Optimality of Finite Parameter Shift Rules for Derivatives of Variational Quantum Circuits

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Abstract

Variational (or, parameterized) quantum circuits are quantum circuits that contain real-number parameters, that need to be optimized/"trained" in order to achieve the desired quantum-computational effect. For that training, analytic derivatives (as opposed to numerical derivation) are useful. Parameter shift rules have received attention as a way to obtain analytic derivatives, via statistical estimators.

In this paper, using Fourier Analysis, we characterize the set of all shift rules that realize a given fixed partial derivative of a multi-parameter VQC. Then, using Convex Optimization, we show how the search for the shift rule with smallest standard deviation leads to a primal-dual pair of convex optimization problems.

We study these optimization problems theoretically, prove a strong duality theorem, and use it to establish optimal dual solutions for several families of VQCs. This also proves optimality for some known shift rules and answers the open question.

As a byproduct, we demonstrate how optimal shift rules can be found efficiently computationally, and how the known optimal dual solutions help with that.

This is an extended abstract missing some proofs.

Keywords: Parameterized quantum circuits, variational circuit optimization.

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1 Introduction

Near-term quantum algorithms meant to be run on pre-fault-tolerant quantum computing devices often employ the concept of containing parameters, which are being optimized/"trained" to maximize the utility of the quantum algorithm for the particular application. The concept is known, depending on the application area, as Variational Quantum Program, Parameterized Quantum Circuit, Quantum Neural Network, etc (see [3] and the references therein).

Typical examples include the various types of Quantum Neural Networks for quantum machine learning applications (e.g., [15, 2]), Variational Quantum Eigensolvers for electronic structure computations (e.g., [23]), and, to varying degrees, Quantum Approximate Optimization Algorithms [6].

One way of training the parameters of a variational or parameterized quantum circuit deploys some type of smooth optimization algorithms such as (stochastic) gradient descent or second order methods or whatnot, in other words, it requires derivatives, be they first order (e.g., [15, 18]), or higher order (e.g., [13, 19]). While, of course, the standard formulas of numerical analysis yield approximations for derivatives, the interest is in so-call analytic derivatives, which don’t approximate (with some $\varepsilon > 0$ that has to be chosen carefully) the derivatives, but estimate the exact derivative. Tickling these analytic derivatives, of any order, out of the quantum circuit is the subject matter of this paper.

Interestingly, the interest in efficient methods for estimating derivatives seems to have become more and more interesting, e.g., [4, 9, 1, 11, 10, 22, 12].

In this paper, we consider parameterized quantum circuits which, with parameters set to $x \in \mathbb{R}^d$, apply a quantum operation $\mathcal{E}(x)$ to an initial quantum state $\rho_0$, and in the resulting state, a fixed observable $\mu$ is measured. The expectation value $f(x) := \text{tr}(\mu \mathcal{E}(x)(\rho_0))$ is the quantity of which one wishes to find the derivatives. In other words, we are interested in the (partial) derivatives of the expectation value function

$$f : \mathbb{R}^d \rightarrow \mathbb{R} : x \mapsto \text{tr}(\mu \mathcal{E}(x)(\rho_0)).$$

Moreover, we consider the situation where each of the parameters enter the parameterized quantum circuit via one-parameter subgroups of unitary operators, i.e., mappings $U(\cdot)$.
with \(U(0)\) equal to the identity and for all \(s, t \in \mathbb{R}\), we have \(U(s + t) = U(s)U(t)\). Each parameter of the PQC could appear in one or several places of the quantum circuit, with the same or different one-parameter subgroups. One-parameter subgroups are, of course, of the form \(U(\xi) = e^{i\xi H}\) for a Hermitian operator \(H\). (Note the author’s idiosyncratic scaling factor \(2\pi\), that matches the standard Fourier transform in Harmonic Analysis.)

This is the setting that seems to be considered in the majority of derivative estimation research, although other settings exist, e.g., the “stochastic” parameter shift rules of [1], which applies to parameterized unitaries of the form \(t \mapsto e^{i(tA+B)}\). Our results don’t cover these types of parameterized unitaries.

To our knowledge, analytic derivatives of Parameterized Quantum Circuits have been introduced into near-term quantum programming in [15].

Soon after [15], the trivial observation was made that, in full generality, the expectation value functions of parameterized quantum circuits into which the parameters enter through one-parameter subgroups can be characterized in terms of their Fourier properties [20, 4, 7]. This fact can be exploited directly for the optimization/training of the PQC [20, 17], but it also has bearing on shift rules for derivatives, most notably in [22, 12], the main references of the present paper.

Indeed, the present paper applies Harmonic Analysis and Convex Optimization to prove the optimality, in terms of the standard deviation of the resulting estimator, of some parameter shift rules. Unfortunately, the shift rules for which we prove optimality are mostly known from [22]. However, our paper adds the certainty that no better shift rules (in terms of stddev) exist.

**Basic approach.** We find that things get simpler if we abstract from the quantum-circuit origin of the functions and work with their Fourier analytic properties: Expectation value functions are real valued, and for a parameterized quantum circuit with \(d\) parameters (it’s OK to count only parameters participating in the partial derivative), there exists a finite set \(\Xi \subset \mathbb{R}^d\) which contains the Fourier spectrum of the expectation value function. As the function is real valued, the set \(\Xi\) is symmetric, meaning:

\[
\Xi = -\Xi = \{ -\xi \mid \xi \in \Xi \}. \tag{1}
\]

We refer to finite, symmetric sets \(\Xi \subset \mathbb{R}^d\) as frequency sets of PQCs.

While every such set can occur as the support of the expectation value function of a Parameterized Quantum Circuit (see Proposition 4 below) we acknowledge that, for \(d > 1\), only a small subclass of frequency sets are truly of interest, mostly because a (small) set \(\Xi\) containing the Fourier spectrum has to be somehow read off from the PQC before shift rules can be constructed and applied. See §2.1 below for (mostly known) examples of frequency sets of expectation value functions of PQCs which can be found by inspecting the parameterized quantum circuit.

Before we summarize some of the contributions of this paper, we draw the reader’s attention to Table 1 which lists the notations frequently used in this paper, for easy reference.

**The contributions of this paper.** (1) Using elementary Harmonic Analysis, for any \(d \in \mathbb{N}\) and any given finite symmetric set \(\Xi \subset \mathbb{R}^d\), and for fixed \(\alpha \in \mathbb{N}^d\), we characterize the set of all shift rules which realize the partial derivative\(^1\) \(\partial^\alpha := \prod_{j=1}^{d} \partial_{j}^{\alpha_j}\) for every real-valued function with Fourier spectrum contained in \(\Xi\). We refer to these shift rules as “feasible”. As we explain in §2.3, at the heart of our characterization is a finite, underdetermined linear system of equations, not unlike, but more general than those that occur in [22, 12] where the systems are used to search for shift rules.

\(^1\)In the math sense, en.wikipedia.org/wiki/Partial_derivative.
Table 1: Overview of notations. Habits of notation in Physics and Math / Theoretical Computer Science are very different, which is why we list the notations which are used throughout this paper, particularly the arcane ones.

Our more general characterization is necessary because it allows us to (2) realize the search for the optimal shift rule (among all possible shift rules) as a the problem of minimizing a convex function over that set (§2.5).

The word “optimal”, of course, requires the concept of a “cost” of a shift rule. We use a cost measure closely related to (the same, really) one proposed in [22] and called the “number of shots” there. It can be understood as (a) an (asymptotic) standard deviation of an estimator in the worst case over all parameterized quantum circuits; or (b) for the Functional/Numerical Analyst, as the operator norm of the shift rule when viewed as a linear operator between the obvious normed spaces. As usual, the latter perspective allows us to view the “cost” as the worst-case bound on how noise in the input function (e.g., sampled estimate of the expectation value function) is blown up in the output function (e.g., estimate of the derivative of the expectation value function).

As a nice coincidence, our cost measure can also be understood (c) as a heuristic to minimize the quantity that in [22] is called the “number of unique circuits”, i.e., the number of “shift vectors” used — we refer to it as the size of the support of the shift rule.

See §2.4 for the formal definition of our cost function, and for discussions related to (3a,3b,3c).

We emphasize that in this paper the phrase “cost of a shift rule” refers to one fixed mathematical concept (with three different justifications) — we do not switch between different resource requirement concepts. However, we also emphasize that much of the technical toolkit we develop carries through to other cost functions: For other “linearizable” cost functions (our cost function has that property, see §2.6.b) most of our tools still work; for general convex cost functions the duality concept (see below) will suffer; for cost functions that require
on/off decisions (such as for the provably-optimal minimization of the size of the support), we exit the land of comforting convexity, and enter the realm of NP hardness.

As we are interested only in “finite” shift rules, i.e., where the size of the support is finite, the resulting optimization problem has a finiteness condition which, ostensibly, falls out of the scope of standard convex optimization. Nonetheless, (3) we establish a dual convex optimization problem (this one perfectly standard), and prove strong duality theorems: A pair of primal and dual solutions are both optimal, if, and only if, (4a) so-called complementary slackness holds, (4b) the objective function values are the same; see §2.7.

(5) En passant in §2.6, we outline how, in the cases where optimal shift rules cannot be found on paper, standard computational convex optimization techniques when applied to the dual convex program yield optimal solutions to it, and how, from these dual-optimal solutions, optimal finite feasible shift rules can be obtained computationally.

**Computational Method 1.** Let $d \in \mathbb{N}$ be a fixed parameter.

There exist efficient algorithms for the following task:

Given as input a finite symmetric set $\Xi \subset \mathbb{R}^d$ and $\alpha \in \mathbb{N}^d$, and a precision parameter $\varepsilon > 0$, return a near-optimal near-feasible shift rule (where “near” is controlled through the precision parameter).

Moreover, heuristically, in cases where there are several optimal shift rules, one can hope for a shift rule with small support.

We also have simpler methods for the cases when optimal dual solutions can be obtained analytically (which happens often, see below).

The computational cost of the method depends on $d$ and $1/\varepsilon$. While everything else in this paper is (meant to be) fully rigorous, we will not prove that our method(s) run in polynomial time (for fixed $d$): They are typical standard approaches in mathematical optimization that are widely used both in practice (cutting-plane generation methods) and in computational complexity theory (proofs of poly-time running times based on the Ellipsoid method).

Instead, we invite the reader to check out the supplementary source code written in the mathematical computation programming language Julia\(^3\) demonstrating the methods in the form of Pluto\(^4\) notebooks; see Appendix A. We point out that the source code is only for demonstration of the algorithms, and will run into numerical instabilities when the frequency sets get a little bit nasty.

In \([22, 12]\), searches for shift rules based on more restricted linear-system characterizations are performed manually. But to our knowledge, no method is known to efficiently find, analytically or computationally, low-cost shift rules, except in the cases of the simplest frequency sets.

(6) Finally, we use the duality theorems to prove optimal shift rules for some situations arising from parameterized quantum circuits, see §2.9.

For that, we need to distinguish two types of frequency sets — ones that generate lattices in $\mathbb{R}^d$, which we call lattice generating, and ones that generate dense subgroups of sub-vector spaces of $\mathbb{R}^d$. We’ll elaborate on that distinction (known to every mathematician) below (§2.9). For now we just mention that (a) a function is periodic if, and only if, its Fourier spectrum is lattice generating (Appendix B.1); (b) a set is lattice generating if, and only if, after a change of basis (“re-scaling”), it is integral (mathematical folklore); (c) for example, for $d = 1$, if every element of the frequency set is a rational multiple of a fixed real constant, then the frequency set is lattice generating.

\(^2\)The reason why $d$ has to be fixed is that the methods involve minimizing a function with Fourier spectrum contained in $\Xi \subset \mathbb{Q}^d$, which can be done efficiently only for fixed $d$.

\(^3\)juliablog.org

\(^4\)plutojlab.org
(6a) For any $d, \alpha, \Xi$, we prove that a finite feasible optimal shift rule exists, and Wierichs et al.’s quantity “number of unique circuits” (what we call the size of the support of the shift rule) is at most $|\Xi|$. (Examples are known that show that the bound is tight.)

(6b) For $d = 1$, any frequency set $\Xi$, and any $\alpha$, we quantify the cost of optimal shift rules:

$$\text{It is } (2\pi \max |\Xi|)^\alpha \text{ (note that } \alpha \in \mathbb{N} \text{ if } d = 1).$$

In the simplest case, if the frequency set has the form (for a positive integer $m$ and a positive real number $\xi_1$)

$$\Xi = \{k\xi_1 | k \in \mathbb{Z}, |k| \leq m\},$$

we prove the optimality of the shift rule that was given in [22] for that case. But, for all other lattice generating $\Xi$, we prove that the corresponding shift rule is still optimal in terms of its cost! In other words, it is impossible for a shift rule to exploit “gaps” in the set of frequencies to obtain lower cost. This closes an issue that was left open in [22]. However, regarding the size of the support, in view of (6a), it will become clear that for sparse frequency sets, there are optimal shift rules with different support sizes. As outlined above, our computational method can be heuristically hoped to find a shift rule with small support.

Particularly for $d = 1$, we show that an optimal shift rule exists whose support size is at most $|\Xi| - (\alpha - 1)%2$. This means that there are optimal shift rules among those described in general forms in [22, 12]. We point out that our simple formula for the cost of optimal finite shift rules holds in full generality, i.e., also for non-lattice-generating $\Xi$.

(6c) For $d \geq 2$ our results are not comprehensive. We quantify the cost of optimal shift rules only for frequency sets satisfying a restrictive technical condition (“pointy”). The condition includes the case when $\Xi$ is a product set, which is the only one that if considered in [22] — it is questionable, though, whether more complicated frequency sets can be identified a priori, by inspecting the parameterized quantum circuit or performing a small number of expectation-value estimations that probably shouldn’t depend on any other parameters.

Note that in this paper, we don’t consider savings that can be gained by computing several partial derivatives, e.g., a complete Hessian, as is done in [22].

The results in (6b) and (6c) are obtained by establishing a dual-optimal solution — we consider these dual-optimal solutions to be a major contribution of this paper. Once we have dual-optimal solutions, using our other theorems, the (existence and) cost of optimal shift rules can easily derived, and one of our computational methods (see above) demonstrates a possible way to computationally find a (heuristically) sparse optimal shift rule even for rugged frequency sets, based on the dual-optimal analytic solution.

About non lattice generating frequency sets. It is prudent to point out a danger of misunderstanding [22]: There, the innocent reader might think of a dichotomy between an equi-spaced Fourier spectrum $\{k\xi_1 | k = -K, \ldots, K\}$ on the one hand, and non-periodicity on the other. While functions with equi-spaced Fourier spectrum are periodic, the converse is, of course, not true. Indeed, the periodicity of the function is equivalent to the Fourier spectrum generating a lattice.

Wierichs et al. (Appendix B.1) talk about frequencies which cannot be scaled to be integral, and use the phrase not periodic in that context, in the case $d = 1$. It is not clear to the author of the current paper what they mean.

Note also that a frequency set that is not lattice generating cannot be represented in a computer: A representation of the vectors/points in any basis will always require coefficients that are not rational.

Why bother with non-lattice-generating Fourier spectra at all? Clearly, from a practical point of view, all frequency sets are lattice generating, and the treatment of non-lattice-generating frequency sets brings some difficulty. (For example, it is not clear whether an optimal feasible shift rule exists, i.e., whether the infimum of the costs is not attained.)

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5In this paper, we give the complete proof only for $\alpha \leq 4$ and we refer to a forthcoming paper for the proof of a technical lemma for $\alpha > 4$. 

6
The reason is that lattice generating frequency sets can sometimes blow up the complexity. Consider, say, 10 31-bit unsigned fixed-point numbers $\xi_1, \ldots, \xi_{10} \in [0, 2]$ chosen uniformly at random, and consider a corresponding (random) real-valued function that has, as its Fourier spectrum, the set $\Xi := \{0\} \cup \{\pm \xi_j \mid j = 1, \ldots, 10\}$. Clearly, $\Xi$ is lattice generating, but the probability that its period is smaller than $2^{29}$ is at roughly one in a million. Hence, treating this frequency set as lattice generating, while correct, does not make the problem of finding a finite optimal shift rule feasible. Considering non-lattice-generating frequency sets, on the other hand, and trading elusive optimality (on account of non-representability in a computer memory) for near-optimality (off by at most an arbitrary given $\varepsilon > 0$), immediately leads to tools such as simultaneous Diophantine approximation (and so to continued fractions, LLL algorithm, etc).

While that offer sufficient motivation, we believe, for not excluding non-lattice-generating frequency sets, in the present paper, we do not pursue the algorithmic approaches that they inspire.

Outline of the paper. In the next section, we give a detailed technical overview of our results, along with pointers to the proofs in the the later sections. In Section ?? we cover the set of feasible (finite) shift rules, the non-emptiness of that set, and we discuss some properties of the cost function. Section ?? contains the proofs of the duality theorems. In Section ?? we establish (near-)optimal feasible shift rules for common partial derivatives of variational quantum circuits. We wrap things up in the concluding Section 3.

2 Technical overview

We give an overview with rigorous definitions and statements of theorems, with references to the proof in the later sections.

2.1 Function spaces from expectation values of parameterized quantum circuits

Fix a $d \in \mathbb{N}$, and let $\Xi$ be a fixed finite, symmetric subset of $\mathbb{R}^d$. We define the vector space of functions

$$K_\Xi := \{ f : \mathbb{R}^d \to \mathbb{R} \mid f \text{ smooth and bounded } \supp \hat{f} \subseteq \Xi \}$$

The Fourier transform of the bounded smooth function here is, technically, that of tempered distributions, but the finiteness of the spectrum renders this machinery trivial. Indeed, we have

$$\mathcal{X}_\Xi = \{ f : x \mapsto \sum_{\xi \in \Xi} b_\xi e^{2\pi i \xi \cdot x} \mid c \in \mathbb{C}^\Xi \text{ with } b_{-\xi} = b_\xi^* \};$$

with $u \cdot v := \sum_j u_j v_j$.

We emphasize our conventions for the Fourier transform: $\hat{f}(\xi) = \int f e^{-2\pi i \xi \cdot x} f(x) \, dx$ — the crucial part being the $2\pi$ in the exponent! This choice goes hand in hand with our decision to normalize Hamiltonian evolution to $t \mapsto e^{2\pi i H t}$. It leads to factors of powers of $2\pi$ in the derivatives and hence the standard deviations of the estimators of the derivatives.

As indicated above, we find it adds clarity to the subject matter to think in terms of function spaces rather than in terms of Hamiltonians or parameterized quantum circuits. As this also adds some generality that is not required to address the currently known applications, we find it prudent to restrict to function spaces which arise from practically relevant parameterized quantum circuits whenever that simplifies the mathematics. However, we refer to
the Proposition 4 below (§2.1.c) as a justification for working with function spaces with arbitrary frequency sets: Every function can all be realized as the expectation value function of a parameterized quantum circuit.

We now go through some common examples of parameterized quantum circuits and their function spaces. What follows is well-known and treated in detail elsewhere, e.g., [22].

2.1.a. A single Hamiltonian. The fact that evolution under a Hamiltonian produces a Fourier spectrum consisting of the differences between the eigenvalues has been observed long ago, e.g., [7, 20].

For easy reference, we pack the statement into a proposition. For convenience, let us define the difference set

$$\text{Diff } \Lambda := \{ \lambda' - \lambda \mid \lambda, \lambda' \in \Lambda \}$$

and the spectrum $\text{Spec}(A)$, the set of eigenvalues of an operator $A$.

**Proposition 2.** Consider a parameterized quantum circuit on $n$ qubits of the following form.

Let $\rho$ be an $n$-qubit density matrix, and $\mu$ an $n$-qubit observable. Let $H$ be a Hermitian operator that acts on an arbitrary subset of the $n$ qubits. Consider the expectation value function

$$f : \mathbb{R} \to \mathbb{R} : x \mapsto \text{tr}(\mu e^{-2\pi iH \cdot x} \rho e^{2\pi iH \cdot x}).$$

The Fourier spectrum of $f$ is contained in the set $\text{Diff Spec}(H)$.

**Proof.** Abbreviating $\Lambda := \text{Spec}(H)$ and replacing $H$ by its spectral decomposition $H = \sum_{\lambda \in \Lambda} \lambda P_\lambda$, where the $P_\lambda$ are the spectral projectors, we find, for every $x \in \mathbb{R}$,

$$\text{tr}(\mu e^{-2\pi iH \cdot x} \rho e^{2\pi iH \cdot x}) = \sum_{\lambda' : \lambda \in \Lambda} \text{tr}(\mu e^{-2\pi i\lambda x} P_\lambda \rho e^{2\pi i\lambda' x} P_{\lambda'}) = \sum_{\lambda' : \lambda \in \Lambda} \text{tr}(\mu P_\lambda \rho P_{\lambda'}) \cdot e^{2\pi i(\lambda' - \lambda)x}.$$  

The function space associated with the case of Proposition 2 is $\mathcal{X}_{\text{Diff Spec}(H)}$, the space of all real-valued functions whose Fourier spectrum is contained in $\text{Diff Spec}(H)$.

2.1.b. Several Hamiltonians. In the multi-variate case, Hamiltonians $H_1, \ldots, H_d$ can be paired with variables $x_1, \ldots, x_d$, respectively. For example, for arbitrary quantum operations $E_1, \ldots, E_{d-1}$, and denoting by $[U]$ ($U$ a unitary) the Kraus-form quantum operation $\rho \mapsto U \rho U^\dagger$, we might have

$$f : \mathbb{R}^d \to \mathbb{R} : x \mapsto \text{tr}(\mu \cdot \left( [e^{-2\pi iH_d \cdot x_d}] \circ E_{d-1} \circ [e^{-2\pi iH_{d-1} \cdot x_{d-1}}] \circ \cdots \circ E_1 \circ [e^{-2\pi iH_1 \cdot x_1}] \right)(\rho)).$$

Applying Proposition 2 $d$ times yields, for the Fourier spectrum, the set

$$\text{Diff Spec}(H_1) \times \cdots \times \text{Diff Spec}(H_d).$$

We can add a little more color by applying a linear transformation, i.e., “$x = Au$” for an arbitrary real $(d \times e)$-matrix $A$.

**Proposition 3.** If $f$ is as in (5), and $A$ is a real $(d \times e)$-matrix, then the function $g : u \mapsto f(Au)$ has Fourier spectrum contained in the set

$$\{ A^\dagger \xi \mid \xi \in \text{Diff Spec}(H_1) \times \cdots \times \text{Diff Spec}(H_d) \}.$$
Sketch of proof. Direct verification. With $\Xi_f := \text{Diff Spec}(H_1) \times \cdots \times \text{Diff Spec}(H_d)$, and $\Xi_g := \{A^\top \xi | \xi \in \Xi\}$, there are complex numbers $b_\xi$, $\xi \in \Xi$, such that

$$g(u) = f(Au) = \sum_{\xi \in \Xi_f} b_\xi e^{2\pi i \xi \cdot (Au)} = \sum_{\xi \in \Xi_f} b_\xi e^{2\pi i (A^\top \xi) \cdot u} = \sum_{\eta \in \Xi_g} \left( \sum_{\xi \in \Xi_f} b_\xi \right) e^{2\pi i \eta \cdot u}.$$

The function space associated with the case of Proposition 3 is $\mathcal{K}_{\Xi_g}$ (re-using the notation from the proof), the space of all real-valued functions each of whose Fourier frequencies is of the form $A^\top \xi$ for some $\xi \in \text{Diff Spec}(H_1) \times \cdots \times \text{Diff Spec}(H_d)$.

2.1.c. Quantum circuits for arbitrary frequency sets. We give the following quite obvious result as an argument in support of the generality in which the present paper is written. No attempt has been made to minimize the resources. The proof is in Appendix C.

Proposition 4. Given a $d \in \mathbb{N}$, $\Xi \subset \mathbb{R}^d$ finite, symmetric, and a $f : \mathbb{R}^d \to \mathbb{R}$ with Fourier spectrum equal to $\Xi$, there exists a parameterized quantum circuit on at most $d \log_2(|\Xi| + 1)$ qubits and with $d$ parameters, whose expectation value function equals $f$.

Hence, we see that (a) the frequency sets of parameterized quantum circuits can be completely arbitrary, and (b) every function in $\mathcal{K}_{\Xi}$ arises from a parameterized quantum circuit.

The practical value of Proposition 4 is doubtful, as taking derivatives through shift rules requires that the frequency sets are known.

2.2 Finite shift rules, feasibility

In this paper, a shift rule is defined as a (finite complex Borel) measure $\phi$ on $\mathbb{R}^d$, which is applied to a function $f \in \mathcal{K}_\Xi$ via convolution:

$$\phi * f(x) = \int f(x - u) d\phi(u).$$

We are interested in finite shift rules, i.e., measures with finite support. This restricts $\phi$ to choosing a finite set $A \subset \mathbb{R}^d$ and complex numbers $u \in \mathbb{C}^A$ (we will later restrict, wlog, to real coefficients $u \in \mathbb{R}^A$), and defining

$$\phi_{A,u} := \sum_{a \in A} u_a \delta_a,$$

where $\delta_a$ is the Dirac distribution / point measure at the point $a$, which means $\int f(x) d\delta_a(x) = f(a)$ for all reasonable functions $f$. For the whole convolution, we get

$$\phi_{A,u} * f(x) = \sum_{a \in A} u_a \delta_a * f = \sum_{a \in A} u_a f(x - a).$$

Given $\alpha \in \mathbb{N}^d$, a shift rule $\phi$ is called feasible for $\Xi, \alpha$, if convolution against it realizes the $\partial^\alpha$ partial derivative for all real-valued functions with Fourier spectrum contained in $\Xi$, i.e.,

$$\phi * f = \partial^\alpha f \text{ for all } f \in \mathcal{K}_\Xi.$$  

From now on, when we say “shift rule”, we mean “finite (but not necessarily feasible) shift rule”.

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2.3 System of equations and existence of (finite) feasible shift rules

Given a finite set \( A \subset \mathbb{R}^d \) and \( u \in \mathbb{C}^A \), applying the Fourier transform on both sides of equation (7), we find that \( \phi \) is a feasible shift rule if and only if

\[
\hat{\phi}(\xi) = (2\pi i \xi)^\alpha \quad \text{for all } \xi \in \Xi;
\]

see §?? (Lemma ??). There, using the fact that \( \hat{\delta}_a(\xi) = e^{-2\pi ia \cdot \xi} \) for all \( \xi \in \mathbb{R}^d \), we will continue to (Lemma ??) an equivalent system of equations formulated in the notation \( \phi_{A,u} \) as in (6):

\[
\sum_{a \in A} u_a e^{-2\pi ia \cdot \xi} = (2\pi i \xi)^\alpha \quad \text{for all } \xi \in \Xi.
\]

As one can see, the system is linear in \( u \), with coefficients that are trigonometric functions of the vectors in the set \( A \).

To summarize: \( \phi_{A,u} \) as in (6) is a feasible shift rule for \( \Xi, \alpha \) if, and only if, it is a solution to the system of \( |\Xi| \) equations (9).

It is not, up to this point, obvious that for every wild combination of \( \Xi \)'s and \( \alpha \)'s a feasible (finite!) shift rule should even exist. In the case where \( \Xi \) is equi-spaced the existence is easy (and known in the community, referred to as "equidistant frequencies" for \( d = 1 \) in [22]). The general case is discussed in [22, Eqn. (90)], but the author of the current paper wasn’t able to find in Wierichs et al. any attempt of an argument why their parameterized family of shift rules for the "general case" in \( d = 1 \) should contain one that’s actually feasible (it’s probably obvious and I’m just missing it). We prove the existence of finite feasible shift rules for all \( d, \Xi \) in §?? (Lemma ??).

We also note that, provided a single feasible shift rule exists, there exists a whole “manifold” of them.

2.4 Cost of a shift rule

There are several possibilities to define the “cost” of a shift rule. The first one is what [22] calls “number of unique circuits” and what in our terminology is the size (cardinality) of the support of the measure: For \( \phi_{A,u} \) as in (6), the support is (contained in) the set \( A \), and its size is \( |A| \) (if all \( u_a \) are non-zero).

In this paper the quantity we use as the cost of a shift rule \( \phi \) is the usual norm\(^7\) of a finite measure, which we denote by \( \| \cdot \|_1 \). Specializing to our situation, for \( \phi_{A,u} \) as in (6), we have

\[
\text{cost}(A, u) := \| \phi_{A,u} \|_1 = \sum_{a \in A} |u_a|.
\]

As noted above, this definition is the same as Wierichs et al.’s “number of shots” up to factors.

Before we discuss the justification(s) for the choice of this cost function, we need to address complex vs. real measures. The observant reader has noticed that we allow complex coefficients \( u \in \mathbb{C}^A \) in the shift rules (6), while in the literature, only real numbers have been considered. We will prove in §?? (Lemma ??) that for every feasible shift rule \( \phi \), there always exists a feasible shift rule that is a real signed measure, i.e., has only real coefficients when written in the form (6), and whose cost is at most that of \( \phi \).

Hence, for the rest of this section, we will consider real coefficients \( u \in \mathbb{R}^A \) only.

\(^6\)Read: “lots!”

\(^7\)The one which underlies the total-variation: For a complex measure \( \mu \) on \( \Omega \), it is defined as \( \| \mu \|_1 := \sup_{A_1, A_{-1}} \sum_{\epsilon \in \{-1,1\}} \epsilon \mu(A_{\epsilon}) \), where the supremum ranges over all partitions of \( \Omega \) into 4 measurable sets.
2.4.a. Cost of a shift rule as an error norm. The first justification of the choice of the cost function comes from Harmonic/Numerical Analysis: It is a folklore fact that for every finite signed (i.e., real valued) Borel measures  on , we have

\[ \|\phi\|_1 = \sup \left\{ \| f \|_1 : f \in \mathcal{C}_b(\mathbb{R}^d), \| f \|_\infty \leq 1 \right\}, \] (11)

where we have denoted by the Banach space of continuous bounded functions, with the supremum norm \( \|f\|_\infty := \sup_x |f(x)| \).

This implies that

\[ \|\phi\|_1 = \sup_{\|f\|_\infty \leq 1} \| \phi \ast f \|_\infty, \]

where the supremum extends over the functions in \( \mathcal{C}_b(\mathbb{R}^d) \) again. In other words, \( \|\phi\|_1 \) is equal to the operator norm for the operator

\[ D: \mathcal{C}_b(\mathbb{R}^d) \to \mathcal{C}_b(\mathbb{R}^d): f \mapsto \phi \ast f. \]

As a general principle, norms of operators give error estimates. Suppose for given \( \Xi \subset \mathbb{R}^d \), \( \alpha \), we are interested in the partial derivative \( \partial^\alpha \) of a function \( f \in \mathcal{K}_\Xi \), and we have a feasible finite shift rule \( \phi \) that accomplishes this. But \( f \) is available only with an error (or noise), so the function that we can evaluate is \( \hat{f} := f + h \) where \( h \in \mathcal{C}_b(\mathbb{R}^d) \). In general, the Fourier frequencies of the error function, \( h \), can be outside of the set of frequencies \( \Xi \). In the case of parameterized quantum circuits, where \( \hat{f}(x) \), for given \( x \), is the average of discrete samples, \( h \) can be expected to have arbitrarily large frequencies.

The question how much the error, \( h \), messes up the computation of the derivative via convolution with \( \phi \) is upper bounded by the operator norm \( \|\phi\|_1 \): \n
\[ \| D\hat{f} - Df \|_\infty = \| Dh \|_\infty \leq \| D \| \cdot \| h \|_\infty = \|\phi\|_1 \cdot \| h \|_\infty. \]

The inequality is tight, i.e., there exist \( h \)'s for which equality holds.

This reasoning is, of course, typical in any kind of Harmonic/Numerical Analysis context.

2.4.b. Cost of a shift rule as worst-case standard deviation. In this paragraph, we essentially repeat with a little more detail the calculation and approximation of Wierichs et al. that leads to their definition of the “number of shots” in [22, Eqn. (14)].

Let us specialize to the case that the observable \( \mu \) in (4) and (5) has only \( \pm 1 \) eigenvalues, e.g., is a (tensor product of) Pauli observable(s). If \( f \) is such an expectation value function, then, for all \( x \in \mathbb{R}^d \), the noise is “blown up” by a factor of \( \|\phi\|_1 \):

\[ \| D\hat{f} - Df \|_\infty = \| Dh \|_\infty \leq \| D \| \cdot \| h \|_\infty = \|\phi\|_1 \cdot \| h \|_\infty. \]

\( \hat{f}(x) \) is the total variation measure; the inequality “\( \geq \)” is in the Riesz Representation Theorem.

\( \| h \|_\infty \) is a (tensor product of) Pauli observable(s). If

\[ \phi = \sum_{a \in A} |u_a|^2 (1 - f(x - a)^2), \]

and with optimally distributed shots, the asymptotic variance

\[ \sigma_a = \text{the standard deviation of } X_a, \text{ for all } a. \]

In our case, when estimating a partial derivative at \( x \in \mathbb{R}^d \) by convolution with \( \phi_{A,u} \) as in (6) (with \( u \in \mathbb{R}^d \)), we have

\[ X_a = u_a \cdot F(x - a), a \in A, \text{ where for all } (F(y))_{y \in \mathbb{R}^d} \text{ is family of independent, } \pm 1 \text{-valued random variables with expectations } \mathbb{E}F(y) = f(y) \text{ for all } y. \]

The variance is \( |u_a|^2 (1 - f(x - a)^2) \), and with optimally distributed shots, the asymptotic variance is

\[ \frac{1}{N} \left( \sum_{a \in A} |u_a|^2 \right)^2. \]
We take the square root, to obtain the asymptotic standard deviation
\[
\frac{1}{\sqrt{N}} \sum_{a \in A} |u_a| \sqrt{1 - f^2(x - a)}.
\]

To manage this expression, we are now taking the worst case over \(x\) and \(f\): We are lower bounding \(f^2(x - a)\) by 0, for all \(a \in A\). This results in the upper bound of the standard deviation of, asymptotically,
\[
\frac{1}{\sqrt{N}} \sum_{a \in A} |u_a| = \text{cost}(A, u) / \sqrt{N}.
\]

Taking the worst case is not just a convenient primitive of computational theory, in our case, it is also a bow to the dreaded “Barren Plateaus” phenomenon \([14]\), where the expectation value functions are flat. (Clearly, lower bounding \(f^2\) by a constant(!) other than 0 doesn’t change the comparison relations between asymptotic standard deviations of different shift rules, and hence has no influence on which shift rule is optimal.)

We emphasize that we are very optimistic about the ingenuity of an estimator applying a shift rule given its support: We allow it to somehow magically know how to distribute a budget of shots among the support of the shift rule in an optimal way, depending on the values of the expectation value function at the support points! Alas, in the worst case, it doesn’t help at all.

### 2.4.c. Cost of a shift rule as a heuristic for sparsity minimization.

In the literature, the other cost factor for a shift rule is what \([22]\) call “number of unique circuits”, and what we refer to as the size of the support of the Borel measure, the set \(A\) in the notation of \((6)\). Let us assume for a moment that our goal was not to minimize the standard deviation, but to minimize the support, while a large but finite candidate set \(A\) that allows feasible shift rules with support contained in it has been fixed. The task at hand is to find a solution to a (finite, underdetermined) system of linear equations whose support (number of non-zero entries of a vector) has minimal size:

\[
\min \{ a \mid u_a \neq 0 \} \\
\text{subject to } Eu = k
\]

for an appropriately chosen matrix \(E\) and vector \(k\); see above. This is an NP-hard optimization problem, but, as we all know, the standard heuristic for it is to replace the term under the minimization by the 1-norm: \(\min \sum_{a} |u_a|\):

\[
\min \sum_{a} |u_a| \\
\text{subject to } Eu = k
\]

In many cases, provable guarantees can be made on the effectiveness of that heuristic \([5]\).

Hence, minimizing \(\|\phi\|_1\) over all feasible shift rules can be justified completely independently from error norms and worst-case standard deviations, simply as the goal to heuristically minimize the support of the shift rule, in other words, maximize its sparsity.

### 2.5 “Primal”, “dual” and weak duality

In optimization vernacular, the “primal” optimization problem is the one you want to solve, while the “dual” optimization problem is one which helps you in solving or proving theorems about the primal. The two are related by “duality theorems” which make statements about pairs of primal/dual feasible solutions.
From what we have discussed, given \( d, \Xi, \alpha \), the optimal finite feasible shift rule is the optimal solution (if attained) of the following optimization problem (\( \phi \) is the variable):

\[
\begin{align*}
\text{Infimum of } & \| \phi \|_1 \\
\text{subject to } & \phi \ast f = \partial^\alpha f \text{ for all } f \in K_\Xi, \\
& \text{supp } \phi \text{ finite.}
\end{align*}
\] (14a)

We have noted above that the ostensibly infinite system of linear equations (14b) is equivalent to each of the (finite) systems (8) and (9), but for now, we stick with the form in (14), because it gives an easy motivation for the Weak Duality Theorem.

In terms of optimization theory, the finiteness condition is puzzling: If \( d, \Xi, \alpha \) are such that the infimum is not attained, do we have to pass to some kind of infinite-dimensional closure of our set of finite shift rules? We want to avoid that, mainly because it isn’t necessary, as we will see later. The puzzlement is mitigated by considering the following “dual” optimization problem (\( f \) is the variable):

\[
\begin{align*}
\text{Supremum of } & (-\partial)^\alpha f(0) \\
\text{subject to } & \| f \|_\infty \leq 1 \\
& f \in K_\Xi.
\end{align*}
\] (15a)

Note that \((-\partial)^\alpha = (-1)^{|\alpha|} \partial^\alpha\). (The notation \(|\alpha|\), for \( \alpha \in \mathbb{N}^d \), stands for \( \sum_j \alpha_j \).)

The optimization problem (15) is of a form that is quite common in convex optimization, and both theory and computation are manageable. Indeed, the feasible region (meaning, the set of all dual feasible \( f \), i.e., the \( f \)’s satisfying the constraints (15b),(15c)) is a subset of a finite dimensional real vector space (namely \( K_\Xi \), of dimension \(|\Xi|\)), and the subset is defined by infinitely many linear constraints (15b):

\[
\text{for each } a \in \mathbb{R}^d: \ -1 \leq f(a) \leq 1.
\] (16)

Moreover, the objective function \( f \mapsto (-\partial)^\alpha f(0) \) is linear.

We have the following critical (albeit super easy) fact.

**Theorem 5.** Let \( d \in \mathbb{N}, \Xi \subset \mathbb{R}^d \) finite symmetric, and \( \alpha \in \mathbb{N}^d \) be given.

The dual feasible region is non-empty and compact. In particular, the objective function attains its supremum in at least one of its points.

The theorem will be proven in §??.

**2.5.a. Weak duality.** To give an idea why (15) can be considered a “dual” of (15), we will prove a “weak duality theorem”:

The objective function values of the feasible solutions to the maximization problem are less than or equal to the objective function values of the feasible solutions to the minimization problem.

We give a slightly more general statement where a restriction to finite support of the measure is not necessary.

**Proposition 6 (Weak Duality Theorem).** Let \( \phi \) be a finite signed Borel measure on \( \mathbb{R}^d \) satisfying (14b), and let \( f \) be feasible for (15). Then

\[
(-\partial)^\alpha f(0) \leq \| \phi \|_1.
\] (17)
Proof. Abbreviating $x \mapsto f(-x)$ to $f(-\Box)$, we calculate:

$$(\partial^\alpha \phi)(0) = \phi * (f(-\Box))(0) \quad \text{[by (14b) and (15c)]}$$

$$= \int f(u - 0) \, d\phi(u)$$

$$\leq \|f\|_\infty \cdot \|\phi\|_1 \quad \text{[by (11)]}$$

$$\leq \|\phi\|_1. \quad \text{[by (15b)]}$$

In the second equation, we have also used that for all $f$, if $f \in \mathcal{H}_\Xi$ then $f(-\Box) \in \mathcal{H}_\Xi$. □

2.6 The computational perspective

In this paper, we mostly use optimization as a tool for proving theorems, ultimately proving optimality of some feasible finite shift rules. The author finds that demonstrating how the optimization problems (14) and (15) could be solved computationally is not only fun, but also, importantly, helps understand the theory.

Unlike everything else in this paper, this subsection is not fully rigorous. For example, we will omit cases in the algorithms and gloss over details in the justifications. Making it rigorous would require to discuss too much background Convex Optimization theory. In other words, while we will try to make as concrete and practical as possible how the methods work, we warn the reader that understanding why they work is impossible without solid knowledge of Convex Optimization theory.

2.6.a. Solving the dual optimization problem. We start with the dual problem (15), because its solution is canonical. From a computational theory perspective, the thrust of the matter is that, using the Ellipsoid algorithm, you can solve the optimization problem (to provable optimality) efficiently, if you can (could!) solve efficiently the so-called “separation problem”, which is an algorithmic version of the separating hyperplane theorem: Given a point, either assert that it is feasible (i.e., inside the convex set described by the constraints), or find an inequality that is valid for all feasible points and violated by the given point.

We must supply a precision, $\epsilon > 0$, to the Ellipsoid algorithm indicating that an “$\epsilon$-almost feasible” solution whose objective function value is at most $\epsilon$ worse than the mathematical optimum is sufficient; we refer to [8], Definition (2.1.10), for the exact formulation. The running time will depend polynomially on $\log(1/\epsilon)$. Similarly, the separation problem should accept as input a precision $\delta > 0$ (Definition (2.1.13) in [8]).

In this paper, where the computational aspect is illustrative and not essential for the theoretical part, we ignore the computational complexity theory entirely, describing the practitioner’s approach. In our situation, from a practical point of view, the separation problem is the following:

Given as input $d, \Xi$ and a function $f \in \mathcal{H}_\Xi$, return either the assertion $\|f\|_\infty \leq 1$, or an $a \in \mathbb{R}^d$ such that $|f(a)| > 1$ (where both inequalities are subject to a precision, $\delta > 0$).

The algorithm for solving (15) then consists in iteratively performing the following steps: Solve the optimization problem with the infinitely many inequalities reduced to a finite list defined by a finite set $A \subset \mathbb{R}^d$; feed the resulting optimal (but not necessarily dual feasible) solution $f^*$ into an algorithm solving the separation problem; update the finite set $A$ of constraints and iterate, or exit with an optimal dual (near-)feasible solution.

Let’s start by encoding functions in $\mathcal{H}_\Xi$. Arbitrarily fix $\Xi_+ \subset \Xi$ in such a way that $\Xi$ is the disjoint union of the three sets $\{0\}, \Xi_+, -\Xi_+$. Now, we represent the “$f \in \mathcal{H}_\Xi$” in (15) and

---

10If you find something that you think is not fully rigorous, please contact the author.
also in the input to the separation problem) by its sine-cosine expansion:

\[ f = \mu + \sum_{\xi \in \Xi^+} \cos(2\pi a \cdot \xi) \cdot x_{\xi} - \sin(2\pi a \cdot \xi) \cdot y_{\xi}; \]  

(19)

the actual optimization variables will be \( \mu \in \mathbb{R}, x, y \in \mathbb{R}^\Xi^+ \). In that way the constraint (15c) is automatically satisfied. The number of variables is, of course, equal to the dimension of the real vector space \( \mathcal{K}_\Xi \), namely \( 1 + 2|\Xi^+| = |\Xi| \).

The objective (15a) is obtained by taking \((-\partial)^a\) at 0 of the function in (19). With the convenient abbreviations

\[ c_\xi := \Re((2\pi i^a)^\alpha), \quad \text{and} \quad s_\xi := \Im((2\pi i^a)^\alpha). \]  

(20)

this gives

\[ \sum_{\xi \in \Xi^+} c_\xi \cdot x_{\xi} + s_\xi \cdot y_{\xi}. \]  

(21a)

The constraint (15b) is written out in infinitely many linear inequalities as in (16), two for every \( a \in \mathbb{R}^d \):

\[ -1 \leq \mu + \sum_{\xi \in \Xi^+} \cos(2\pi a \cdot \xi) \cdot x_{\xi} - \sin(2\pi a \cdot \xi) \cdot y_{\xi} \leq +1. \]  

(21b)

Fig. 1 shows the complete algorithm for solving (15) to optimality — provided we could solve the separation problem. We have added a tolerance parameter \( \delta > 0 \) to replace the strict inequality in the separation problem: Instead of the computationally unpractical \(|f(a)| > 1\) we require \(|f(a)| > 1 + \delta\). As a consequence, the algorithm will, of course, return only a near-feasible solution.

Iterated LP algorithms with “cutting plane generation” (i.e., adding inequalities violated by the current optimal point), often based on the Simplex algorithm for Linear Programming, are a standard tool in computational optimization to solve to optimality convex optimization problems with linear objective where there is a large number of inequalities.

We invite the reader to try it out: The author has coded a toy demonstration, for \( d = 2 \) only, of the algorithm as a notebook; see Appendix A.

2.6.b. Finding an optimal shift rule. A similar iterative approach, referred to as “column generation” in Linear Programming literature, would help us with the primal problem (14). Since we have the finiteness-of-the-support condition (14c), a minimum may or may not be attained, but we can still hope for a shift rule that is feasible and whose cost is at most \( \varepsilon \) larger than the infimum, for a given \( \varepsilon > 0 \). In that approach, in every iteration, for a fixed finite set \( A \subset \mathbb{R}^d \), we would be solving the following Linear Program. The variables are \( u^+, u^- \in \mathbb{R}^A \):

\[
\begin{align*}
\text{Minimum of} & \quad \sum_{a \in A} u^+_a + u^-_a \\
\text{subject to} & \quad \sum_{a \in A} u^+_a - u^-_a = 0, \\
& \quad \forall \xi \in \Xi^+ : \sum_{a \in A} (u^+_a - u^-_a) \cos(2\pi a \cdot \xi) = c_\xi, \\
& \quad \forall \xi \in \Xi^+ : \sum_{a \in A} (u^+_a - u^-_a) \sin(-2\pi a \cdot \xi) = s_\xi, \\
& \quad u^+, u^- \geq 0.
\end{align*}
\]  

(22)

\[ ^{11}\text{A small calculation is necessary to see this. The reason why we set things up like this is because it goes nicely with duality.} \]
Algorithm 1: Solve-Dual

| Step |
|------|
| **Input**: d, Ξ⁺ ⊂ Rᵈ, α ∈ Nᵈ; δ ≥ 0 |
| **Output**: Optimal near-feasible solution to (15) (in µ, x, y variables) |
| 1 | Initialize A to some (finite) subset of Rᵈ; e.g., A := ∅. |
| 2 | Repeat |
| 3 | Solve the following Linear Program, in the variables µ ∈ R, x, y ∈ Ξ⁺: |
| 4 | maximize expression (21a) |
| 5 | subject to inequalities (21b), for all a ∈ A |
| 6 | Obtain an optimal LP solution µ⁺, x⁺, y⁺, with objective function value v⁺. |
| 7 | **Separation Routine** |
| 8 | Initialize A⁺ := ∅ |
| 9 | Find argmin a⁺ and argmax a⁻ of the function |
| 10 |  \[ f^* : a \mapsto \mu^* + \sum_{\xi \in \Xi^+} \cos(2\pi a \cdot \xi) \cdot x^+ \xi - \sin(2\pi a \cdot \xi) \cdot y^+ \xi \] |
| 11 | If \( f^*(a⁺) \) < \(-1 - \delta\), update \( A⁺ := \{a⁺\} \) |
| 12 | If \( f^*(a⁻) \) > \(1 + \delta\), update \( A⁺ := A⁺ \cup \{a⁻\} \) |
| 13 | **Return** A⁺ |
| 14 | Update A := A \∪ A⁺ |
| 15 | Until A⁺ = ∅ |
| 16 | **Return** Optimal near-feasible solution µ⁺, x⁺, y⁺ with objective function value v⁺. |

---

The non-linear absolute value |u| that occurs in (14) via (10) has been “linearized” by replacing the optimization variable u from (14) by its positive and negative parts u⁺, i.e.,

\[ u = u⁺ - u⁻. \]

Solving the LP will return either in the optimal feasible shift rule with support contained in A⁺, or the assertion that no feasible shift rule with support contained in A exists.

We are not pursuing the column-generation approach here, mainly because it requires a lot of LP theory while not adding much magic. Indeed: The primal column generation method is mathematically exactly the same the dual column generation method: Each step in one is the LP-dual of the corresponding step in the other.

Finding an optimal shift rule when a dual-optimal basis is available. Instead, we will explain how we can computationally find a feasible finite shift rule whose cost equals that returned by Algorithm 1, with ε, δ set to 0 to simplify the exposition. Indeed, the support of the resulting shift rule will be contained in the last set A that was used to solve the LP in line 3 there. With the notations used in Algorithm 1, take the values of the variables in the iteration where the Separation Routine returns A⁺ = ∅, i.e., the last iteration. We also assume that the optimal solution is a so-called “vertex solution” which comes with what is called a “basis” in LP vernacular: A set of inequalities that are satisfied with equality by the vertex solution, and whose left-hand-side vectors are linearly independent spanning a space of dimension |Ξ|. (In other words: The coefficients of the selected inequalities form a square, invertible matrix.) We index the inequalities of the basis by the (disjoint) sets A⁺ and A⁻, where the elements \( a ∈ A⁺ \) index inequalities of the form “\( f(a) ≤ 1 \)”, and the elements of \( a ∈ A⁻ \) index inequalities of the form “\(-1 ≤ f(a)\)”. 

---

Figure 1: Algorithm “Solve-Dual”
To obtain a feasible shift rule with support contained in $A^+ \cup A^- \subseteq A$ whose cost equals $v^*$, we need to solve for $u^+, u^-$, the system of linear equations consisting of equations (22b),

$$
\begin{align*}
  u^+_a &= 0 & \text{for all } a \notin A^+ \\
  u^-_a &= 0 & \text{for all } a \notin A^-.
\end{align*}
$$

(23)

Linear Programming theory guarantees:

- The existence of a solution;
- That the obtained $(u^+, u^-)$ is a feasible solution for the LP (22);
- That the cost of $u^+, u^-$ in the LP (22) is equal to $v^*$, and hence optimal by weak LP duality.

Set $u_a := u^+_a - u^-_a$ for all $a \in A$, et voilà, $\phi_{A,u}$ defined as in (6) is a the desired shift rule.

From the definition of an LP-basis above, we see that the size of the support $A^+ \cup A^-$ of the shift rule is at most $2|\Xi| + 1 = |\Xi|$. In our source code, see Appendix A, we don’t have to explicitly solve the system of linear equations: That is implicitly done inside the LP solver: We can just query the result from the “dual LP-solution”.

2.6.c. Finding an optimal shift rule when a dual solution is known. We conclude this subsection by giving a method that, in the lattice-generating case, given an optimal dual solution “on paper” but no dual optimal basis, recovers an optimal shift rule by solving a single Linear Program.

Let $\Xi \subset \mathbb{R}^d$ be (finite, symmetric, and) lattice generating, so that, wlog, we may assume that $\Xi \subset \mathbb{Z}^d$, so that the functions in $\mathcal{K}_\Xi$ are $\mathbb{Z}^d$-periodic.

Denoting the known dual optimal solution by $f^*$, let

$$
A^\pm := \{a \in [-1/2, 1/2]^d \mid f^*(a) = \pm 1\},
$$

and (to simplify the notation) $A := A^+ \cup A^-$. Now, the LP is easily described: it is (22), with the additional equations (23).

The LP is of the form (13) from §2.4.c in the motivation of the cost of a shift rule based on a sparsity minimizing Linear Program. This means that, if, for a given $A$, several optimal solutions exist, we can hope that one that is sparse will be returned. That turns out to be true in practice: We have implemented a demonstration of the method as a notebook, see Appendix A. The sparsest optimal shift rule is not always found.

Now finally back to mathematical rigor. Phew!

2.7 Strong duality and complementary slackness

Weak duality already has useful consequences: If you happen to stumble upon a feasible shift rule $\phi$ along with a dual-feasible function $f$, such that their objective function values coincide, i.e., $(-\partial)\alpha f(0) = \|\phi\|_1$ holds, then you can conclude that $\phi$ is an optimal shift rule, and $f$ is optimal for the dual. If you are not lucky enough to have that equation, you can still conclude from weak duality that the cost of your shift rule $\phi$ is at most $\|\phi\|_1 - (-\partial)\alpha f(0)$ larger than the infimum.

2.7.a. Strong duality. Strong duality adds to weak duality the certainty that if primal and dual optimal solutions exist, then their objective function values coincide. Our theorem is tailored for our situation.

**Theorem 7** (Strong duality of shift rule optimization). Let $d \in \mathbb{N}$, $\Xi$ finite symmetric $\subset \mathbb{R}^d$, and $\alpha \in \mathbb{N}^d$ be given.
(a) The infimum in the primal optimization problem is equal to the maximum in the dual optimization problem.

(b) If \( \phi^* \) is a finite feasible shift rule that is an optimal solution of the primal optimization problem, then there exists a dual feasible \( f \) such that

\[
\|\phi^*\|_1 = (-\partial)^\alpha f(0).
\]  

(24)

The way how Theorem 7 will appear a bit odd once the complete picture is known: Optimal finite shift rules always exist. However, Theorem 7 follows from Linear Programming theory, while for the existence of optimal shift rules, we have to raise the stakes to graduate level math — which is why we prove strong duality before we prove existence. The proof of Theorem 7 is in §??.

2.7.b. Complementary slackness. “Complementary slackness” is the Linear Programming theory equivalent of the Karush-Kuhn-Tucker (first-order) optimality conditions in general (convex) optimization. KKT is the inequality-constrained extension of Lagrange multipliers in multi-variable calculus. In the complementary slackness conditions, the dual solution takes the role of the multiplier.

**Theorem 8** (Complementary slackness for shift rule optimization). Let \( d \in \mathbb{N} \), \( \Xi \) finite symmetric \( \subseteq \mathbb{R}^d \), and \( \alpha \in \mathbb{N}^d \) be given.

If \( \phi \) is a finite feasible shift rule, and \( f \) dual feasible (i.e., feasible for (15)), then the following are equivalent:

1. Both \( \phi \) and \( f \) are optimal;
2. supp \( \phi \subseteq \{ a \in \mathbb{R}^d \mid |f(a)| = 1 \} \) in such a way that for all \( a \in \mathbb{R}^d \) the following logical implications hold:

\[
\phi(a) < 0 \implies f(a) = -1, \quad \text{and} \quad \phi(a) > 0 \implies f(a) = +1.
\]  

(25a)

The proof of the theorem is in §??.

In applications of Linear Programming theory to other fields of theoretical computer science / mathematics, complementary slackness is a powerful\(^{12}\) tool for proving theorems. Not surprisingly, Theorem 8 is our main ingredient when proving optimality for some shift rules.

2.8 Existence of optimal finite shift rules, and size of the support

The attentive reader will have noticed that the question whether optimal (finite!) shift rules exist, is unto this point unresolved. Here is the answer.

**Theorem 9.** Let \( d \in \mathbb{N} \), let \( \alpha \in \mathbb{N}^d \), and \( \Xi \subseteq \mathbb{R}^d \) non-empty and symmetric.

The optimization problem (14) attains an optimal solution, i.e., there exists a feasible (finite) shift rule \( \phi \) in which the infimum is attained.

Moreover, there always exists an optimal shift rule whose support has size at most \( |\Xi| \).

The proof of the theorem is in Section ??.

We also prove a strengthening of the size-of-the-support statement for \( d = 1 \) to \( |\Xi| - (\alpha \% 2) \) (where “\( \% \)” stands for remainder upon division). Wierichs et al. consider only shift-rules with that support, as they come out of their particular construction of shift rules. But they never ask the question whether shift rules with larger support but smaller cost (i.e., “number of shots”) might exist.

\(^{12}\)Even if somewhat . . . vintage.
**Theorem 10.** Let $\alpha \in \mathbb{N}$, and $\Xi \subset \mathbb{R}$ non-empty and symmetric. There always exists an optimal shift rule whose support has size at most $|\Xi| - (\alpha/2)$.

The proof of Theorem 10 is in §??.

### 2.9 Optimal primal and/or dual solutions

Before we approach the examples, we recall the formal definition of what we call a “lattice generating” set of vectors, as promised in the introduction.

Consider the sub-group (wrt addition) of $\mathbb{R}^d$ generated by $\Xi$. There are two cases: This sub-group is a lattice, or this sub-group is dense in a linear subspace of $\mathbb{R}^d$. A lattice is a subgroup that is generated as a group by a linearly (over the real numbers) independent set of vectors. For $\Xi$ to generate a lattice is equivalent to the matrix whose columns are the elements of $\Xi$ having rank over the rational numbers equal to (instead of strictly greater than) the rank over the real numbers. If $\Xi$ generates a lattice, we say, in this paper, that it is lattice generating.

#### 2.9.a. Dimension $d = 1$. We will prove the following.

**Theorem 11.** Let $\alpha \in \mathbb{N}$, and $\Xi \subset \mathbb{R}$ non-empty and symmetric. The optimal solution to the “dual” optimization problem (15) is

$$a \mapsto (\partial^\alpha \cos)(2\pi \max \Xi \cdot a).$$

In particular, the cost of an optimal shift rule is $(2\pi \max \Xi)^\alpha$.

Note that the theorem holds without conditions on $\Xi$ (beyond symmetry): It holds whether $\Xi$ is equi-spaced or not; whether $\Xi$ is lattice-generating or not; whether the space $\mathcal{K}_\Xi$ consists of periodic functions or not. Indeed, we prove Theorem 11 in three steps, each of which is of interest in its own right.

1. For $\Xi = \{-K, \ldots, K\} \subset \mathbb{Z}$ we establish primal and dual feasible solutions and prove complementary slackness. Complementary slackness relies on a fact about signs of derivatives of modified Dirichlet kernels; in this paper we give the proof of that lemma only for the practically relevant cases $\alpha = 1, 2, 3, 4$, and refer to a separate paper for the more technical general case.

   This proves that the shift rules in [22] for equi-spaced Fourier spectra are, indeed, optimal.

   This part of the proof is Theorem ?? in §??.

2. The case of lattice-generating Fourier spectra is reduced to Step 1. by a cheap trick, as Corollary ?? in §??.

   As the proof establishes, in particular, the dual optimal value, and since an optimal finite shift rule exists (Theorem 9), by strong duality (Theorem 7(b)), we also know the cost of the best possible feasible shift rule — which answers a question left open in [22]. Moreover, knowing the dual optimal solution allows us to realize the computational search for a sparse optimal shift rule through standard Linear Programming techniques:

   Solving a single LP as described in §2.6.c.

3. Finally we use simultaneous Diophantine approximation to reduce the non-lattice-generating case to the lattice generating one. The proof is in §??.

#### 2.9.b. Dimension $d \geq 2$. We give optimal dual solutions only in a special case, for which we need some notation and terminology. Our notation for the canonical projection mappings is the following:

$$\text{pr}_j : \mathbb{R}^d \to \mathbb{R} : x \mapsto x_j.$$
Let us say that a frequency set $\Xi \subset \mathbb{R}^d$ is pointy, if

there exists $\epsilon \in \{\pm 1\}^d$ such that $(\epsilon_1 \cdot \max \text{pr}_1(\Xi), \epsilon_2 \cdot \max \text{pr}_2(\Xi), \ldots, \epsilon_d \cdot \max \text{pr}_d(\Xi))^\top$. (26)

**Theorem 12.** Let $d \geq 2$, $\alpha \in \mathbb{N}^d$, and $\Xi \subset \mathbb{R}^d$ non-empty and symmetric.

If $\Xi$ is pointy with $\epsilon$ as in (26), then the optimal solution to the “dual” optimization problem (15) is

$$a \mapsto \prod_{j=1}^d (\partial^{\alpha_j} \cos)(2\pi \cdot \max \text{pr}_j(\Xi) \cdot a_j).$$

In particular, the cost of an optimal shift rule is $\prod_{j=1}^d (2\pi \max \text{pr}_j(\Xi))^{\alpha_j}$.

We prove Theorem 12 in two steps.

1. If $\Xi$ is a product set, i.e., if there exist symmetric sets $\Xi_j \subset \mathbb{R}$, $j = 1, \ldots, d$, with $\Xi = \prod_{j=1}^d \Xi_j$, then we can reduce to (11) together and Theorem 9.

2. If $\Xi$ is pointy, then (we will show) it is contained in a fitting product set, so the same cheap trick we used above gives a reduction to 1.
3 Conclusion

This paper contributes what the author believes to be novel and useful tools to the study of efficient shift rules, culminating in dual optimal solutions for a number of situations. The tools inspire efficient computational methods for practically computing optimal, hopefully sparse, shift rules for the many situations where (at least to date) no analytic description of the optimal (sparse) shift rules are known.

Some questions remain, some of them “merely” mathematical, others with practical relevance.

Dual optimal solutions for $d > 2$. The present papers offers dual optimal solutions for $d > 2$ only for a restricted family of frequency sets (the “pointy” ones). Is it possible to write down and prove dual optimal solutions for all (lattice generating) frequency sets? Is it true that (in the lattice generating case), the dual optimal solution is always of the form $a \mapsto \prod_{j=1}^{d} (\partial^{\alpha_j} \cos)(2\pi \xi_j \cdot a_j)$ for a $\xi$ in the lattice generated by $\Xi$? Or even $\xi \in \Xi$?

Numerically stable implementations of the methods computing shift rules. In the supplementary material (see Appendix A) we have given quick-and-dirty implementations of the computational methods in this paper, based on cheap Linear Programming solvers, and with no thought given to stability. Obviously, a proper, numerically stable implementation of these methods is needed in order to apply them practically. The most interesting method is certainly that in §2.6.c, when the optimal dual solution is known on paper as it allows to exploit all the theory of this paper.

Several partial derivatives at the same point Wierichs et al. give combined shift rules for estimating the whole Hessian. Is their construction optimal? The present paper only shows how to estimate each individual entry of the Hessian optimally, but it does not consider estimators which “recycle” previously made measurements to estimate several partial derivatives at the same time. (It can be shown that, for estimating $\partial f(x)$, measurements at $x$ cannot be used to reduce the cost, but that’s a silly scenario.)

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APPENDIX

A Example source code

The author of this paper has implemented some of the techniques discussed here in the mathematical computation programming language Julia\textsuperscript{14}, in the form of Pluto\textsuperscript{15} notebooks.

The notebooks are available on GitHub\textsuperscript{16} for download. Here we go through the files in that repository with a quick description of what the notebook does.

\textsuperscript{14}julialang.org
\textsuperscript{15}plutojl.org
\textsuperscript{16}github.com/dojt/ShiftRulesPluto
File `solve-for-u.jl`  The main function in this notebook, `solve_it(;Ξ, α, A)`, takes a set \( Ξ + \subset Q \) of (positive) frequencies, and a set \( A \subset \mathbb{R} \), and finds a shift rule of the form (6). If a feasible shift rule with that support exists, it will be found; if none exists, one that is closest to being feasible is returned. Closest to being feasible refers to the 2-norm, in frequency space \( \| \partial^α - φ \|_2^Ω \).

The function uses floating point arithmetic, and the precision can be chosen between 64 bits and 16384 bits. Changing the precision can sometimes help recognizing a set \( A \) that yields no feasible shift rule, but where the error with 64-bit precision is small, say \( 10^{-16} \).

File `dual-opt.jl`  This notebook implements the method that is described in the subsection §2.6.a. After terminating with an optimal set \( A \), the optimal shift rule is obtained: This can be done directly from the dual variables, which, is equivalent to the method described in §2.6.b, in the case when an optimal basis is known.

File `sparse-optimal-1d.jl`  In this notebook, knowledge about the optimal dual solution for lattice-generating frequency sets with \( d = 1 \) is used to compute an optimal feasible shift rule using a finite, i.e., “normal”, Linear Program, as described in §2.6.c.

### B Miscellaneous math background

#### B.1 Lattices

We sketch the proof of the equivalence of the periodicity of a function and the lattice-generating property of its Fourier spectrum:

**Lemma 13.** If \( f \) is a tempered distribution on \( \mathbb{R}^d \) that is periodic (i.e., there exists an additive subgroup \( M \) of \( \mathbb{R}^d \) such that \( δ_μ * f = f \) for all \( μ \in M \)), then the support of the Fourier transform of \( f \) is a lattice.

If a function \( f : \mathbb{R}^d \to \mathbb{R} \) has a Fourier spectrum \( Ξ \) that generates a lattice \( Λ \), then the function is periodic modulo the dual lattice (which is, indeed, a lattice)

\[
Λ^⊥ := \{ μ \in \mathbb{R}^d \mid \forall λ \in Λ: μ • λ = 0 \},
\]

i.e., for all \( x \in \mathbb{R}^d \) and every \( μ \in Λ^⊥ \) we have \( f(x + μ) = f(x) \).

For the other direction, we skip the part where you have to prove that the Fourier spectrum is discrete, and go right to the part where we prove that it also generates a discrete set (i.e., a lattice). If a smooth, bounded function \( f : \mathbb{R}^d \to \mathbb{R} \) is periodic, meaning, there exists an additive subgroup \( M \) of \( \mathbb{R}^d \) such that for all \( x \in \mathbb{R}^d \) and all \( μ \in M \) we have \( f(x + μ) = f(x) \), then either \( f = 0 \) or \( M \) is a lattice. In the case when \( M \) is a lattice, \( \hat{f} = e^{2πiμ • ξ} \hat{f} \), which implies that, for all \( ξ \) in the support of \( f \), we have \( μ • ξ \in \mathbb{Z} \), in other words \( Ξ \subset M^⊥ \), so that the group generated by \( Ξ \) is also contained in \( M^⊥ \), and hence a lattice.

#### B.2 Convexity

**B.2.a. Convex cones.** For a set of vectors \( R \), let us denote by \( cvxcone(R) \) the convex cone generated by \( R \), i.e., the set of all (finite) linear combinations with non-negative coefficients of elements of \( R \). A convex cone \( C \) is called **polyhedral**, if there exists a finite set \( R \) such that \( C = cvxcone(R) \).

**Lemma on infinitely-generated convex cones.** We use the following math notation only in this subsection. For a set \( C \) in a finite-dimensional real vector space, we denote: by \( C^\circ \) its topological closure; and by \( C^o \) its topological interior. Recall that, if \( C \) is a convex set (in a finite-dimensional real vector space) then \( C \) is also convex.

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The following strengthened version of Carathéodory’s theorem is one of those things in convexity theory about which the professor says “It’s obvious” and then a student asks, “Why?” and the professor spends 60 min proving it. Carathéodory’s theorem is the case \( \overline{C} = C \).

**Lemma 14.** Let \( C \) be a convex cone in an \( m \)-dimensional real vector space, and suppose \( C \) is generated by a set of vectors \( R \). If \( c \in (\overline{C})^\circ \) then there exist \( r_1, \ldots, r_m \in R \) with \( c \in \text{cvxcone}\{r_1, \ldots, r_m\} \).

**C Complexity of function estimation**

In this section we briefly consider the following questions, ignoring “subtleties” about processing real numbers in classical algorithms.

Given a \( d \in \mathbb{N} \), \( \Xi \subset \mathbb{R}^d \) finite & symmetric, and a \( f : \mathbb{R}^d \to \mathbb{R} \) with Fourier spectrum equal to \( \Xi \):

1. Does there exist a parameterized quantum circuit (with \( d \) parameters) whose expectation value function is \( f \)?
2. Does there exist a uniform family of these circuits, i.e., a polynomial time classical algorithm which, upon input of \( d, \Xi, \hat{f} \), produces the PQC as in (1)?
3. How does the minimum depth (or other complexity measure) of the quantum circuits in (1) relate to the complexity of estimating the function with a (randomized) classical circuit/algorithm?

The questions are informally inspired by the complexity theory of Boolean functions. We give the obvious, cheap answer to (1), Proposition 4, as an argument in support of the generality in which the present paper has been written, making absolutely no attempt to search for an efficient parameterized quantum circuit — and express the hope that the other questions might be picked up by smart people.

Recall the definition of \( \text{Diff} \) from (3), and, for conciseness, denote by \( \text{Spec}(A) \) the set of eigenvalues of a given operator \( A \).

**Proof of Proposition 4.** For each \( j = 1, \ldots, d \), consider the set \( \Xi_j = \{ \xi_j \mid \xi \in \Xi \} \) — the projection of \( \Xi \) onto the \( j \)th coordinate. For each \( j = 1, \ldots, d \), apply Lemma 15 below to each of the \( \Xi_j \), and define \( q_j := \lceil \log_2((|\Xi_j| + 1)/2) \rceil \). Letting

\[
q := \sum_{j=1}^{d} q_j \quad < d \log_2(|\Xi| + 1),
\]

we take \( q \) qubits, split into \( d \) quantum registers, where, for \( j = 1, \ldots, d \), register number \( j \) has \( q_j \) qubits. Let us denote by \( H_j \) the operator from Lemma 15 below applied to \( \Xi_j \), acting on the \( j \)th quantum register. We then let

\[
H := \sum_{j=1}^{d} H_j,
\]

and consider the parameterized circuit with initial state \( |\psi_0\rangle \), multi-parameterized unitary evolution \( U(x) \), as follows:

\[
|\psi_0\rangle := 2^{-q/2} \sum_{\gamma \in \{0,1\}^q} |\gamma\rangle
\]

\[
U(x) := e^{2\pi i \sum_{j=1}^{d} x_j H_j}.
\]
Now we define a Hermitian $q$-qubit operator $\mu$ as follows.

First of all, we interpret each of the $d$ quantum registers in the computational basis as encoding an unsigned integer. For $\ell_j, \ell_j' \in \{0,\ldots,2^q\}$, $j = 1,\ldots,d$, we say that $(\ell, \ell')$ fits, if, for all $j = 1,\ldots,d$, we have both $\ell_j, \ell_j' \leq (|\Xi| - 1)/2$ and $\ell_j, \ell_j' = 0$. Now, for $\ell_j, \ell_j' \in \{0,\ldots,2^q\}$, we define

$$
\langle \ell_1', \ell_2', \ldots, \ell_d' | \mu | \ell_1, \ell_2, \ldots, \ell_d \rangle := \begin{cases} 2^{q/2} f(\xi), & \text{if } (\ell, \ell') \text{ fits and } \left(\xi_{\ell_1'} - \xi_{\ell_1}, \ldots, \xi_{\ell_d'} - \xi_{\ell_d}\right) \in \Xi \\ 0, & \text{otherwise.} \end{cases}
$$

Note that, as $f$ is real valued, $\mu$ is indeed Hermitian.

The final quantum circuit is the following: Starting from $|0\rangle$, prepare a uniform superposition over all computational basis states, then apply the parameterized unitary (using the usual tools, as the exponent is a linear combination of tensor-products of $\ell$-operators), finally measure $\mu$. The last step is done by diagonalizing $\mu$ using a basis change unitary $W$ from the computational basis, i.e., $W\mu W^{\dagger}$ is diagonal in the computational basis, and implementing $W$ as a quantum circuit, based on the usual universality theorems (e.g., Section 4.5.2 in [16]). \hfill \square

**Lemma 15 (Trivial Helper Lemma).** Let $\Xi \in \mathbb{R}$ be finite and symmetric, and let $0 =: \xi^{(0)} < \xi^{(1)} < \cdots < \xi^{(m)}$, where $m := (|\Xi| - 1)/2$, be the non-negative elements of $\Xi$. There exists a Hermitian $[\log_2(m + 1)]$-qubit operator $H$ such that $\text{Diff Spec}(H) \supseteq \Xi$.

More precisely, the operator $H$ is diagonal in the multi-qubit Z-basis (computational basis), and for $\ell, \ell' \in \{0,\ldots,m\}$ (coded in binary):

$$
\langle \ell' | H | \ell \rangle = \delta_{\ell', \ell} \cdot \xi^{(\ell)}.
$$

(27)

Let $\gamma \in \mathbb{N}^q$, and a 1-qubit operator $A$, we use the shorthand

$$
A^{\otimes \gamma} := A^{\otimes 1} \otimes A^{\otimes 2} \otimes \cdots \otimes A^{\otimes q}.
$$

**Proof of Lemma 15.** To define $H$, follow (27), and choose the remaining $2^q - m - 1$ diagonal entries arbitrarily. We have $\text{Diff Spec}(H) \supseteq \text{Diff}\{\xi^{(0)}, \ldots, \xi^{(m)}\} \supseteq \Xi$. \hfill \square

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