Spectral Invariance and Maximality Properties of the Frequency Spectrum of Quantum Neural Networks

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Abstract

Quantum Neural Networks (QNNs) are a popular approach in Quantum Machine Learning. We analyze this frequency spectrum using the Minkowski sum for sets and the set of differences, which makes it particularly easy to express and calculate the frequency spectrum algebraically, and prove different maximality results for a large class of models. Furthermore, we prove that under some mild conditions there exists a bijection between classes of models with the same area $A := R \cdot L$ that preserves the frequency spectrum, where R denotes the number of qubits and L the number of layers, which we consequently call spectral invariance under area-preserving transformations. With this we explain the symmetry in R and L in the results often observed in the literature and show that the maximal frequency spectrum depends only on the area A = RL and not on the individual values of R and L. Moreover, we collect and extend existing results and specify the maximum possible frequency spectrum of a QNN with arbitrarily many layers as a function of the spectrum of its generators. In the case of arbitrary dimensional generators, where our two introduces notions of maximality differ, we extend existing results based on the so-called Golomb ruler and introduce a second novel approach based on a variation of the turnpike problem, which we call the relaxed turnpike problem.

Keywords: Quantum Computing, Quantum Neural Networks, Frequency Spectrum, Spectral Invariance

1 Introduction

A frequently studied approach to Quantum Machine Learning (QML), a field combining quantum computing and classical Machine Learning (ML), is based on Variational Quantum Algorithms (VQAs) [1-3]. VQAs are hybrid algorithms that use parameterised quantum circuits (PQCs) to build a target function. PQCs are quantum circuits $U(\boldsymbol{\theta})$ dependent on some real parameters $\boldsymbol{\theta} \in \mathbb{R}^P$. While the evaluation of the target function is done on quantum hardware, the training or optimisation of the parameters θ is done on classical hardware. VQAs are considered as a promising candidate for practical applications on Noisy Intermediate-Scale Quantum (NISQ) computers [2, 4, 5]. Different types of architectures or ansätze for PQCs have been proposed, like the Quantum Alternating Operator Ansatz (QAOA) [6], Variational Quantum Eigensolver (VQE) [7, 8], Quantum Neurons [9] and Quantum Neural Networks (QNNs), which appear under different names in the literature [10-16]. There are also variations and extension of the QNN ansatz like Dissipative Quantum Neural Networks (dQNNs) [17–19] or Hybrid Classical-Quantum Neural Networks (HQNNs) [13, 20, 21]. More hardware near approaches [22] or higher dimensional qubits (qudits) are also investigated [23]. Additionally, there is no standardized definition in the literature for a QNN, similar to classical neural networks. Therefore, there are slight variations in the approaches used. The application of PQCs and QNNs in finance [24–26], medicine [27, 28], chemistry [29] and other domains has also been investigated.

Following [9, 10, 30], this work focuses solely on pure QNNs. A QNN is a function of the form

$$f_{\theta}(\mathbf{x}) = \langle 0|U^{\dagger}(\mathbf{x}, \boldsymbol{\theta})MU(\mathbf{x}, \boldsymbol{\theta})|0\rangle$$
 (1)

for some observable M, $x \in \mathbb{R}^N$ and parameter $\theta \in \mathbb{R}^P$, where the parameterised quantum circuit $U(x,\theta)$ consists of embedding layers of a certain form. The dimension of the underlying Hilbert space is denoted by $d := 2^R$, where the number of qubits is denoted by R. If N = 1, then $x \in \mathbb{R}$ and $f : \mathbb{R} \to \mathbb{R}$ is a real valued univariate function. In this case, each layer consists of a data encoding circuit of the form $S_l(x) = e^{-ixH_l}$ for some Hamiltonian H_l called generator, and a trainable parameter encoding circuit $W_{\theta}^{(l)}$. Concretely, the parameterised quantum circuit takes the form

$$U(x, \boldsymbol{\theta}) = W_{\boldsymbol{\theta}}^{(L+1)} \underbrace{S_L(x) W_{\boldsymbol{\theta}}^{(L)}}_{\text{Layer } L} \cdots W_{\boldsymbol{\theta}}^{(2)} \underbrace{S_1(x) W_{\boldsymbol{\theta}}^{(1)}}_{\text{Layer } 1}$$
(2)

The reuse of the input x is called data re-uploading or input redundancy and has been shown to be necessary to increase the expressiveness of the model [9, 20, 31].

The univariate model can be extended to a multivariate model with $x \in \mathbb{R}^N$ for N > 1 in multiple ways, we present two typically used approaches called sequential and parallel ansatz. In the sequential ansatz, there is a parametrized quantum circuit $U_n(x_n, \boldsymbol{\theta})$ for each univariate variable x_n . The full parameterised circuit is then defined

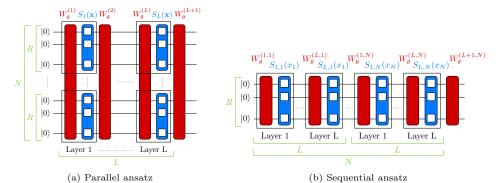


Fig. 1 Circuits of the parallel and the sequential ansatz. R is the number of qubits, L the number of layers per variable x_n and N is the dimension of $x \in \mathbb{R}^N$. The parameter encoding layers are coloured red, the data encoding layers are coloured blue. The data encoding layers have the form $S(x) = e^{-ixH}$ for some Hamiltonian H called generators. The generators are typically composed of smaller sub-generators. We have illustrated that all generators are composed of 2×2 matrices and thus acting on a single qubit each. The sub-generators have been marked as white squares.

via concatenation

$$U(\boldsymbol{x}, \boldsymbol{\theta}) := \prod_{n=1}^{N} U_n(x_n, \boldsymbol{\theta}). \tag{3}$$

In the parallel ansatz, the data encoding circuits $S_{n,l}(x_n)$ for each univariate variable x_n and each layer l are glued together in parallel via tensor product

$$S_l(\boldsymbol{x}) := \bigotimes_{n=1}^N S_{l,n}(x_n). \tag{4}$$

The circuits $U(x, \theta)$ of the sequential and parallel ansatz are shown in Figure 1.

For univariate functions, the two cases collapse into a single ansatz.

The QNN is trained iteratively by evaluating $f_{\theta}(x)$ on a dataset \mathcal{D} on quantum hardware, computing some loss of the output and updating the parameters θ by some classical algorithm. To update the parameters, one can use the parameter shift rule [32] to compute the gradient with respect to θ efficiently by two further evaluations of the QNN and use it for gradient descent.

An immediate question to ask is what kind of functions are represented by the class of QNN. In [10] it was shown that every QNN can be represented by a finite Fourier series

$$f_{\theta}(x) = \sum_{\omega \in \Omega} c_{\omega}(\theta) e^{i\omega \cdot x},$$
 (5)

where $\boldsymbol{\omega} \cdot \boldsymbol{x} \in \mathbb{R}$ denotes the standard scalar product of $\boldsymbol{\omega}$ and \boldsymbol{x} , and $\boldsymbol{\Omega} \subseteq \mathbb{R}^N$ is a finite set called the *frequency spectrum*. It can be shown that the frequency spectrum only depends on the data encoding Hamiltonians $H_{n,l}$ and is the same for the parallel and

sequential ansatz, while the Fourier coefficients $c_{\omega}(\boldsymbol{\theta})$ also depend on the parameter encoding circuits $W_{\boldsymbol{\theta}}^{(l)}$ and the observable M. More precisely, let $\Delta S := S - S := \{s_1 - s_2 | s_1, s_2 \in S\}$ and $\sum_{l=1}^L S_l := \{\sum_{l=1}^L \lambda_l | (\lambda_1, ..., \lambda_L) \in S_1 \times \cdots \times S_L\}$ for all sets $S, S_1, ..., S_L \subseteq \mathbb{R}^N$, and let $\sigma(H_l) \subseteq \mathbb{R}$ be the spectrum of H_l , then the frequency spectrum of the univariate model is given by

$$\Omega = \Delta \sum_{l=1}^{L} \sigma(H_l). \tag{6}$$

The frequency spectrum of the multivariate model Ω , regardless whether it is constructed by the parallel or the sequential approach, is given by the Cartesian product $\Omega = \Omega_1 \times \cdots \times \Omega_N$ of the frequency spectra $\Omega_n = \Delta \sum_{l=1}^L \sigma\left(H_{n,l}\right)$ of the associated univariate models. Thus, maximising Ω can be reduced to maximising all univariate spectra Ω_n .

In this work, we focus on the frequency spectrum and presents various maximality results for different architectures and assumptions made to the QNN. There are at least two ways to define maximality here. One is to maximise the size $|\Omega|$ of the frequency spectrum, the other is to maximize the number $K \in \mathbb{N}$ such that

$$\mathbb{Z}_K := \{-K, ..., 0, ..., K\} \subseteq \Omega \tag{7}$$

to ensure proper approximation properties. In some cases, as we will see, the answers to these two questions are related. A useful concept to study maximality is the degeneracy of the quantum model [9, 33]. The $degeneracy \deg(\omega) \in \mathbb{N}$ of the frequency $\omega \in \Omega$ of a given QNN is defined as the number of representations

$$\omega = \sum_{l=1}^{L} \left(\lambda_{k_l}^{(l)} - \lambda_{j_l}^{(l)} \right), \tag{8}$$

where $\lambda_1^{(l)},...,\lambda_d^{(l)}\in\mathbb{R}$ denotes the eigenvalues of H_l . Maximizing the set Ω is equivalent to minimizing the degeneracies.

Schuld et al. [10] have shown further that for any square integrable function there exists a QNN approximating that function with the given precision. More precisely, they have shown that for any square-integrable function $g \in L_2([0,2\pi]^N)$ and all $\epsilon > 0$ there exists an observable $M_{g,\epsilon}$ and a single layer QNN

$$f(\boldsymbol{x}) = \langle 0 | \left(W^{(1)} \right)^{\dagger} S^{\dagger}(\boldsymbol{x}) \left(W^{(2)} \right)^{\dagger} M_{g,\epsilon} W^{(2)} S(\boldsymbol{x}) W^{(1)} | 0 \rangle$$
 (9)

with a sufficiently large number of qubits $R \in \mathbb{N}$ such that $||f - g||_2 < \epsilon$ under some mild constraints on the generators of the data encoding layers called *universal Hamiltonian property*. This property guarantees that the frequency spectrum is rich enough to approximate the target function. For example, if all generators are constructed out of Pauli matrices, this condition is satisfied. This underlines the importance of studying

the properties of the frequency spectrum of QNNs. The broader the frequency spectrum, the better the potential for approximating target functions, at least if there is enough degree of freedom in the parameter circuits $W^{(l)}$. It should be noted, however, that although this universality theorem undoubtedly answers an important question regarding the class of functions that can be approximated by QNNs, the dependence of the observables M on the Fourier coefficients of the approximated function g is a too strong restriction to be an analogue of the universal approximation property of classical neural networks [34]. In practice, M is typically set to $M = Z \otimes \operatorname{Id} \otimes \cdots \otimes \operatorname{Id}$ or similar with sufficiently many copies of the identity. In theory, it could be that a function cannot be well approximated with this class of observables, no matter how many qubits are used. So as far as we know, it is still an open question whether this class of observables can approximate any square integrable function with arbitrary precision, or, more generally, whether there exists a sequence of observables $(M_k)_{k\in\mathbb{N}}$ such that for all target functions g and all $\epsilon > 0$ there exists an index K such that for all $k \geq K$ there exist unitaries $W^{(1)}, W^{(2)}$ such that $\|g - f\|_2 < \epsilon$, where M_k is used as observable in f and $W^{(1)}, W^{(2)}$ as parameter unitaries.

1.1 Related Work and Our Contribution

In order to present the results of related work and our contribution on the frequency spectrum Ω , we need to introduce some additional terms and notations regarding various assumptions that can be made on the QNN ansatz. In [10] it is assumed that the data encoding circuits are all equal in a QNN, i.e., $S_1(x) = ... = S_L(x)$. We refer to this case as a QNN with equal data encoding layers. If we do not make this addition, then we do not make any further assumptions about the layers. Note that in a single-layer model both cases collapse into one. Further, for practical and theoretical considerations, it is often assumed that the generators, and hence the data encoding circuits, are built up of smaller sub-generators, typically $S_l(x) = \bigotimes_{r=1}^R e^{-ixH_{r,l}} = e^{-ix\bigoplus_{r=1}^R H_{r,l}}$ (which should not be confused with the formula for the data encoding layers in the parallel ansatz), where $H_{r,l} \in \text{End}(\mathcal{B})$ is Hermitian. Moreover, the sub-generators $H_{l,r}$ are often set to some multiple of the Pauli matrices X, Y, Z, where

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{10}$$

If the QNN is only built by generators of dimension $k \times k$, we refer to the QNN as QNN with k-dimensional sub-generators. We write QNN with Pauli sub-generators when only multiples of Pauli matrices are used. If not clear from the context, we name the sub-generators explicitly and write QNN with k-dimensional sub-generators $H_{l,r}$.

In [10, 19], it was shown that the frequency spectrum of a single layer QNN with Pauli sub-generators $\mathbb{Z}/2$ is given by

$$\Omega = \mathbb{Z}_R = \{-R, ..., 0, ..., R\}. \tag{11}$$

In [33], this setting is called Hamming encoding. If instead a single qubit QNN with Pauli sub-generators $\mathbb{Z}/2$ and equal data encoding layers is used, the frequency

spectrum is

$$\Omega = \mathbb{Z}_L = \{-L, ..., 0, ..., L\}. \tag{12}$$

The result is symmetrical and linear in R and L. While these results consider the special case of L=1 and R=1, we extend this result to arbitrary L, R and 2-dimensional sub-generators H. In this case, the frequency spectrum is given by

$$\Omega = (\lambda - \mu) \cdot \mathbb{Z}_{RL} = \{ (\lambda - \mu) \cdot k | k \in \mathbb{Z}_{RL} \}, \tag{13}$$

where $\lambda, \mu \in \mathbb{R}$ are the two eigenvalues of H. The previous results can be derived directly from this.

In [9], two ansätze for an exponential encoding scheme were presented, leading both to the same frequency spectrum. In their so called *sequential exponential* ansatz, which is in our terminology a singe qubit QNN with Pauli sub-generators, where each H_l is set to $H_l = \beta_l \cdot Z/2$ with

$$\beta_l := \begin{cases} 2^{l-1}, & \text{if } l < L \\ 2^{L-1} + 1, & \text{if } l = L, \end{cases}$$
 (14)

the resulting frequency spectrum is given by $\Omega = \mathbb{Z}_{2^L}$ and therefore exponential in L. The second ansatz suggested called parallel exponential, which is in our terminology a single layer QNN with Pauli sub-generators $H_r = \beta_r \cdot Z/2$ with β_r as before, only the variable names are interchanged. This ansatz leads to the frequency spectrum $\Omega = \mathbb{Z}_{2^R}$, which is exponential in R. Almost the same encoding strategy was presented in [33] for the single layer QNN with Pauli encoding layers $H_r = \beta_r \cdot Z/2$. The only difference here is that no exception is made for the last term, i.e. $\beta_l = 2^{l-1}$ for all l = 1, ..., L. The authors have named the approach binary encoding strategy. The frequency spectrum for this ansatz is given by frequency spectrum $\Omega = \mathbb{Z}_{2^R-1}$, therefore, only the two terms at the boundary are omitted compared to the parallel exponential ansatz.

The same approach was chosen in [30, 33] for single layer QNNs with Pauli subgenerators of the form $H_r = \beta_r \cdot \mathbb{Z}/2$, but here the generators were multiplied by powers of 3. More precisely, $\beta_r = 3^{r-1}$. In [33], this ansatz is called ternary encoding strategy. The frequency spectrum in this case is given by $\Omega = \mathbb{Z}_{\frac{3^R-1}{2}}$. Unlike the previous approaches, this ansatz is maximal in both senses, meaning that there is no Ω' such that $|\Omega'| > |\Omega|$ and that there is no $K > \frac{3^R-1}{2}$ such that $\mathbb{Z}_K \subseteq \Omega'$ for a QNN with that ansatz. This is due to the fact that the degeneracy is 1 for all frequencies $\omega \in \Omega \setminus \{0\}$, hence each frequency is given by a unique combination of differences of the eigenvalues [33]. We extend these results to QNNs with arbitrary number of layers $L \geq 1$ and arbitrary 2-dimensional Hermitian sub-generators $H_{l,r}$, both for the equal layer approach and the non equal layer approach. If the data encoding layers are equal, the maximal frequency spectrum in both senses is given by

$$\Omega_{\text{max}} = \mathbb{Z}_{\frac{(2L+1)^R - 1}{2}},\tag{15}$$

if no restrictions to the layers are made, the maximal frequency spectrum is given by

$$\Omega_{\text{max}} = \mathbb{Z}_{\frac{3^{RL} - 1}{2}}.\tag{16}$$

It is no coincidence that the results for the Hamming ansatz, the sequential and parallel ansatz, as well as the ternary encoding strategy with non equal data encoding layers are symmetrical in L and R and depend only on $L \cdot R$.

We show that there exists a bijection

$$\mathcal{B}_b: \{\text{QNN}_k | \text{QNN}_k \text{ has shape } (R, L)\} \longrightarrow \{\text{QNN}_k | \text{QNN}_k \text{ has shape } (R', L')\}$$
 (17)

between the set of all QNNs with R qubits and L layers with k-dimensional subgenerators and the set of all QNNs with R' qubits and L' layers with k-dimensional sub-generators such that the frequency spectrum is invariant under that transformation, as long as $R \cdot L = R' \cdot L'$ holds. We denote that observation as spectral invariance under area-preserving transformations and $A := R \cdot L$ as the area of the QNN. The symmetries in the results mentioned above can be directly derived from this. Additionally, the results for QNNs with any number of layers can be derived straight from the single-layer results and the spectral invariance under area-preserving transformations, if no assumptions such as equal data-coding layers on the structure are made.

The previous results only considered QNNs with 2-dimensional generators, i.e. Hermitian operators acting on a single qubit. In [9, 33], Peters et al. presented how to extend these results to single layer QNNs with a d-dimensional generator, which is nothing other than allowing an arbitrary data-encoding H. In this case, the frequency spectrum Ω is maximal in size with $|\Omega| = 2\binom{d}{2} + 1$ if and only if the eigenvalues of H are a so called $Golomb\ ruler$. A Golomb ruler is a set of real numbers $\lambda_1 < \ldots < \lambda_k$ such that each difference $\lambda_i - \lambda_j$ except 0 only occur once. Since there are maximally $2\binom{k}{2} + 1$ possible pairs, $\lambda_1 < \ldots < \lambda_k$ are a Golomb ruler if and only if

$$\left| \Delta \left\{ \lambda_1, ..., \lambda_k \right\} \right| = 2 \binom{k}{2} + 1. \tag{18}$$

Hence, the frequency spectrum Ω is maximal in size because it is non-degenerate. We extend this result to arbitrary k-dimensional sub-generators and provide an instruction how to build a QNN whose frequency spectrum is maximal in size with

$$|\Omega_{\text{max}}| = (4^q - 2^q + 1)^{RL/q},$$
 (19)

where $q = \log_2(k)$.

To maximize the number $K \in \mathbb{N}$ such that $\mathbb{Z}_K \subseteq \Omega$, we introduce a novel approach similar to the turnpike problem. The turnpike problem goes like this: given a multiset ΔS , find S. We relax prerequisites of the problem and name it consequently relaxed turnpike problem. The relaxed turnpike problem asks for an S of size d such that $K(S) := \max \{K \in \mathbb{N}_0 | \mathbb{Z}_K \subseteq \Delta S\}$ is maximal over all sets of size d. We propose an algorithm with complexity $\mathcal{O}\left(d^{2d}\right)$ to solve the relaxed turnpike problem. With this

Encoding strategy	R	L	Н	$\beta_{r,l}$	Equal	Ω	$ \Omega $	Maximal	Source
Hamming	1	N	P/2	1	1	\mathbb{Z}_L	2L + 1	×	[10, 19]
Hamming	N	1	P/2	1	-	\mathbb{Z}_R	2R + 1	×	[10, 19, 33]
Sequential exponential	1	N	P/2	$1, 2, 2^2,, 2^{L-1} + 1$	Х	\mathbb{Z}_{2^L}	$2^{L+1}-1$	Х	[9]
Parallel exponential	N	1	P/2	$1, 2, 2^2,, 2^{R-1} + 1$	-	\mathbb{Z}_{2^R}	$2^{R+1} + 1$	×	[9]
Binary	N	1	P/2	2^{r-1}	-	\mathbb{Z}_{2^R-1}	$2^{R+1}-1$	×	[33]
Ternary	N	1	P/2	3^{r-1}	-	$\mathbb{Z}_{\frac{3^R-1}{2}}$	3^R	$ \Omega , K$	[30, 33]
Golomb	N	1	d	1	-	varies	$2\binom{d}{2} + 1$	$ \Omega $	[9, 33]
Hamming	N	N	P/2	1	1	\mathbb{Z}_{RL}	2RL + 1	×	Our
Equal Layers	\mathbb{N}	N	2	$(2L+1)^{r-1}$	1	$\mathbb{Z}_{\frac{(2L+1)^R-1}{2}}$	$(2L+1)^{R}$	$ \Omega , K$	Our
Ternary	N	N	2	$3^{l-1+L(r-1)}$	Х	$\mathbb{Z}_{\frac{3^{RL}-1}{2}}$	3^{RL}	$ \Omega , K$	Our
Golomb	N	N	k	$(2\ell(\sigma(H)) + 1)^{l-1+L(r-1)}$	Х	varies	$(4^q - 2^q + 1)^{RL/q}$	$ \Omega $	Our
Turnpike	N	N	k	$(2K+1)^{l-1+L(r-1)}$	Х	varies	$\geq (2K+1)^{RL/q}$	K / X	Our

Table 1 Summary of the frequency spectra results for QNNs. Our contributions are highlighted with bold letters. If R or L are arbitrary for a given encoding scheme, we denote that with \mathbb{N} . All encoding schemes use sub-generators of the form $H_{l,r}=\beta_{l,r}\cdot H$. If $H\in\{X/2,Y/2,Z/2\}$ is a multiple of a Pauli matrix, we abbreviate that by H=P/2. Otherwise, the dimension of the arbitrary Hermitian matrix H is stated in column H. If we write k, an arbitrary power of 2 is allowed. The column named "Equal" indicates if equal data encoding layers are required. If the encoding scheme is maximal, we denote the type of maximality in the maximal column, either it is maximal in size $|\Omega|$ or maximal in K such that $\mathbb{Z}_K\subseteq\Omega$. In the Golomb encoding scheme the eigenvalues of H are a Golomb ruler and $q:=\log_2(k)$ with q|R. Similarly, in the turnpike encoding scheme, the eigenvalues of H are a solution to the relaxed turnpike problem. Only when L=1 and k=d this scheme guaranteed to be maximal.

we show that for k = d the number $K \in \mathbb{N}$ such that $\mathbb{Z}_K \subseteq \Omega$ is maximal if and only if the eigenvalues of the generator H are a solution of the relaxed turnpike problem. We further give a construction to extend this to arbitrary k and L, yielding

$$\mathbb{Z}_{\frac{(2K+1)^{RL/q}-1}{2}} \subseteq \Omega, \tag{20}$$

where $K := K(\sigma(H))$ for some k-dimensional sub-generator H whose eigenvalues are a solution of the relaxed turnpike problem and $q := \log_2(k)$. However, in this case $K' = \frac{(2K+1)^{RL/q}-1}{2}$ is not necessarily maximal. For $k \le 4$ and therefore especially for Pauli sub-generators, the Golomb approach and the turnpike approach lead to the same results and in particular reproduce the results for k = 2.

We collect all mentioned results on the frequency spectrum and our contributions in Table 1.

Overall, this work contributes to our understanding of spectral properties of Quantum Neural Networks, particularly clarifying the underlying symmetry and maximality conditions associated with their frequency spectra. We use Minkowski sums and difference sets to obtain a compact algebraic expression for the frequency spectrum, which can be easily calculated with the given formula. This allows us to standardize existing results and extend them to more general cases. We also explain the symmetry of the already known results by spectral invariance. Furthermore, we introduce two precise notions of maximality, namely maximality in size and maximality in K. While they

do not differ for QNNs with only 2-dimensional sub-generators, this is not the case for arbitrary dimensional generators. While the Golomb encoding is maximal in size, we introduce a new problem, the relaxed turnpike problem, which is related to the turnpike problem and whose solutions imply encodings that are maximal in K.

1.2 Structure of the Paper

The paper is structured as follows. Section 2 serves to define the notation and to introduce some necessary concepts such as the Kronecker and Minkowski sum, as well as to describe some of their useful properties. In Section 3, we discuss the representation of Quantum Neural Networks (QNNs) as finite Fourier series and explain how the frequency spectrum can be expressed in terms of the generator's spectrum. This holds true for various selections of N and L, encompassing both parallel and sequential approaches. In Section 4, we show that the frequency spectrum of a QNN solely relies on the area A=RL and remains independent of the specific assignment of subgenerators to layers and qubits. This observation elucidates the symmetry observed between single-qubit and single-layer QNNs commonly reported in the literature. In section 5 we prove maximality results for the frequency spectrum of QNNs with 2-dimensional sub-generators, while section 6 addresses the case of arbitrary-dimensional sub-generators.

2 Notations

Let \mathcal{B} denote the two-dimensional Hilbert space $\mathbb{C}^2 = \mathbb{C} |0\rangle + \mathbb{C} |1\rangle$ endowed with the standard inner product $\langle \cdot, \cdot \rangle$. For $R \in \mathbb{N}$ let $\mathcal{B}^{\otimes R}$ be the R-fold tensor product of \mathcal{B} and $\mathcal{U}_R := \{U \in \operatorname{End}(\mathcal{B}^{\otimes R}) | UU^{\dagger} = \operatorname{Id} \}$ the unitary group of $\mathcal{B}^{\otimes R}$. With R we always denote the number of considered qubits. The overall dimension of $\mathcal{B}^{\otimes R}$ is denoted by $d = 2^R$. Sometimes it will also be useful to consider the standard inner product on \mathbb{R}^N . To avoid confusion with the Dirac notation, we write $\mathbf{x} \cdot \mathbf{y} = \mathbf{x}_1 \mathbf{y}_1 + \ldots + \mathbf{x}_N \mathbf{y}_N$ for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^N$.

For $n \in \mathbb{N}_0 = \{0, 1, 2, 3, ...\}$ we define

$$[n] := \{0, 1, \dots, n-1\} \subseteq \mathbb{N}_0$$

and

$$\mathbb{Z}_n := \{-n, \dots, 0, \dots, n\} \subseteq \mathbb{Z}.$$

We will make use of the natural identification of elements $j \in [d]$ with the vectors of the computational basis $|j\rangle$ of $\mathcal{B}^{\otimes R}$.

The data encoding layers $S_l(x)$ of QNNs typically consist of smaller building blocks $S_l(x) = \bigotimes_{r=1}^R e^{-ixH_{r,l}}$ with sub-generators $H_{r,l}$. To see that $S_l(x)$ can be rewritten in the form $S_l(x) = e^{-ix\tilde{H}}$ for some generator \tilde{H} as required, the following construction is useful.

Definition 1 (Kronecker Sum) Let V_r be some finite dimensional vector spaces and $H_i \in End(V_r)$ be linear maps for all r = 1, ..., R. Define

$$H'_r := Id_1 \otimes \cdots \otimes Id_{r-1} \otimes H_r \otimes Id_{r+1} \cdots \otimes Id_R,$$

where $Id_r \in End(V_r)$ denotes the identity map. The Kronecker sum of the linear maps is defined as

$$\bigoplus_{r=1}^R H_r := \sum_{r=1}^R H_r'.$$

The Kronecker sum has the following well-known properties:

Lemma 2 (Properties of the Kronecker Sum) Let V_r be some finite dimensional vector spaces and $H_r \in End(V_r)$ be Hermitian for all r = 1, ..., R.

(1) It holds

$$\bigotimes_{r=1}^{R} e^{H_r} = e^{\bigoplus_{r=1}^{R} H_r}.$$

In particular, $\bigotimes_{r=1}^R e^{-ixH_r} = e^{-ix\tilde{H}}$ for some Hermitian \tilde{H} and all $x \in \mathbb{R}$.

(2) We have

$$\sigma\left(\bigoplus_{r=1}^{R} H_r\right) = \sum_{r=1}^{R} \sigma(H_r),$$

where $\sigma(\cdot)$ denotes the spectrum of the operator.

As mentioned in the introduction, we are interested in the frequency spectra of QNNs, which can be represented via sums and differences of the sets of eigenvalues of the sub-generators. For this reason, the following notations will be useful in this work.

Definition 3 Let $A, A_1, A_2, \ldots, A_n \subseteq \mathbb{R}^N$ be arbitrary subsets.

(a) The Minkowski sum of A_1, \ldots, A_n is defined as

$$\sum_{i=1}^{n} A_i := \{ a_1 + \ldots + a_n | a_1 \in A_1, \ldots, a_n \in A_n \}.$$

- (b) For any $r \in \mathbb{R}$, we define $r \cdot A := \{r \cdot a | a \in A\}$.
- (c) The special case where n=2 and $A_2=(-1)\cdot A_1$ is abbreviated as $\Delta A:=\{a-b|a,b\in A\}$. We also write $A_1\Delta A_2:=(A_1-A_2)\cup (A_2-A_1)$, which is not to be confused with the symmetric difference of sets, which we do not use in this work.

We note some well-known properties of the Minkowski sum.

Lemma 4 Let $A_1, A_2, \ldots, A_n, B_1, B_2, \ldots, B_n \subseteq \mathbb{R}^N$ be arbitrary subsets.

- (a) $\sum_{i=1}^{n} \Delta A_i = \Delta(\sum_{i=1}^{n} A_i).$ (b) $\Delta(A_1 \times \ldots \times A_n) = \Delta A_1 \times \ldots \times \Delta A_n.$ (c) $\sum_{i=1}^{n} (A_i \times B_i) = (\sum_{i=1}^{n} A_i) \times (\sum_{i=1}^{n} B_i).$

Quantum Neural Networks and Fourier Series

Let us first recall the definition of Quantum Neural Networks. For that, we consider two types of ansätze.

Definition 5 (Parallel and Sequential Ansatz) Let $R, L \in \mathbb{N}$ and $x \in \mathbb{R}^N, \theta \in \mathbb{R}^P$.

(a) A parallel ansatz is a parametrized circuit of the form

$$U(\boldsymbol{x},\boldsymbol{\theta}) = W_{\boldsymbol{\theta}}^{(L+1)} S_L(\boldsymbol{x}) W_{\boldsymbol{\theta}}^{(L)} \cdots W_{\boldsymbol{\theta}}^{(2)} S_1(\boldsymbol{x}) W_{\boldsymbol{\theta}}^{(1)}$$

with

$$S_l(\boldsymbol{x}) = \bigotimes_{n=1}^N e^{-ix_n H_{l,n}},$$

where each $H_{l,n} \in End(\mathcal{B}^{\otimes R})$ is Hermitian and each $W_{\theta}^{(l)} \in End(\mathcal{B}^{\otimes R \cdot N})$ is unitary. (b) A sequential ansatz is a parametrized circuit of the form

$$U(\boldsymbol{x}, \boldsymbol{\theta}) = \prod_{n=1}^{N} U_n(\boldsymbol{x}_n, \boldsymbol{\theta}),$$

with

$$U_n(\boldsymbol{x}_n, \boldsymbol{\theta}) = W_{\boldsymbol{\theta}}^{(L+1,n)} S_L(x_n) W_{\boldsymbol{\theta}}^{(L,n)} \cdots W_{\boldsymbol{\theta}}^{(2,n)} S_1(x_n) W_{\boldsymbol{\theta}}^{(1,n)}$$

and

$$S_l(x_n) = e^{-ix_n H_{l,n}}.$$

Again, each $H_{l,n} \in End(\mathcal{B}^{\otimes R})$ is Hermitian and each $W_{\theta}^{(l,n)} \in End(\mathcal{B}^{\otimes R})$ is unitary.

In both cases, the Hermitians $H_{l,n}$ are called the *generators* of the ansatz. We briefly mention some simplifying assumptions we can make when working with these ansätze. First, we can omit the dependence of $W_{\boldsymbol{\theta}}^{(l)}$ on $\boldsymbol{\theta}$ from the notation since we

are not applying any optimization process and assume that all unitaries $W \in \mathcal{U}_R$ can

be represented by some $W_{\boldsymbol{\theta}}$. Therefore we write $W^{(l)} := W^{(l)}_{\boldsymbol{\theta}}$ from now on. Second, since the $H_{l,n}$ are Hermitian, there exists unitaries $U_{l,n} \in \mathcal{U}_R$ such that $U^{\dagger}_{l,n}H_{l,n}U_{l,n} = \mathrm{diag}\left(\lambda^{(l,n)}_0,...,\lambda^{(l,n)}_{d-1}\right)$ in the computational basis $|0\rangle, |1\rangle,..., |d-1\rangle \in$ $\mathcal{B}^{\otimes R}$. In the sequential ansatz, we can "absorb" the $U_{l,n}$ in the unitaries $W^{(l,n)}$ via $\tilde{W}^{(l,n)} := U_{l,n} W^{(l,n)} U_{l-1,n}^{\dagger}$. In the parallel ansatz, we can use the unitary $\bigotimes_{n=1}^{N} U_{l,n}$ and let it be absorbed by the $W^{(l)}$. Hence, without loss of generality, the $H_{l,n}$ are diagonal with eigenvalues

$$\lambda_0^{(l,n)},...,\lambda_{d-1}^{(l,n)} \in \mathbb{R}.$$

Definition 6 (Quantum Neural Networks) Let U(x) be a parallel or sequential ansatz. A Quantum Neural Network (QNN) is a function of the form

$$f: \mathbb{R}^N \longrightarrow \mathbb{R}$$

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

with some Hermitian M. We call the tuple $(R, L) \in \mathbb{N}^2$ the shape of the QNN.

In [10] it was shown that QNNs with equal data encoding layers can be written in the form

$$f(\boldsymbol{x}) = \sum_{\omega \in \Omega} c_{\boldsymbol{\omega}} e^{i\boldsymbol{x} \cdot \boldsymbol{\omega}},$$

where $c_{\omega} \in \mathbb{C}$ and $\Omega \subseteq \mathbb{R}^N$ is a finite set, called the frequency spectrum. If $\Omega \subseteq \mathbb{Z}^N$, then this sum is the partial sum of a Fourier series. To start with, we show the proof of the above representation for N=1 and, in the process, generalize it to the situation where the data encoding layers may be different. Recall that for N=1, the parallel and sequential ansatz are equal and we write $H_l := H_{l,1}$.

Theorem 7 (Univariate QNN is a Fourier Series) Let $f(x) = \langle 0|U^{\dagger}(x)MU(x)|0\rangle$ be a univariate QNN with arbitrary generators $H_l \in End(\mathcal{B}^{\otimes R})$. Then

$$f(x) = \sum_{\omega \in \Omega} c_{\omega} e^{-i\omega \cdot x},$$

with

$$\Omega = \sum_{l=1}^{L} \Delta \sigma(H_l).$$

Proof For each l=1,...,L let $\lambda_0^{(l)},...,\lambda_{d-1}^{(l)}$ be the eigenvalues of H_l . The action of $W^{(l)}$ and e^{-ixH_l} on some basis vector $|j\rangle$ for $j \in [d]$ are given by

$$W^{(l)}|j\rangle = \sum_{i=0}^{d-1} W_{i,j}^{(l)}|i\rangle$$

and

$$S_l(x)|j\rangle = e^{-ixH_l}|j\rangle = e^{-ix\lambda_j^{(l)}}|j\rangle,$$

where $W_{i,j}^{(l)} := \langle i|W^{(l)}|j\rangle \in \mathbb{C}$. Hence

 $= \sum_{j_{L+1}=0}^{d-1} \sum_{j \in [d]^L} \left(\prod_{l=1}^{L+1} W_{j_l, j_{l-1}}^{(l)} \right) e^{-ix\Lambda_j} |j_{L+1}\rangle,$

where $j_0 := 0$ and $\Lambda_j := \sum_{l=1}^L \lambda_{j_l}^{(l)} \in \sum_{l=1}^L \sigma(H_l)$. This yields

$$\langle 0|U^{\dagger}(x) = \sum_{j_{L+1}=0}^{d-1} \langle j_{L+1}| \sum_{j \in [d]^L} \left(\prod_{l=1}^{L+1} \left(W^{\dagger} \right)_{j_{l-1}, j_l}^{(l)} \right) e^{ix\Lambda_j}.$$

Hence

$$f(x) = \langle 0|U^{\dagger}(x)MU(x)|0\rangle = \sum_{\boldsymbol{j},\boldsymbol{k}\in[d]^L} a_{\boldsymbol{k},\boldsymbol{j}} e^{ix(\Lambda_{\boldsymbol{k}}-\Lambda_{\boldsymbol{j}})}$$

with

$$a_{\boldsymbol{k},\boldsymbol{j}} = \sum_{k_{L+1},j_{L+1}=0}^{d-1} \left(\prod_{l=1}^{L+1} W_{k_{l},k_{l-1}}^{(l)}\right) \cdot \left(\prod_{l=1}^{L+1} \left(W^{\dagger}\right)_{j_{l-1},j_{l}}^{(l)}\right) \cdot M_{j_{L+1},k_{L+1}}$$

and $k = (k_1, ..., k_L), j = (j_1, ..., j_L) \in [d]^L$. If we group all terms with the same frequencies together, we obtain

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

where

$$c_{\omega} := \sum_{\substack{\boldsymbol{j}, \boldsymbol{k} \in [d]^L \\ \Lambda_{\boldsymbol{k}} - \Lambda_{\boldsymbol{j}} = \omega}} a_{\boldsymbol{k}, \boldsymbol{j}}$$

and

$$\Omega = \left\{ \Lambda_{\boldsymbol{k}} - \Lambda_{\boldsymbol{j}} | \boldsymbol{j}, \boldsymbol{k} \in [d]^L \right\} = \Delta \sum_{l=1}^L \sigma(H_l).$$
 (21)

By Lemma 4, the difference Δ can be shifted inside the sum, proving the claim.

The result above can be generalized to multivariate QNNs. We skip the technical details and just give the final result here, the details and a proof can be found in Appendix A.

Theorem 8 (Frequency Spectrum of a Multivariate QNN) The frequency spectrum $\Omega_{L,N}$ of a multivariate QNN with generators $H_{l,n} \in End(\mathcal{B}^{\otimes R})$, regardless of whether the parallel or sequential approach is chosen, is given by

$$\mathbf{\Omega}_{L,N} = \Omega_L \left(H_{1,1}, ..., H_{L,1} \right) \times \cdots \times \Omega_L \left(H_{1,N}, ..., H_{L,N} \right),$$

where $\Omega_L(H_{1,n},...,H_{L,n})$ denotes the frequency spectrum of the univariate model with generators $H_{1,n},...,H_{L,n}$ for all n=1,...,N.

According to Theorem 8, the frequency spectrum of a multivariate QNN depends only on the generators of the ansatz. Specifically, it is 'rectangular', that is, the Cartesian product of the corresponding univariate frequency spectra $\Omega_L\left(H_{n,1},...,H_{n,L}\right)$ to the variable x_n . In the following we are only interested in the frequency spectrum of a QNN. In particular, our goal is to maximise it, so by Theorem 8, maximising the multivariate frequency spectrum is equivalent to maximising each univariate frequency spectrum. It is therefore sufficient to consider only univariate models, i.e. N=1, in the following.

4 Spectral Invariance Under Area-Preserving Transformations

We have seen that the frequency spectrum of a QNN depends only on the eigenvalues of the generators H_l , or, if it is composed of smaller sub-generators $H_{r,l}$, on their eigenvalues. In this section, we show how to transform the QNN in such a way that the frequency spectrum remains invariant and the resulting QNN uses the same sub-generators. More precisely, given a QNN of shape (R, L), we show that one can rearrange the sub-generators without changing the frequency spectrum as long as the area $A := R \cdot L$ of the QNN is preserved. We summarise the previous idea in the following theorem.

Theorem 9 (Spectral Invariance Under Area-Preserving Transformations) Let $k = 2^q$ and let $R, R', L, L' \in \mathbb{N}$ with $R \cdot L = R' \cdot L'$ such that q divides R and R'. Then every bijection

$$b: [R'/q] \times [L'] \to [R/q] \times [L] \tag{22}$$

induces a bijection

$$\mathcal{B}_b: \{QNN_k \mid QNN_k \text{ has shape } (R, L)\} \longrightarrow \{QNN_k \mid QNN_k \text{ has shape } (R', L')\}$$
 (23)

between univariate QNNs which only consists of k-dimensional sub-generators such that the frequency spectrum of the models is invariant under that transformation.

In particular, if we make no further assumptions on the generators like equal data encoding layers, the maximal possible frequency spectrum of a QNN with k-dimensional sub-generators is only dependent on the area $A(R,L) := R \cdot L \in \mathbb{N}$ and not on the individual R,L. We call \mathcal{B}_h an area-preserving transformation.

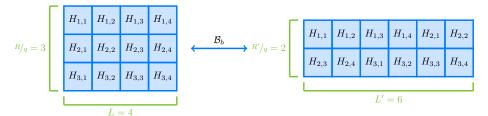


Fig. 2 Visualisation of Theorem 9. By Theorem 7, the frequency spectrum only depends on the subgenerators $H_{r,l}$. The QNN can thus be represented by a rectangle containing these sub-generators as squares in the arrangement matching their occurrence in the quantum circuit. By Theorem 9, the arrangement is irrelevant for the frequency spectrum, as there exists an area-preserving transformation for all other compatible rectangles.

Proof Let $k = 2^q$ and $H_{r,l} \in \text{End}(\mathcal{B}^{\otimes q})$ be the k-dimensional sub-generators of a univariate QNN of shape (R, L). By Theorem 7 and Lemma 4, the frequency spectrum of that QNN is given by

$$\Omega = \sum_{l=1}^{L} \sum_{r=1}^{R/q} \Delta \sigma(H_{r,l}).$$

The QNN of shape (R', L') with sub-generators $H_{b(r-1,l-1)+(1,1)}$ (we have to do an index shift here), then has trivially the same frequency spectrum, as it is only a permutation of the sub-generators and the Minkowski sum remains the same.

Note that two QNNs are considered equal if and only if they have the same shape and all their sub-generators $H_{r,l}$ and $H'_{r,l}$ for all $r=1,\ldots,R$ and $l=1,\ldots,L$ are equal. Strictly speaking, however, the QNNs also depend on the parameter encoding layers. Therefore, we have only constructed a bijection between equivalence classes of QNNs, which is sufficient for our cases here. Using the Schröder-Bernstein theorem of set theory and the axiom of choice, it is possible to extend this to a bijection of QNNs considering the parameter encoding layers.

By Theorem 7, the only relevant information for the frequency spectrum are the generators or sub-generators. Thus, the QNN can be represented by a rectangular plot containing these sub-generators as squares in the arrangement matching their occurrences in the circuit. Theorem 9 now implies that this arrangement is irrelevant, since we can transform each QNN with an area preserving transformation in all other compatible rectangles. We sketch this in Figure 2.

If no requirements are made on the generators, such as equal data coding layers, Theorem 9 implies that, without loss of generality, we can consider single-layer models to study the maximum frequency spectrum of QNNs with k-dimensional generators. The results depending on R can then be generalised to the multi-layer case by simply replacing the dependence on R by $R \cdot L$.

The technical requirement that q divides R is only necessary because we have made the assumption that the QNN consists only of sub-generators of dimension k, which is only possible if this is satisfied. We briefly sketch how to generalize Theorem 9 allowing mixed-dimensional generators. In this case, the squares representing the sub-generators like in Figure 2 are replaced by rectangles with side-length $q_{r,l} \times 1$,

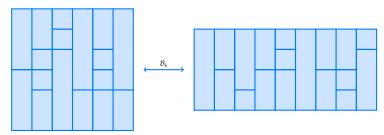


Fig. 3 Example of how to extend Theorem 9 to QNNs without the requirement that all generators are k-dimensional. The sides of the individual rectangles representing a $k_{r,l} = 2^{q_{r,l}}$ -dimensional subgenerator $H_{r,l}$ have side lengths $q_{r,l} \times 1$. In this example, we used q = 1, 2, 3, 4, (R, L) = (6, 6) and (R', L') = (4, 9). An area-preserving transformation is only possible if the target rectangular could be tiled with the given sub-generator rectangles.

where $k_{r,l} = 2^{q_{r,l}}$ is the dimension of the sub-generator $H_{r,l}$. An area-preserving transformation thus is only possible into rectangular shapes which can be constructed out of these rectangular tiles, see Figure 3 for an example.

We emphasise that the invariance is only for the frequency spectrum, we do not necessarily obtain the same Fourier series, since the parameter encoding layers $W^{(l)}$ and the observable M remain unchanged and therefore have incompatible dimensions for other shapes (R', L'). Therefore, the parameter encoding layers and the observable would also need to be transformed for a bijection that preserves the full Fourier series. The consequence of a Fourier series preserving transformation would be that there would be no advantage in terms of expressibility and approximation in considering models with more than one layer or with more than one qubit. Thus, it is important to keep in mind that area-preserving transformations preserve only the frequency spectrum and not necessarily the entire Fourier series.

While the frequency spectrum depends only on the area A and not on the concrete shape (R, L), for practical applications the number of available qubits and error rates could play an important role in choosing a well-suited shape of the QNN.

In [10] it was shown that the frequency spectrum of a single layer model with Pauli sub-generators $\mathbb{Z}/2$ is given by $\Omega = \mathbb{Z}_R$, while the frequency spectrum of a single qubit QNN with the same sub-generators is given by $\Omega = \mathbb{Z}_L$. The symmetry in these results is a direct consequence of Theorem 9. If one allows an arbitrary 2-dimensional sub-generator H to replace $\mathbb{Z}/2$ and arbitrary many layers and qubits, the resulting QNN has the following frequency spectrum.

Theorem 10 (Frequency Spectrum of the Hamming Encoding Strategy) Let $H \in End(\mathcal{B})$ be Hermitian and $\lambda, \mu \in \mathbb{R}$ its eigenvalues. The frequency spectrum Ω of the univariate QNN with 2-dimensional sub-generators $H_{r,l} = H$ is given by

$$\Omega = (\lambda - \mu) \cdot \mathbb{Z}_{RL}. \tag{24}$$

Proof By Theorem 9, w.l.o.g. we can assume R = 1 and replace L by $R \cdot L$ afterwards. By Theorem 7 and Lemma 2, the frequency spectrum is given by

$$\Omega = \sum_{l=1}^{L} \Delta \sigma(H) = \sum_{l=1}^{L} (\lambda - \mu) \cdot \mathbb{Z}_1 = (\lambda - \mu) \cdot \mathbb{Z}_L.$$
 (25)

In [9], two exponential coding schemes were presented, namely the parallel exponential and the sequential exponential ansatz, both of which lead to the same frequency spectrum. This relationship can be explained using Theorem 9, as one ansatz is just the image under an area-preserving transformation of the other.

5 2-Dimensional Sub-Generators

In this section we consider univariate QNNs with 2-dimensional generators. In [30, 33] it was shown that the maximal frequency spectrum in both senses of a single layer QNN with Pauli sub-generators $^P\!/_2$ is given by $\Omega_{\max} = \mathbb{Z}_{\frac{3^R-1}{2}}$, i.e. it is maximal in size and maximal in K such that $\mathbb{Z}_K \subseteq \Omega$. For the ansatz with no further restrictions to the data encoding layers, we can extend this result directly by Theorem 9 to QNNs with arbitrary many layers $L \geq 1$, i.e. $\Omega_{\max} = \mathbb{Z}_{\frac{3^R \cdot L}{2}}$. However, we follow another approach. We first show that the maximal frequency spectrum of a univariate QNN with equal data encoding layers and arbitrary 2-dimensional generators is given by $\Omega_{\max} = \mathbb{Z}_{\frac{(2L+1)^R-1}{2}}$. We then use Theorem 9 to extend this result to QNNs without the restriction of equal data encoding layers.

The following purely number theoretic lemma is necessary for the following maximallity results. A proof is provided in Appendix B.

Lemma 11 Let $R, L \in \mathbb{N}$ and $z_1, ..., z_R \in \mathbb{R}_{\geq 0}$ with $z_1 \leq ... \leq z_R$ such that

$$\sum_{r=1}^{R} z_r \cdot \mathbb{Z}_L = \mathbb{Z}_{\frac{(2L+1)^R - 1}{2}}.$$
 (26)

The unique solution in $z_1,...,z_R$ is given by

$$z_r = (2L+1)^{r-1}$$

for all r = 1, ..., R.

From the previous lemma, we can give the maximum frequency spectrum of QNNs with equal data encoding layers.

Theorem 12 (Maximal Frequency Spectrum with Equal Data Encoding Layers) Let Ω be the frequency spectrum of a univariate QNN with equal data encoding layers and 2-dimensional generators $H_{r,l} := H_r \in End(\mathcal{B})$ for all $r = 1, \ldots, R$. Further, let $\lambda_r, \mu_r \in \mathbb{R}$ be the two eigenvalues of H_r and w.l.o.g. assume $0 \le \lambda_1 - \mu_1 \le \ldots \le \lambda_R - \mu_R$.

(a) Let $K \in \mathbb{N}$ be maximal with respect to the property

$$\mathbb{Z}_K \subseteq \Omega$$
.

Then $K \leq \frac{(2L+1)^R-1}{2}$ with equality if and only if $\lambda_r - \mu_r = (2L+1)^{r-1}$ for all r=1,...,R.

(b) In particular, if one fixes $H \in End(\mathcal{B})$ with eigenvalues $\lambda, \mu \in \mathbb{R}$ and $\lambda - \mu = 1$, one can set $H_r := (2L+1)^{r-1}H$ to obtain

$$\Omega = \mathbb{Z}_{\frac{(2L+1)^R - 1}{2}}.$$

Proof By Theorem 7 and Lemma 2, the frequency spectrum Ω is given by

$$\Omega = \sum_{l=1}^{L} \sum_{r=1}^{R} \Delta \sigma(H_r) = \sum_{l=1}^{L} \sum_{r=1}^{R} (\lambda_r - \mu_r) \cdot \mathbb{Z}_1 = \sum_{r=1}^{R} (\lambda_r - \mu_r) \cdot \mathbb{Z}_L$$
 (27)

The upper bound can be derived from counting elements

$$|\Omega| < (2L+1)^R,$$

which yields $K \leq \frac{(2L+1)^R-1}{2}$ by the symmetry $\Omega = -\Omega$ and $0 \in \Omega$. By defining $z_r := \lambda_r - \mu_r$ for all r = 1, ..., R, the rest is the exact statement of Lemma 11.

We extend the above results to QNNs with arbitrary 2-dimensional data encoding layers.

Theorem 13 (Maximal Frequency Spectrum for Arbitrary Data Encoding Layers) Let Ω be the frequency spectrum of a univariate QNN with 2-dimensional generators $H_{r,l} \in End(\mathcal{B})$ for all $r = 1, \ldots, R$. Further, let $\lambda_r, \mu_r \in \mathbb{R}$ be the two eigenvalues of H_r and w.l.o.g. assume $0 \leq \lambda_1 - \mu_1 \leq \ldots \leq \lambda_R - \mu_R$.

(a) Let $K \in \mathbb{N}$ be maximal with respect to the property

$$\mathbb{Z}_K \subseteq \Omega$$
.

Then $K \leq \frac{3^{RL}-1}{2}$ with equality if and only if $\left\{\lambda_r^{(l)} - \mu_r^{(l)} | r, l\right\} = \left\{3^0, 3^1, \dots, 3^{R\cdot L-1}\right\}$.

(b) In particular, if one fixes $H \in End(\mathcal{B})$ with eigenvalues $\lambda, \mu \in \mathbb{R}$ and $\lambda - \mu = 1$, one can set $H_{r,l} := 3^{l-1+L\cdot(r-1)}H$ to obtain

$$\Omega = \mathbb{Z}_{\frac{3^{R \cdot L} - 1}{2}}.$$

Proof By Theorem 9, each QNN of shape (R, L) with 2-dimensional generators has the same frequency spectrum as a single layer model (L' = 1) with 2-dimensional generators and $R' := R \cdot L$ many qubits. For a single layer model, Theorem 12 states that

$$K \le \frac{(2L'+1)^{R'}-1}{2} = \frac{3^{R \cdot L}-1}{2}$$

with equality if and only if $\left\{\lambda_r^{(l)} - \mu_r^{(l)} | r, l\right\} = \left\{3^0, 3^1, \dots, 3^{R'-1}\right\}$. Note that the bijection

$$[R] \times [L] \to [RL] \tag{28}$$

$$(r,l) \mapsto l - 1 + L \cdot (r - 1) \tag{29}$$

is arbitrarily chosen and can be replaced by any other bijection.

6 Arbitrary Dimensional Sub-Generators

6.1 Golomb Ruler

So far, we only considered QNNs under the constraint that all subgenerators are 2-dimensional, i.e. Hermitian operators acting on a single qubit. In [9, 33], this was extended to single layer QNNs with a $d = 2^R$ -dimensional generator, which is nothing other than allowing an arbitrary data-encoding H. In this case, the the frequency spectrum Ω is maximal in size with

$$|\Omega| = 2\binom{d}{2} + 1 = 2^R (2^R - 1) + 1$$
 (30)

if and only if the eigenvalues of H are a so called Golomb ruler. We extend this approach to QNNs with $k = 2^q$ -dimensional subgenerators and arbitrary many layers.

Definition 14 (Golomb Ruler) Let $\lambda_1, ..., \lambda_k \in \mathbb{R}$ with $\lambda_1 \leq ... \leq \lambda_k$. They are a Golomb ruler if all differences of pairs $\lambda_i - \lambda_j$ for $i \neq j$ are pairwise different. Equivalently, the set of differences has size

$$\left|\Delta\left\{\lambda_{1},...,\lambda_{k}\right\}\right| = 2\binom{k}{2} + 1. \tag{31}$$

The order of a Golomb ruler $G = \{\lambda_1, ..., \lambda_k\}$ is defined as

$$ord(G) := k, (32)$$

 $and\ its\ length\ as$

$$\ell(G) := \lambda_k - \lambda_1. \tag{33}$$

An optimal Golomb ruler is one with a minimal length over all Golomb rulers with the same order. A Golomb ruler is called perfect if $\mathbb{Z}_{\ell(G)} = \Delta G$, i.e. there are no gaps in ΔG .

Golomb rulers first appeared in [35] and have applications in astronomy [36], radio engineering [37, 38] and information theory [39].

Golomb rulers are linked to the maximum frequency spectrum in size. This is precisely the notion needed to avoid degeneracy, i.e. all frequencies except 0 occur

only once. We explain how to construct a single layer QNN using only k-dimensional generators with a maximum frequency spectrum. First, we need that the number of qubits q per generator divides R, otherwise it would be impossible to use only kdimensional generators with R qubits. Next, find a Golomb ruler $G = \{\lambda_1, ..., \lambda_k\}$ of order $k = 2^q$ and let $H \in \text{End}(\mathcal{B}^{\otimes q})$ be some Hermitian with eigenvalues $\lambda_1, ..., \lambda_k$. Then scale H by some appropriate factors $\beta_r \in \mathbb{R}$ to obtain the final generators $H_r := \beta_r \cdot H$. The key idea is to find a scaling such that the resulting frequency spectrum remains non-degenerate. However, choosing arbitrary Golomb rulers for Hand large factors β_r will lead to gaps in the resulting frequency spectrum Ω . For approximation properties, as in [10], one does not only want a large set Ω , but the largest possible $K \in \mathbb{N}$ such that $\mathbb{Z}_K \subseteq \Omega$, or at least as few gaps as possible. There are two ways to reduce the number of gaps. First, use an optimal Golomb ruler. If the Golomb ruler is even perfect, there are no gaps and both notions of maximality are equivalent. However, it can be shown that there is no perfect Golomb ruler of order $k \geq 5$ [40] and finding optimal Golomb rulers of large orders is a difficult task and sometimes conjectured to be NP-hard [41]. Second, choose the factors β_r as small as possible.

We would like to emphasise that in this work we do not investigate whether such non-separable generators H_r can be easily implemented on real physical hardware. This being said, the maximum frequency spectrum with respect to size is as follows.

Theorem 15 ($|\Omega|$ -Maximal Frequency Spectrum) The maximal frequency spectrum $\Omega_{\rm max}$ of a univariate single layer QNN with $k=2^q$ -dimensional generators $H_r \in End(\mathcal{H}_k)$, where q divides R, has size

$$|\Omega_{\text{max}}| = (4^q - 2^q + 1)^{R/q}.$$

By Theorem 9, if the QNN has more than one layers, the maximal frequency spectrum is hence given by

$$|\Omega_{\text{max}}| = (4^q - 2^q + 1)^{RL/q}.$$

Proof The frequency spectrum of any univariate single layer QNN with with no further restrictions to the data encoding layers and $k=2^q$ -dimensional generators $H_r \in \text{End}(\mathcal{B}^{\otimes q})$ is given by

$$\Omega := \Omega_1 \left(\bigoplus_{r=1}^{R/q} H_r \right) = \sum_{r=1}^{R/q} \Delta \sigma(H_r). \tag{34}$$

An upper bound to the size of the frequency spectrum is given by

$$|\Omega| \le |\Delta\sigma(H_r)|^{R/q} \le \left(2\binom{k}{2} + 1\right)^{R/q} = \left(4^q - 2^q + 1\right)^{R/q},$$
 (35)

where equality holds if and only if $\sigma(H_r)$ is a Golomb ruler of order k for all r=1,...,R/q and each sum $\sum_{r=1}^{R/q} \omega_r \in \sum_{r=1}^{R/q} \Delta \sigma(H_r)$ is unique. We explicitly construct a set of generators $H_r = \beta_r \cdot H$ such that these conditions are

satisfied. Let $H \in \text{End}(\mathcal{B}^{\otimes q})$ such that $\sigma(H) \subseteq \mathbb{Z}$ is a Golomb ruler. Choose any integer $\beta \geq 1$

 $2\ell(\sigma(H))+1$ and set $\beta_r:=\beta^{r-1}\in\mathbb{N}$. Then all $\sigma(H_r)$ are Golomb rulers since $\sigma(H_r)=\beta_r\cdot\sigma(H)$ and Golomb rulers are independent from scaling. Now assume $\sum_{r=1}^{R/q}\beta_r\omega_r=\sum_{r=1}^{R/q}\beta_r\omega_r'$ with $w_r,w_r'\in\Delta\sigma(H)$ for all r=1,...,R/q. Re-arranging the sums yields

$$eta \cdot \left(\sum_{r=2}^{R/q} eta^{r-2} (\omega_r - \omega_r')
ight) = \omega_1' - \omega_1.$$

Since $|\omega_1' - \omega_1| \leq 2\ell(\sigma(H))$ and $\beta > 2\ell(\sigma(H))$, this is only possible if $\omega_1 = \omega_1'$ and $\sum_{r=2}^{R/q} \beta^{r-2}(\omega_r - \omega_r') = 0$. Repeating this argument inductively, this yields $w_r = w_r'$ for all r = 1, ..., R/q. Hence the sums are unique and therefore the H_r build a set of generators with maximal frequency spectrum as mentioned.

Note that we can recover the results of the previous section for k=2. In this case q=1 and therefore $|\Omega_{\max}|=3^{RL}$. Moreover, since k<5, using a perfect Golomb ruler and minimal β_r as in the proof of Theorem 15, there are no gaps in the frequency spectrum, thus obtaining the results of Theorem 13. If q=R and therefore k=d, the result matches that in [33] for single layer models.

6.2 Relaxed Turnpike Problem

While a Golomb ruler is the right concept to maximise the size of the frequency spectrum, it is unsuitable for maximising $K \in \mathbb{N}$ such that $\mathbb{Z}_K \subseteq \Omega$. However, for the universality result in [10], it was crucial to have a wide range of integers without gaps in the frequency spectrum, hence such a maximally large K. Technically speaking, whereas in the Golomb ruler setting we were looking for a set S such that ΔS has no degeneracy, here we are looking for a set $S \subseteq \mathbb{Z}$ of a given size S such that S for a maximally large S is somewhat related to what is known as the turnpike problem or the partial digest problem [42].

Definition 16 (Turnpike Problem) Given a multiset M of $\binom{d}{2}$ integers, find a set $S \subseteq \mathbb{Z}$ (of size d) such that $\Delta S = M$ (here, the difference is also understood as a multiset) if possible, else prove that there is no such set S.

The turnpike problem occurs for example in DNA analysis [43], X-ray crystallography [44, 45] and other fields. Algorithms have been proposed to solve the turnpike problem based on, for example, backtracking [46] or factoring polynomials with integer coefficients [47].

However, the turnpike problem is not precisely what we need here in our setting. For the frequency spectrum, the number of occurrences of a frequency is irrelevant, so here we only need M to be a set. Furthermore, we do not want to set $\mathbb{Z}_K = M$, but rather $\mathbb{Z}_K \subseteq M$, hence relaxing some constraints. For this reason, we call this modification the relaxed turnpike problem.

Definition 17 (Relaxed Turnpike Problem) Given $d \in \mathbb{N}$, find a set $S \subseteq \mathbb{Z}$ of size d such that

$$K(S) := \max \left\{ K \in \mathbb{N}_0 \middle| \ \mathbb{Z}_K \subseteq \Delta S \right\} \tag{36}$$

is maximal, i.e. for all sets $S' \subseteq \mathbb{Z}$ of size d one has $K(S') \leq K(S)$. S is called a solution of the relaxed turnpike problem. Note that always $K(S) \leq \binom{d}{2}$.

To find a solution to the relaxed turnpike problem, we propose a not necessarily efficient algorithm.

Theorem 18 (Algorithmic Solution of the Relaxed Turnpike Problem) For a given size $d \in \mathbb{N}$, define the finite set of candidates

$$C := \left\{ \{s_1, s_2, ..., s_d\} \subseteq \mathbb{Z} | \ 0 < s_{i+1} - s_i \le \begin{pmatrix} d \\ 2 \end{pmatrix} \ \forall i = 1, ..., d-1, \ s_1 = 0 \right\}.$$
 (37)

Then C contains a solution to the relaxed turnpike problem. It can be found by iterating over all $S' \in C$ and returning the set S with the largest K(S').

Proof Let $S = \{s_1, ..., s_d\} \subseteq \mathbb{Z}$ with $s_1 < ... < s_d$ be a solution of the relaxed turnpike problem. Given that $\Delta S = \Delta S'$ for $S' = \{0, s_2 - s_1, ..., s_d - s_1\}$, we may assume without loss of generality that $s_1 = 0$ and $s_i \geq 0$ for all $i \in \{1, ..., d\}$. Suppose there exists an index $j \in \{1, ..., d-1\}$ for which $s_{j+1} - s_j > {d \choose 2}$. We then partition S into two subsets:

$$A := \{s_1, ..., s_j\}$$
$$B := \{s_{j+1}, ..., s_d\}.$$

Let K := K(S). For every element $e \in A\Delta B$ it holds

$$|e| \ge s_{j+1} - s_j > \binom{d}{2} \ge K. \tag{38}$$

The assumption

$$k \in \Delta S = \Delta A \cup \Delta B \cup A \Delta B \tag{39}$$

implies that $k \in \Delta A$ or $k \in \Delta B$ for all $k \in \{1, ..., K\}$. Define $c := s_{j+1} - s_j - K - 1 \ge 0$ and set

$$B' = \{s'_{j+1}, ..., s'_d\} := B - c = \{s_{j+1} - c, ..., s_d - c\},\$$

$$S' := A \cup B'.$$

Because $\Delta B' = \Delta B$, the set $\Delta S'$ also contains all integers $k = 1, \ldots, K$. However, it would also contain $K + 1 = s'_{j+1} - s_j$, contradicting the premise that S is a solution to the relaxed turnpike problem where K is maximal over all sets of size d. Thus, our assumption that there exists an index j with $s_{j+1} - s_j > {d \choose 2}$ must be false. Consequently, the solution S to the turnpike problem must be an element of the candidate set C.

Note that the size of the candidate set C is $\binom{d}{2}^{d-1}$, making it impractical to iterate over all candidates, even for small d. For $d=1,\ldots,8$ we computed all solutions of the relaxed turnpike problem, see Table 2. Note that in the context of QNNs, d must be a power of 2. For $d \leq 4$ the solutions are also perfect Golomb rulers, so the first case where the maximality in size and the maximality in K differ is d=8.

With the previous thoughts we are prepared to return to the initial problem of searching for a QNN such that its frequency spectrum Ω contains \mathbb{Z}_K with maximally large $K \in \mathbb{N}$.

d	Example S	K	Number of solutions	$ \mathbf{C} $
1	{0}	0	1	1
2	$\{0, 1\}$	1	1	1
3	{0,1,3}	3	2	9
4	{0,1,4,6}	6	2	216
5	{0,1,2,6,9}	9	8	10,000
6	{0,1,2,6,10,13}	13	14	759,375
7	$\{0, 2, 7, 13, 16, 17, 25\}$	18	8	85,766,121
8	{0, 8, 15, 17, 20, 21, 31, 39}	24	2	13,492,928,512

Table 2 Example solution $S \in C$, K = K(S) and number of solutions found in C of the relaxed turnpike problem for d = 1, ..., 8. The shown example is the solution with the lowest lexicographical order, defined from left two right.

Theorem 19 (K-Maximally Frequency Spectrum) For a given dimension $d=2^R$, $K \in \mathbb{N}$ is maximal such that $\mathbb{Z}_K \subseteq \Omega$ for some univariate single layer QNN with a d-dimensional generators $H \in End(\mathcal{B}^{\otimes R})$ and frequency spectrum Ω if and only if the eigenvalues of H are a solution of the relaxed turnpike problem.

Proof For any univariate single layer QNN with one arbitrary generator $H \in \text{End}(\mathcal{B}^{\otimes R})$, the frequency spectrum is given by

$$\Omega = \Delta \sigma(H).$$

By definition K is maximal if and only if $\sigma(H)$ is a solution of the turnpike problem (cases in which eigenvalues occur twice can be excluded directly).

The previous theorem cannot be extended in a trivial way to QNNs with k-dimensional generators and an arbitrary number of layers. By scaling we can construct a QNN such that $\mathbb{Z}_{K'} \subseteq \Omega$ with $K' = (2K+1)^{L \cdot R/q} - 1$, where K = K(S) and S is a solution of the relaxed turnpike problem of size k, but it is not guaranteed that this K' is maximal.

Theorem 20 (Extension to more General Settings) Let $k = 2^q$ with $q \mid R$ and let $H \in End(\mathcal{B}^{\otimes q})$ be Hermitian, such that $\sigma(H)$ is a solution of the relaxed turnpike problem of size k. Further, let $K := K(\sigma(H))$, $\beta_r := (2K+1)^{r-1}$ and $H_r := \beta_r \cdot H$. Then

$$\mathbb{Z}_{\underbrace{(2K+1)^{R/q}-1}} \subseteq \Omega \tag{40}$$

for the frequency spectrum Ω of the single layer QNN with the k-dimensional generators H_r . By Theorem 9, this can be extended to multi layer models with non equal layers, hence there exists a QNN with

$$\mathbb{Z}_{\frac{(2K+1)^{R \cdot L/q} - 1}{2}} \subseteq \Omega. \tag{41}$$

Proof Again, the frequency spectrum Ω is given by

$$\Omega = \sum_{r=1}^{R/q} \beta_r \Delta \sigma(H). \tag{42}$$

Each
$$k \in \left\{0, \dots, \frac{(2K+1)^{R/q}-1}{2}\right\}$$
 can be (uniquely) written as $k = \sum_{r=1}^{R/q} k_r (2K+1)^{r-1}$ with $k_r \in \{-K, \dots, K\} \subseteq \Delta \sigma(H)$, thus $k \in \Omega$.

7 Conclusion and Outlook

In this work, we have examined the properties of the frequency spectrum of QNNs in more detail. We focused on models whose approach consists of alternating parameterized encoding layers.

First, we introduced the parallel and sequential ansatz and discussed the representability of QNNs by finite Fourier series. It was observed that the frequency spectrum of the multivariate model is the Cartesian product of the frequency spectrum of univariate models. Therefore, we could restrict ourselves to univariate models. We then introduced the concept of spectral invariance under area-preserving transformations. This states that the frequency spectrum of a QNN is invariant under certain transformations of the ansatz that leave the area A=RL unchanged, where R is the number of qubits and L the number of layers. The consequence of this is that, from a frequency spectrum point of view, the maximum frequency spectrum depends only on the area A=RL and not on the individual R and L. In addition, one can consider single-layer or single-qubit models and extend frequency-spectrum results to QNNs of arbitrary shape. This explains various symmetry results in R and L in the literature. We emphasize that we do not make any statement about possible changes in the coefficients or expressibility of the finite Fourier series under such transformations.

Furthermore, we have comprehensively clarified how the generators of a QNN must be chosen in order to obtain a maximal frequency spectrum. For that, we have distinguished two cases of maximality, namely maximal in the size $|\Omega|$ of the frequency and maximal in K such that $\mathbb{Z}_K \subseteq \Omega$. Second, we distinguish between cases where the generators can be decomposed into 2-dimensional and arbitrary-dimensional subgenerators. For 2-dimensional sub-generators, we have extended known exponential encoding methods to QNNs with arbitrary number of layers, both under the assumption of equal data encoding layers and for arbitrary data encoding layers. While the terms of maximality coincide for 2-dimensional generators, this is not the case for generators of arbitrary dimensions. To maximize the size $|\Omega|$ of the frequency spectrum, we extended existing results to QNNs with arbitrary number of layers and arbitrary dimensional generators based on the concept of a Golomb ruler. For maximality in K, we introduced the relaxed turnpike problem, which is a variation of the classical turnpike problem, and proved that a univariate single layer QNN with one generator is maximal if and only if the eigenvalues are a solution to the relaxed turnpike problem. We explained how to extend that result to models with an arbitrary number of layers and sub-generators. However, the result may not be maximal in this case.

Although the focus was solely on the frequency spectrum, future work could expand the area-preserving transformations to include a transformation of the parameter encoding layers $W^{(l)}$ and the observable M. This would allow to study their impact on the entire Fourier series and could provide insights into the expressiveness and trainability of QNNs. An extension to other architectures of parametrized circuits could also be fruitful as a next step for further insights.

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Not applicable.

Author Contribution

Patrick Holzer and Ivica Turkalj contributed equally to this work.

Competing Interests

The authors declare no competing interests.

Appendix A Frequency Spectrum of Multivariate QNNs

We extend Theorem 7 to multivariate models and give a proof of Theorem 8 in this section. First, we begin with models with a parallel ansatz.

Theorem 21 (Multivariate Frequency Spectrum - Parallel Ansatz) Let $f(x) = \langle 0|U^{\dagger}(x)MU(x)|0\rangle$ be a multivariate QNN with a parallel ansatz. Then

$$f(x) = \sum_{\omega \in \Omega} c_{\omega} e^{-i\omega \cdot x}, \tag{A1}$$

with

$$\Omega = \sum_{l=1}^{L} \Delta(\sigma(H_{l,1}) \times \ldots \times \sigma(H_{l,N})).$$

Proof If $\lambda_0^{(l,n)},...,\lambda_{d-1}^{(l,n)}$ are the eigenvalues of $H_{l,n},$ we write

$$\boldsymbol{\lambda}_{\boldsymbol{j}}^{(l)} := \left(\lambda_{j_1}^{(l,1)}, ..., \lambda_{j_N}^{(l,N)}\right)^T \in \sigma(H_{l,1}) \times ... \times \sigma(H_{l,N}) \subseteq \mathbb{R}^N$$

for all $j \in [d]^N$ (recall that $d = 2^R$). To obtain the representation as a finite Fourier series, we again have to determine the action of $W^{(l)}$ and $S_l(x)$ on arbitrary vectors as in the proof of Theorem 7.

Let

$$|\boldsymbol{j}\rangle := |j_1,...,j_N\rangle := \bigotimes_{n=1}^N |j_n\rangle \in \bigotimes_{n=1}^N \mathcal{B}^{\otimes R} = \mathcal{B}^{\otimes R\cdot N}$$

for all $j \in [d]^N$, where $|0\rangle, ..., |d-1\rangle \in \mathcal{B}^{\otimes R}$ denotes the computational basis. The action of $W^{(l)}$ and $S_l(\boldsymbol{x})$ on some basis vector $|\boldsymbol{j}\rangle$ for $\boldsymbol{j}\in[d]^N$ are given by

$$W^{(l)}|\boldsymbol{j}\rangle = \sum_{\boldsymbol{i} \in [d]^N} W^{(l)}_{\boldsymbol{i},\boldsymbol{j}}|\boldsymbol{i}\rangle$$

and

$$S_{l}(\boldsymbol{x})|\boldsymbol{j}\rangle = \bigotimes_{n=1}^{N} e^{-ix_{n}H_{l,n}}|j_{n}\rangle$$
$$= e^{-i\sum_{n=1}^{N} x_{n}\lambda_{j_{n}}^{(l,n)}}|\boldsymbol{j}\rangle$$
$$= e^{-i\lambda_{\boldsymbol{j}}^{(l)} \cdot \boldsymbol{x}}|\boldsymbol{j}\rangle$$

where $W_{i,j}^{(l)} := \langle i|W^{(l)}|j\rangle \in \mathbb{C}$. We obtain the same equations as in the proof of Theorem 7, we only have to replace each index j by a multiindex j and the complex product $\lambda_j^{(l)} \cdot x$ by the scalar product $\lambda_{j}^{(l)} \cdot x$. We therefore obtain

$$U(\boldsymbol{x})|0\rangle = \sum_{\boldsymbol{j}^{(1)},...,\boldsymbol{j}^{(L+1)} \in [d]^N} \left(\prod_{l=1}^{L+1} W_{\boldsymbol{j}^{(l)},\boldsymbol{j}^{(l-1)}}^{(l)} \right) e^{-i\boldsymbol{x} \cdot \left(\sum_{l=1}^{L} \boldsymbol{\lambda}_{\boldsymbol{j}^{(l)}}^{(l)}\right)} |\boldsymbol{j}^{(L+1)}\rangle,$$

where $j^{(0)} := (0, ..., 0)$. Hence

$$f(\boldsymbol{x}) = \langle 0|U^{\dagger}(\boldsymbol{x})MU(\boldsymbol{x})|0\rangle = \sum_{\substack{\boldsymbol{k}^{(1)},...,\boldsymbol{k}^{(L+1)} \in [d]^{N} \\ \boldsymbol{j}^{(1)},...,\boldsymbol{j}^{(L+1)} \in [d]^{N}}} a_{\boldsymbol{k}^{(1)},...,\boldsymbol{k}^{(L)},\boldsymbol{j}^{(1)},...,\boldsymbol{j}^{(L)}} e^{i\boldsymbol{x} \cdot \left(\sum_{l=1}^{L} \left(\boldsymbol{\lambda}_{\boldsymbol{k}^{(l)}}^{(l)} - \boldsymbol{\lambda}_{\boldsymbol{j}^{(l)}}^{(l)}\right)\right)}$$

with

$$a_{\boldsymbol{k}^{(1)},...,\boldsymbol{k}^{(L)},\boldsymbol{j}^{(1)},...,\boldsymbol{j}^{(L)}} = \sum_{\boldsymbol{k}^{(L+1)},\boldsymbol{j}^{(L+1)} \in [d]^N} \left(\prod_{l=1}^{L+1} W_{\boldsymbol{k}^{(l)},\boldsymbol{k}^{(l-1)}}^{(l)} \right) \cdot \left(\prod_{l=1}^{L+1} \left(W^\dagger \right)_{\boldsymbol{j}^{(l-1)},\boldsymbol{j}^{(l)}}^{(l)} \right) \cdot M_{\boldsymbol{j}^{(L+1)},\boldsymbol{k}^{(L+1)}}.$$

Again, grouping all terms with the same frequencies together yields

$$f(x) = \sum_{\boldsymbol{\omega} \in \mathbf{\Omega}} c_{\boldsymbol{\omega}} e^{i\boldsymbol{\omega} \cdot \boldsymbol{x}}$$

with

$$\mathbf{\Omega} = \sum_{l=1}^{L} \Delta(\sigma(H_{l,1}) \times \dots \times \sigma(H_{l,N})). \tag{A2}$$

We now show that the parallel and the sequential ansatz lead to the same frequency spectrum.

Theorem 22 (Multivariate Frequency Spectrum - Sequential Ansatz) Let $f(x) = \langle 0|U^{\dagger}(x)MU(x)|0\rangle$ be a multivariate QNN with a sequential ansatz. Then

$$f(x) = \sum_{\omega \in \Omega} c_{\omega} e^{-i\omega \cdot x}$$
 (A3)

with the frequency spectrum Ω being the same as in the corresponding parallel ansatz from Theorem 21.

Proof The proof works very similarly to Theorem 7. We use the same notation for the eigenvalues of $H_{l,n}$ as in Theorem 21. The ansatz circuit is of the form

$$U(\mathbf{x}) = U_N(x_N) \cdots U_1(x_1). \tag{A4}$$

In the proof of Theorem 7 we have seen that

$$U_n(x_n)|j\rangle = \sum_{j_{L+1} \in [d]} \sum_{j \in [d]^L} \left(\prod_{l=1}^{L+1} W_{j_l, j_{l-1}}^{(l)} \right) e^{-ix_n \Lambda_j^{(n)}} |j_{L+1}\rangle$$
 (A5)

with $j_0 := j$ (we only considered j = 0 in the proof of Theorem 7) and $\Lambda_{\boldsymbol{j}}^{(n)} := \sum_{l=1}^{L} \lambda_{j_l}^{(l,n)}$. Applying all $U_n(x_n)$ consecutively, $U(\boldsymbol{x})$ has the form

$$U(\boldsymbol{x})|0\rangle = \sum_{\boldsymbol{j}^{(1)},...,\boldsymbol{j}^{(N+1)} \in [d]^L} c_{\boldsymbol{j}^{(1)},...,\boldsymbol{j}^{(N+1)}} e^{-i\sum_{n=1}^N x_n \Lambda_{\boldsymbol{j}^{(n)}}^{(n)}} |j_L^{(L+1)}\rangle.$$

The rest follows analogously to Theorem 21.

Finally, we proof Theorem 8 and show, that the frequency of the multivariate model is just the Cartesian product of the frequency spectra of the corresponding univariate models.

Proof This follows from Lemma 4 about the Minkowski sum.

$$\Omega_{L,N}\left(\left(H_{l,n}\right)_{l,n}\right) = \sum_{l=1}^{L} \Delta(\sigma(H_{l,1}) \times \ldots \times \sigma(H_{l,N}))$$

$$= \sum_{l=1}^{L} \Delta(\sigma(H_{l,1})) \times \ldots \times \Delta(\sigma(H_{l,N}))$$

$$= \sum_{l=1}^{L} \Delta(\sigma(H_{l,1})) \times \ldots \times \sum_{l=1}^{L} \Delta(\sigma(H_{l,N})))$$

$$= \Omega_{L}\left(H_{1,1}, \ldots, H_{L,1}\right) \times \cdots \times \Omega_{L}\left(H_{1,N}, \ldots, H_{L,N}\right).$$

Appendix B Proof of Lemma 11

Proof One can easily check that $z_r = (2L+1)^{r-1}$ for all r = 1, ..., R is indeed a solution of the problem.

To prove the uniqueness, we first show that $\sum_{r=1}^{R} z_r \cdot \mathbb{Z}_L = \mathbb{Z}_{\frac{(2L+1)R-1}{2}}$ if and only if

$$\sum_{r=1}^{R} z_r \cdot [2L+1] = \left[(2L+1)^R \right]. \tag{B6}$$

Since all $z_1,...,z_R$ are non negative, one has $T:=\sum_{r=1}^R z_r\cdot L=\frac{(2L+1)^R-1}{2}$ as it is the maximal element of both sides. Then

$$\sum_{r=1}^{R} z_r \cdot [2L+1] = \sum_{r=1}^{R} z_r \cdot (\mathbb{Z}_L + L) = \left(\sum_{r=1}^{R} z_r \mathbb{Z}_L\right) + T = \mathbb{Z}_{\frac{(2L+1)^R - 1}{2}} + T = \left[(2L+1)^R\right]. \tag{B7}$$

The opposite direction is analogue. Hence we consider the equation $\sum_{r=1}^{R} z_r \cdot [2L+1] = \left[(2L+1)^R \right]$ from now on. The set on the left hand side has maximally size

$$\left| \sum_{r=1}^{R} z_r \cdot [2L+1] \right| \le (2L+1)^R, \tag{B8}$$

thus it could only be equal $\left[(2L+1)^R\right]$ if all sums $\sum_{r=1}^R z_r \cdot s_r \in \sum_{r=1}^R z_r \cdot [2L+1]$ are pairwise different. Further, all $z_1, \ldots, z_R \in \mathbb{N}_0$, since

$$z_r \in \sum_{r=1}^R z_r \cdot [2L+1] = \left[(2L+1)^R \right] \subseteq \mathbb{N}_0.$$
 (B9)

As a consequence $z_1 \geq 1$, else

$$0 = 0 \cdot z_1 + \ldots + 0 \cdot z_R = 1 \cdot z_1 + 0 \cdot z_2 + \ldots 0 \cdot z_R$$
(B10)

and the sums would therefore not be pairwise different. We can conclude further that $z_1=1$ from $1\leq z_1\leq\ldots\leq z_R$, else

$$1 < z_1 \le s_1 \cdot z_1 + \ldots + s_R \cdot z_R \tag{B11}$$

if at least one coefficient is non zero, contradicting $1 \in \left[(2L+1)^R \right] = \sum_{r=1}^R z_r \cdot [2L+1]$. Since $z_1 = 1$ and $s = z_1 \cdot s$ for all $s \in [2L+1]$, we conclude that $z_2 \geq 2L+1$, again by uniqueness of the sums. By the same reasons, $z_2 > 2L+1$ would lead to a contradiction because then

$$2L + 1 < z_2 \le s_1 \cdot z_1 + \ldots + s_R \cdot z_R \tag{B12}$$

if at least one of $s_2, \ldots s_R$ is non zero and therefore $2L+1 \notin \sum_{r=1}^R z_r \cdot [2L+1] = \left[(2L+1)^R \right]$. Repeating this argument, one concludes $z_r = (2L+1)^{r-1}$.

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