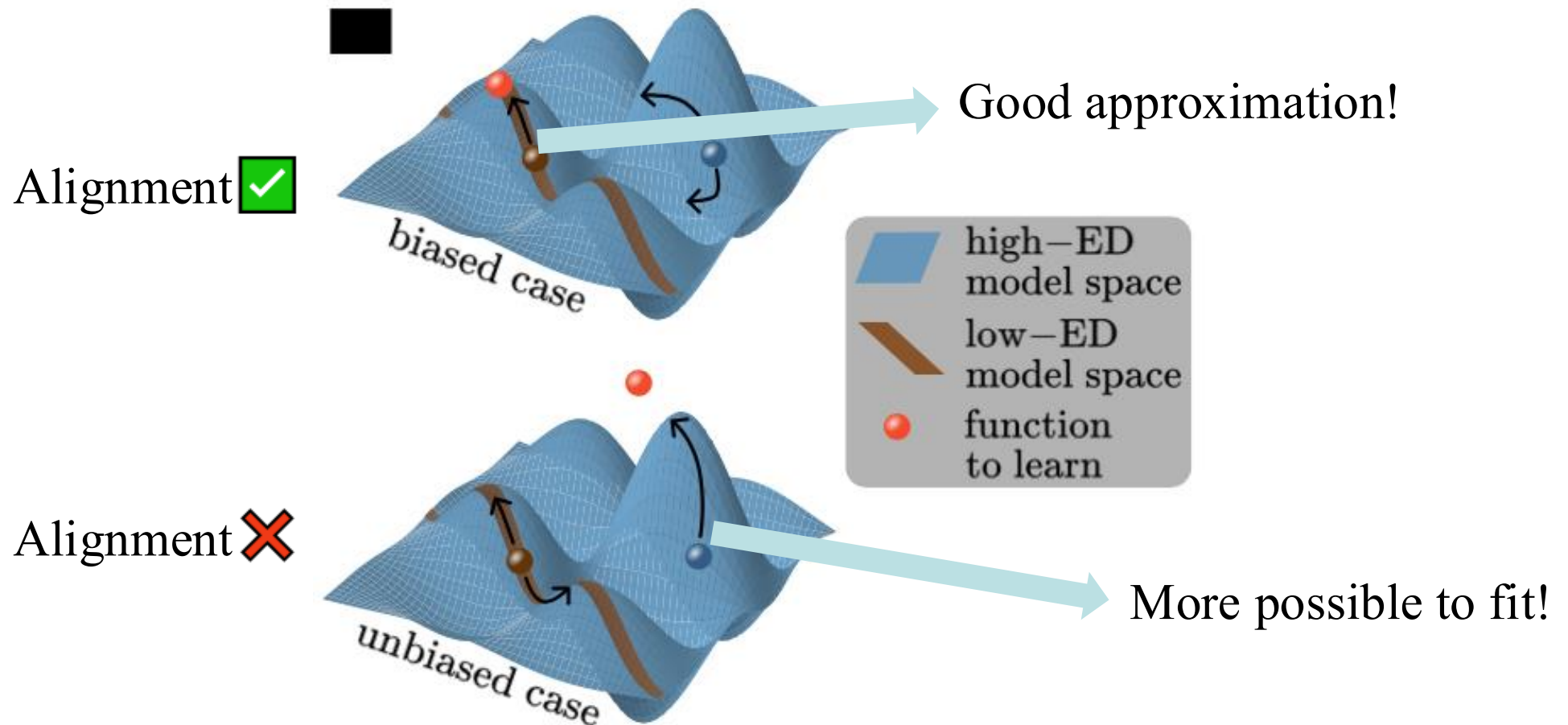
Trainability: Which Fourier Components Are Easier to Learn?

Finding 1: QNNs with same spectrum can have different training performance



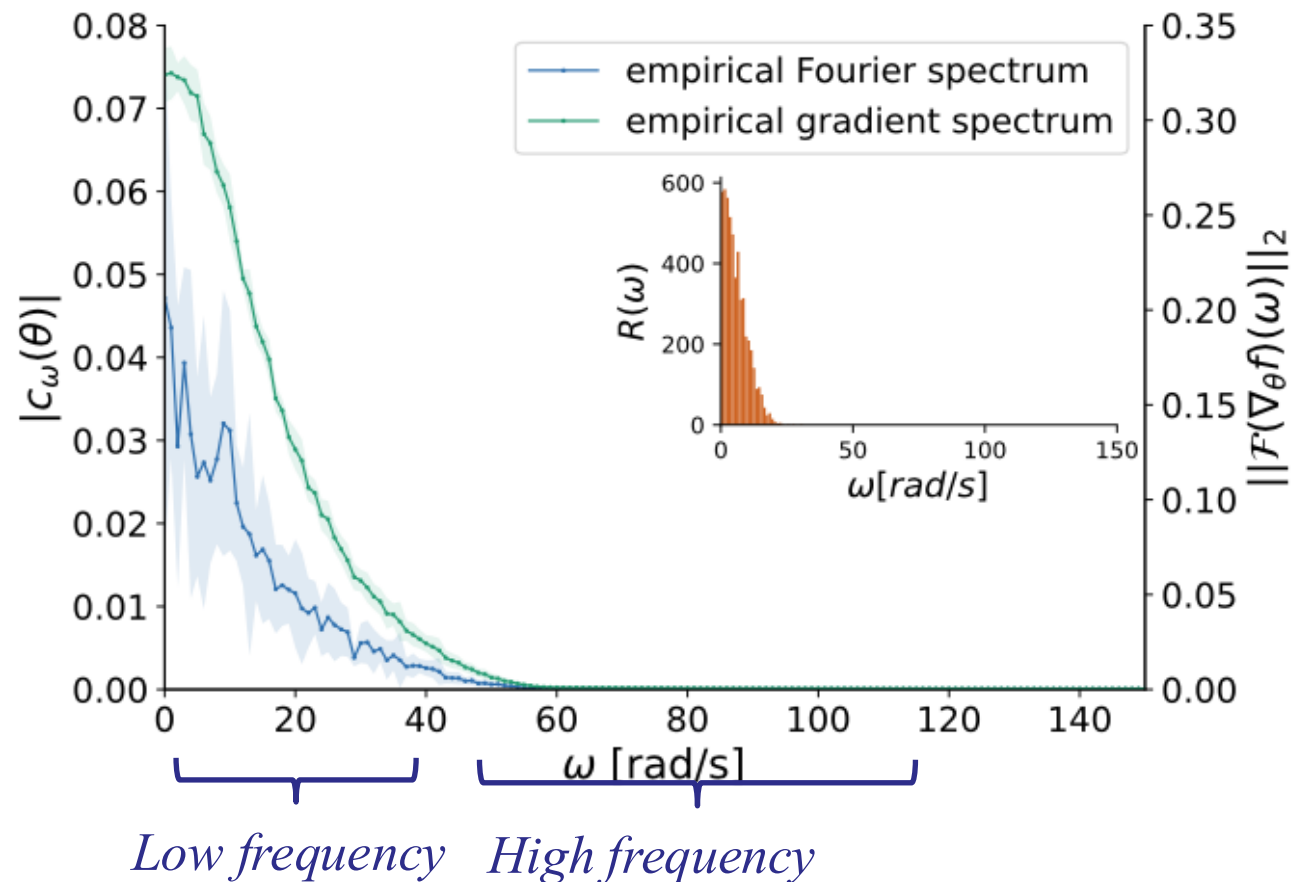
Trainability: Which Fourier Components Are Easier to Learn?

Finding 2: Model-task alignment matters



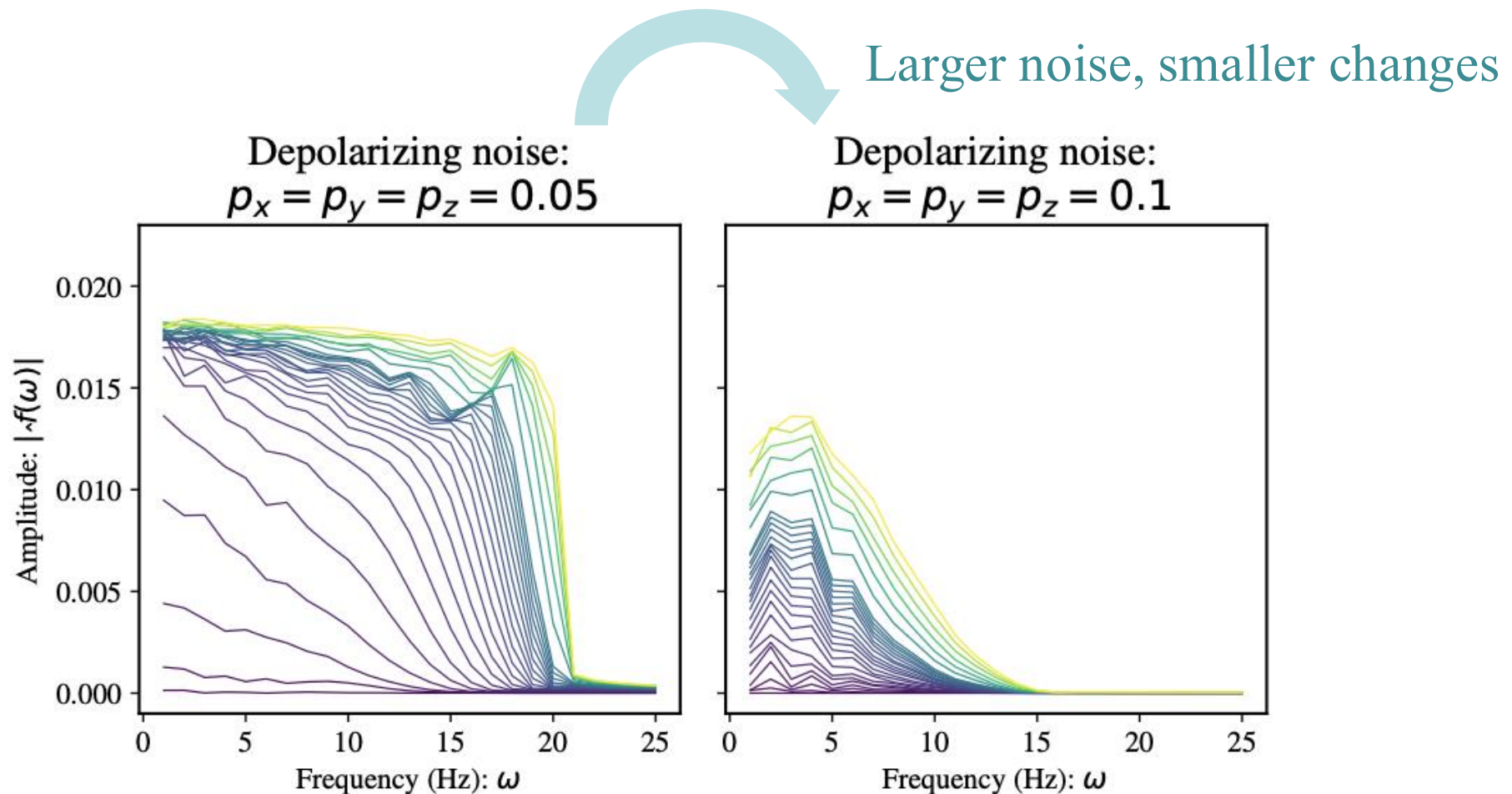
Trainability: Which Fourier Components Are Easier to Learn?

Finding 3: QNNs show spectral bias Lower frequency converges faster.



Trainability: Which Fourier Components Are Easier to Learn?

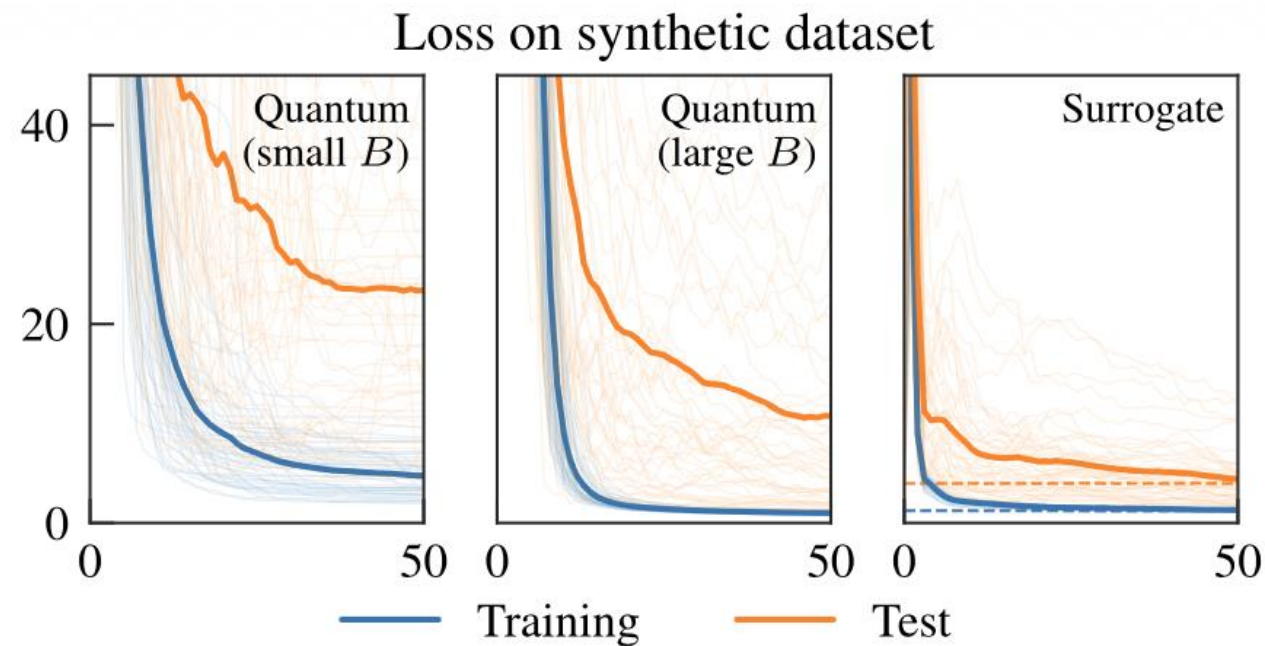
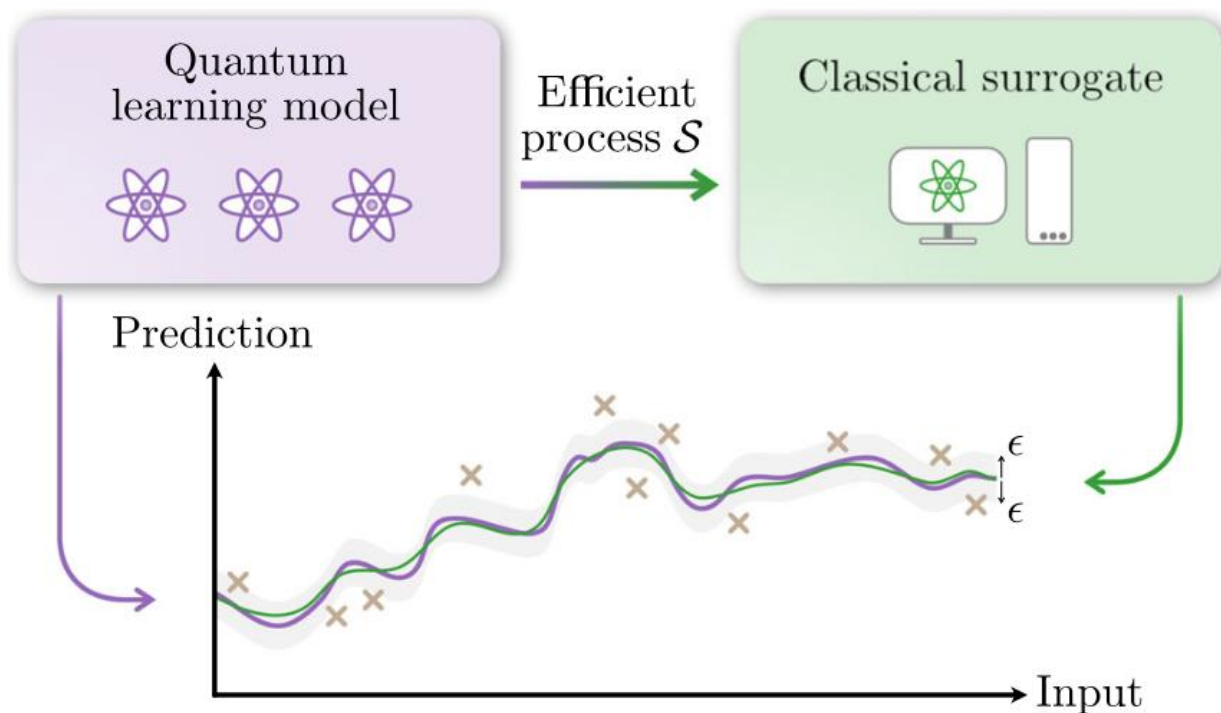
Finding 4: Noise suppresses high frequency



Dequantization: Can QNN Be Approximated Classically?

***Finding 1:* QNNs can be approximated by a fast
Random Fourier Features**

Quantum advantage?
High-dimensional space?

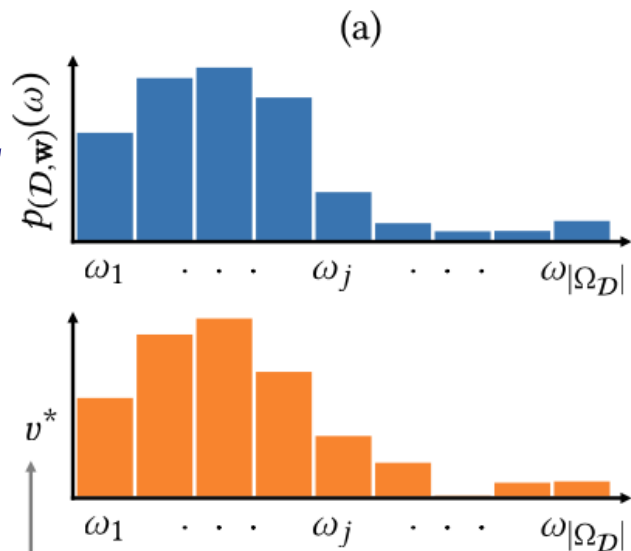


Dequantization: Can QNN Be Approximated Classically?

Finding 2: Alignment and concentration are necessary for efficient approximation

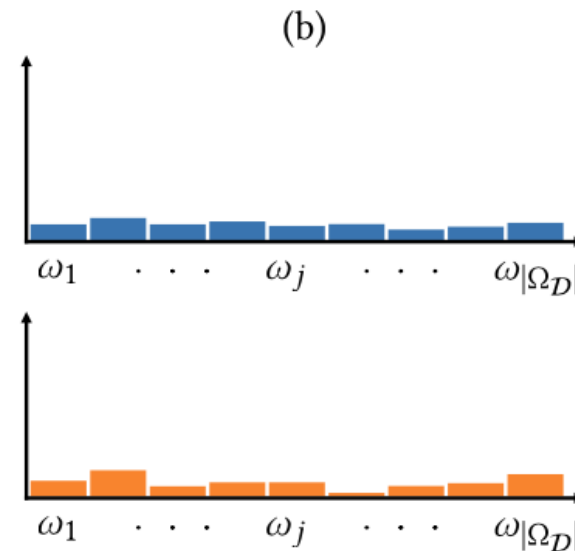
Sampling from QNNs

Target function



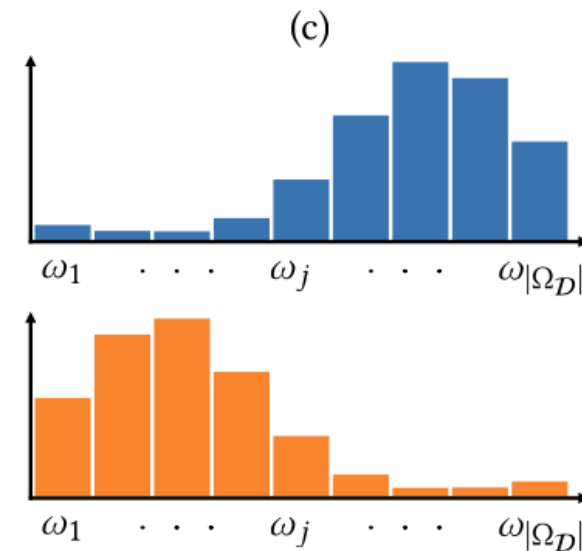
f^* sufficiently concentrated ✓
 f^* and $\mathbf{w}$ sufficiently aligned ✓

RFF dequantization is efficient
 (Assuming efficient sampling from ω)



f^* not sufficiently concentrated ✗
 f^* and $\mathbf{w}$ sufficiently aligned ✓

RFF dequantization is not efficient



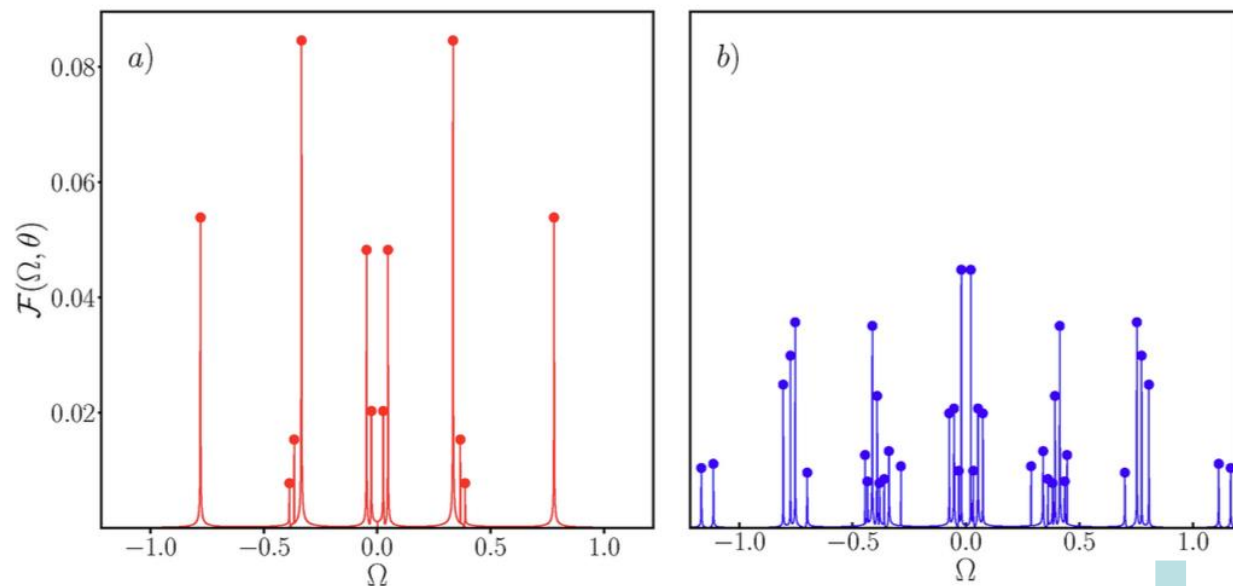
f^* sufficiently concentrated ✓
 f^* and $\mathbf{w}$ not sufficiently aligned ✗

RFF dequantization is not efficient

Architecture Design: Can Spectral Information Guide QNN Design?

Finding 1: More entanglement and global measurement benefit

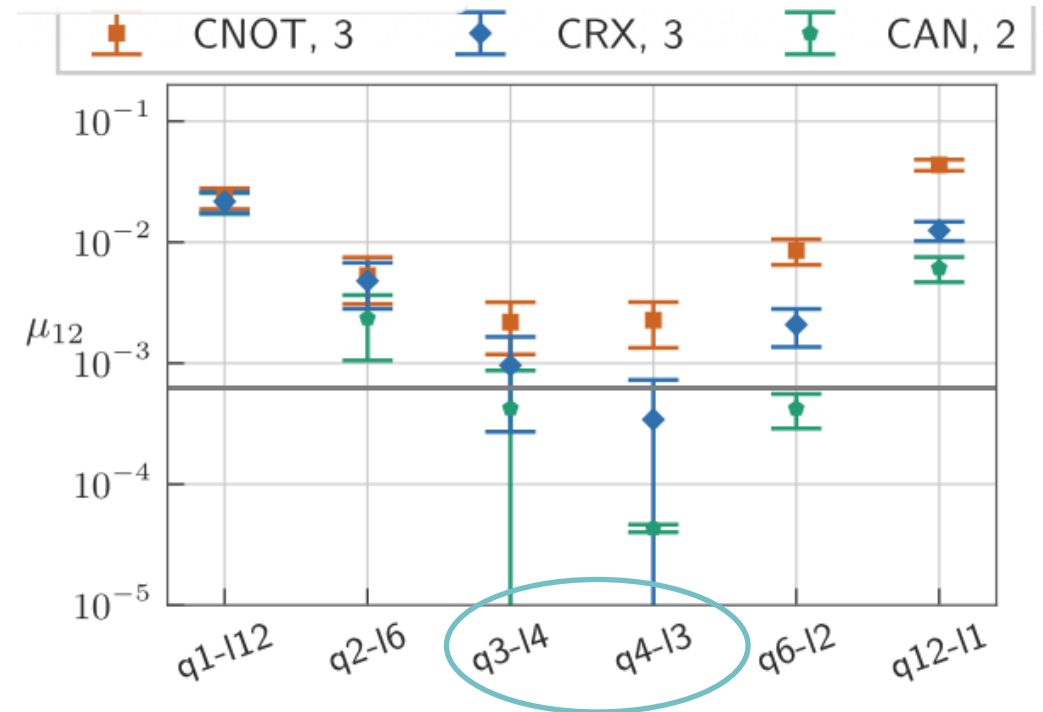
Finding 2: Balance width, depth and entanglement layers



Without entanglement

With entanglement

More frequencies with non-0 coefficients!



Width 3+Depth 4 > Width 1+Depth 12

What is Still Missing

- They have answered
 - What a QNN can represent
 - Which ansatz may be better
 - Whether it can be classically approximated
- However...
 - What is the actual spectrum used by a trained QNN in real-world tasks?
 - Which frequencies are important to the function and spectral energy?
 - How can Fourier information explain the behaviors of original circuit?

Future Work

Direction and possible problems

General Plan: Explain trained QNNs from a Fourier View

- Research target
 - A random target function  A trained QNN
 - Real-world task: image classification
- Problem
 - How to obtain exact Fourier frequencies and coefficients?
 - Which frequencies are important?
 - How can Fourier representation explain the model behaviors?

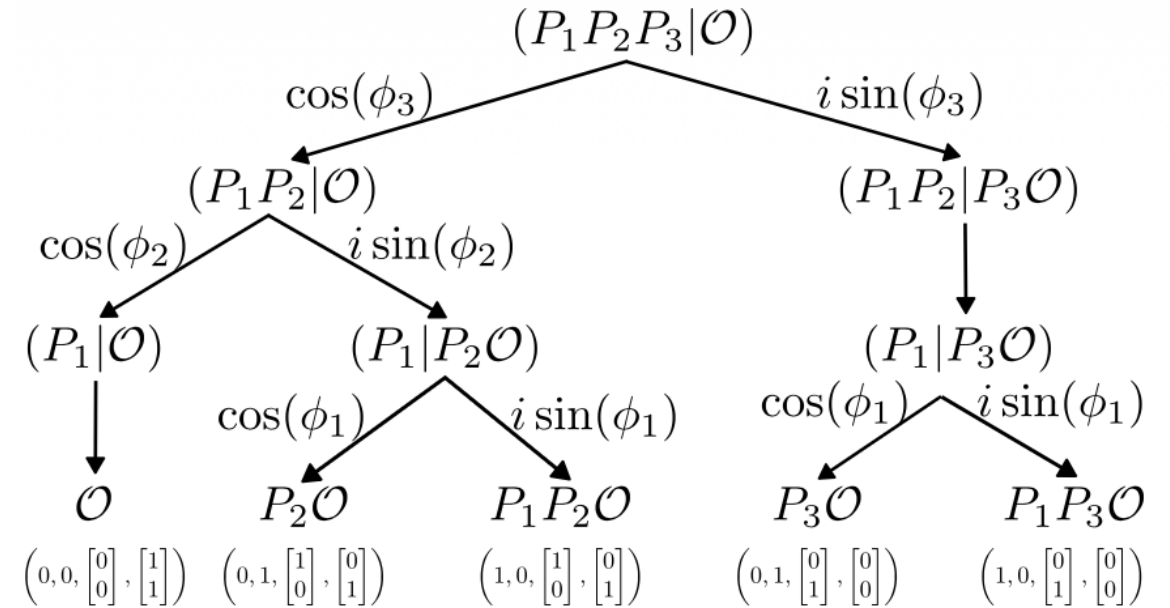
Trained QNN $\rightarrow$ Fourier analysis $\rightarrow$ Behavior explanation

How to Obtain Exact Spectrum for Trained QNNs?

- Build binary tree [1]
 - Generate nodes gate by gate
 - Merge branches
 - Compute coefficients

Scalability

- More qubits, more gates
- Exponential increase of nodes



$$\begin{aligned}
 \langle \mathcal{O} \rangle = & \cos(\phi_3) \cos(\phi_2) \langle 0 |^{\otimes n} \mathcal{O} | 0 \rangle^{\otimes n} \\
 & + i \cos(\phi_3) \sin(\phi_2) \cos(\phi_1) \langle 0 |^{\otimes n} P_2 \mathcal{O} | 0 \rangle^{\otimes n} \\
 & - \cos(\phi_3) \sin(\phi_2) \sin(\phi_1) \langle 0 |^{\otimes n} P_1 P_2 \mathcal{O} | 0 \rangle^{\otimes n} \\
 & + i \sin(\phi_3) \cos(\phi_1) \langle 0 |^{\otimes n} P_3 \mathcal{O} | 0 \rangle^{\otimes n} \\
 & - \sin(\phi_3) \sin(\phi_1) \langle 0 |^{\otimes n} P_1 P_3 \mathcal{O} | 0 \rangle^{\otimes n}
 \end{aligned}$$

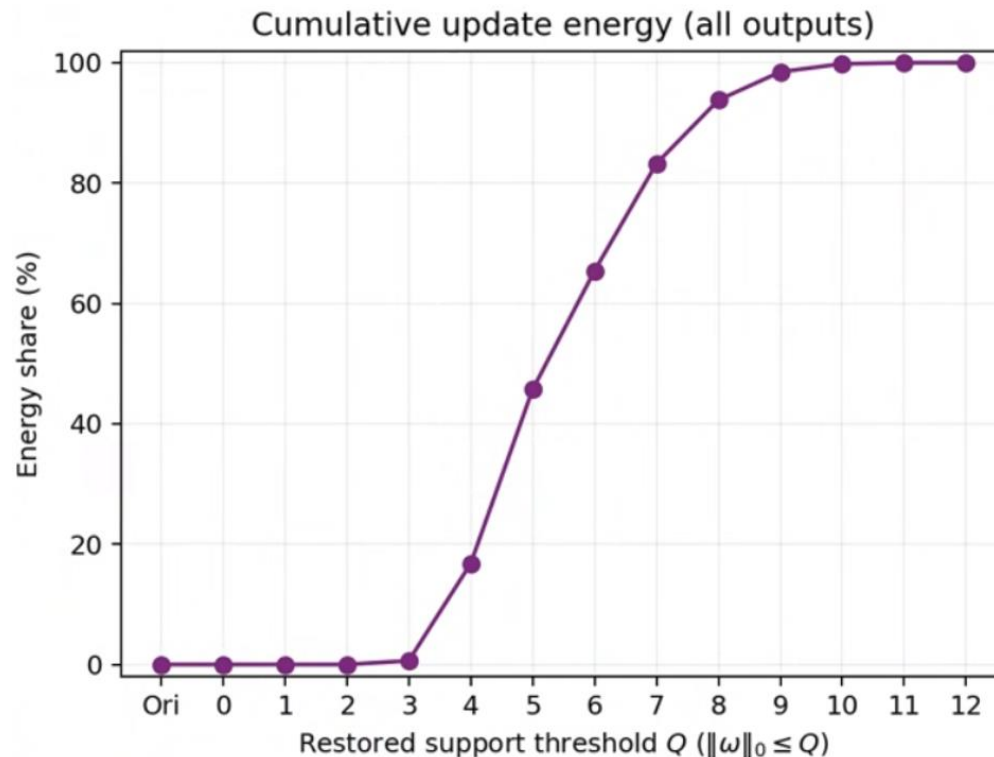
Which Frequencies are Important?

- Order $q(\omega) = \|\omega\|_0 = \sum_{j=1}^d \mathbb{I}(\omega_j \neq 0)$

- Current finding:

Low-order frequencies: smooth features

High-order frequencies: sharp features



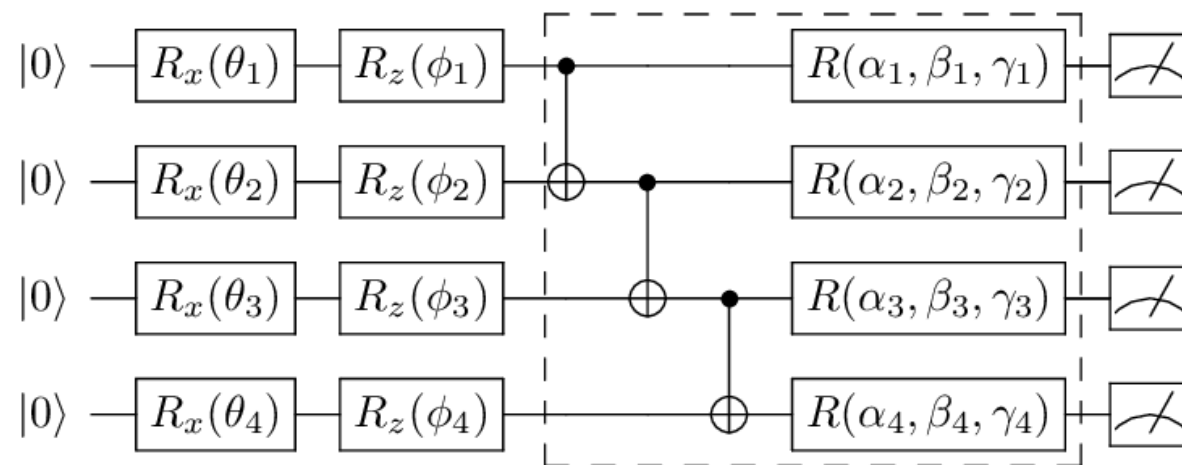
How much does each frequency order contribute to the function?

Low order contributes more?
High order contributes less?

What is Connection between Fourier Representation and Gates

- Gap between Fourier form and circuit structure

$$f_{\theta}(x) = \sum_{\omega \in \Omega} c_{\omega}(\theta) e^{i\omega x}$$



Which gates can affect the Fourier function?



Which gates can affect the model behaviors more significantly?

Fault Localization?

Thank you for your listening



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