Optimal compilation of parametrised quantum circuits

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A quantum circuit is built out of small unitary gates that together make it possible to perform an arbitrary quantum computation. In a *parametrised* quantum circuit, we allow certain quantum gates to be specified by a classical parameter that is determined before running the circuit on a quantum device. Usually parametrised gates are either phase gates or controlled-phase gates, and the parameter, a real number, specifies the phase to be applied. Parametrised quantum circuits are an increasingly important construction for quantum algorithms, especially for near-term applications. For instance, variational algorithms such as QAOA [13] and VQE [20] use a feedback loop between a classical side and a quantum side where the parameters are updated by a classical optimisation procedure, based on measurement outcomes of the quantum device. Each training step of a typical optimisation procedure involves estimating the gradient of the cost function with respect to each parameter (e.g. using the parameter-shift rule [23]). In order to be as efficient as possible with our resources we should hence make sure that we are not using superfluous parameters. We then would like some classical optimisation algorithm for parametrised quantum circuits that reduces the circuit to a form that has the minimal number of parameters, while still being able to express the same set of unitaries.

Parameter optimisation is also relevant in the field of measurement-based quantum computation (MBQC) [21, 22]. In most literature on MBQC the measurement patterns have to be deterministic regardless of the chosen measurement angles [5, 6, 12]. We can hence view this as a computation parametrised by those measurement angles. In this setting minimising the number of parameters corresponds to minimising the number of measurements needed [5], while still preserving deterministic realisability of the pattern.

There are numerous techniques for simplifying universal families of circuits by decreasing the number of non-Clifford gates, such as T gates. Such techniques not only decrease the number of non-Clifford gates themselves (which may be costly to implement, e.g. on fault-tolerant architectures [7]), but often decrease the overall size of the circuit, since sequences of Clifford gates can always be reduced to depth that is linear in the number of qubits (see e.g [18]).

While some of these techniques, such as [3, 10, 15], include special-case behaviour for certain non-Clifford phases such as $T := R_Z[\pi/4]$ or more generally $R_Z[\pi/2^k]$ (k > 1), others act uniformly on all non-Clifford phases [1, 11, 17, 19, 24]. Consequently, the latter can immediately be applied to parametrised phase gates, as we can then just treat these as 'black-box' non-Clifford phase gates.

There are only a small number of rewrites known that we can do with such black-box phase gates. Most of these correspond to a 'fusing' of two parameters. The simplest case is when we have two parametrised phase gates next to each other on the same qubit:

$$R_Z(\alpha_1) R_Z(\alpha_2) = R_Z(\alpha_1 + \alpha_2)$$
(1)

We see that the two different parameters α_1 and α_2 are combined into one gate, so that we can build the same set of unitaries using a single parameter α' by making the identification $\alpha' := \alpha_1 + \alpha_2$. More complicated versions of the same basic idea can be made by using the sum-of-paths approach [2], which allows us to fuse phases that apply to the same parity of qubits [1], or by compiling the circuit into a series of Pauli exponentials and exploiting the Pauli commutation relations [17, 24].

There are also more complicated rewrites that can in principle be performed on parametrised phase gates, for instance by exploiting the different Euler angle decompositions of a single-qubit unitary:

$$- R_Z(\alpha_1) - R_X(\alpha_2) - R_Z(\alpha_3) - = - R_X(\alpha_1') - R_Z(\alpha_2') - R_X(\alpha_3') - (2)$$

Here the parameters on the right depend on those on the left by some trigonometric relations, and are in particular discontinuous as a function of $(\alpha_1, \alpha_2, \alpha_3)$. Hence, when the use-case is for instance QAOA, this might not be desirable to apply, as it transforms the parameter space in pathological ways.

All this then raises a number of questions:

- What is the right notion of equivalence of parametrised quantum circuits?
- What are the possible rewrites we can do to transform parametrised quantum circuits while preserving equivalence?
- Is there an efficient algorithm to find an equivalent parametrised quantum circuit that uses the minimal number of parameters?

In this work, we answer each of these questions in the case of parametrised quantum circuits without repeated parameters. Regarding the first point, we show that a broad set of parameter transformations (analytic functions on the unit circle) actually already forces the relations between parameters in equivalent quantum circuits to be given by simple additive relations that correspond to just 'fusions' of parameters. We answer the second point by finding that the Clifford rewrite rules of the ZX-calculus [4] suffice to prove any equality between parametrised Clifford circuits, under the condition that each parameter occurs uniquely.

Our main result is an answer to the third question: we find that an existing optimisation approach, previous work of some of the authors [17], finds the optimal number of parameters, under the condition that every parameter in the circuit occurs on a unique gate:

Theorem. Given a parametrised circuit which consists of Clifford gates and parametrised Z phase gates, each of which is parametrised by a unique parameter, we can efficiently find an equivalent parametrised circuit with an optimal number of parameters. Furthermore, these new parameters correspond to sums and differences of the original parameters, and the algorithm for finding the circuit is that described in [17].

Note that if we drop the requirement here on the non-parametrised gates being Clifford that the problem likely no longer has an efficient solution:

Proposition. The parameter optimisation problem for parametrised Clifford+T circuits is NP-hard.

We conjecture that parameter optimisation for Clifford circuits where parameters are allowed to be used multiple times on different gates is also NP-hard. If that conjecture holds, this would make the types of circuits we specified the largest possible for which an efficient minimisation algorithm exists. While we do not prove this conjecture, we do provide two pieces of evidence for it. The first piece of evidence is an example of a circuit equation with repeated parameters that require more powerful versions of the ZX calculus to prove, such as the Clifford+T [16] and universal [14] variants, which do not in general admit efficient proofs of equality. The second piece of evidence is that we *do* prove that the optimisation problem involving repeated parameters is NP-hard for *post-selected* circuits, even though optimising post-selected circuits where the parameters occur uniquely is also efficiently optimally solvable by our algorithm.

In order to specify what an 'optimal number of parameters' is, we need to specify what types of equivalences between parametrised circuits we allow. We will consider a parametrised quantum circuit to be a quantum circuit consisting of gates from a discrete set, together with *parametrised phase gates* $Z[\alpha]$. Here $\alpha \in \mathbb{R}$ is a classical parameter that has to be determined prior to running the quantum circuit. A parametrised quantum circuit C depending on a vector of values $\vec{\alpha} \in \mathbb{R}^k$ can then be viewed as a map from parameter space \mathbb{R}^k to the space of unitaries \mathcal{U} as $C : \mathbb{R}^k \to \mathcal{U}$. A specific instantiation of C, which we will write as $C[\vec{\alpha}]$, is then just a regular quantum circuit where the phases have been filled in. We then say a circuit C_1 with parameter space \mathbb{R}^k reduces to C_2 with parameter space \mathbb{R}^l when there exists a function $f : \mathbb{R}^k \to \mathbb{R}^l$ such that $C_1[\vec{\alpha}] = \lambda(\vec{\alpha})C_2[f(\vec{\alpha})]$ for all $\vec{\alpha} \in \mathbb{R}^k$ where $\lambda : \mathbb{R}^k \to \mathbb{C} \setminus \{0\}$ is a function representing a global scalar $\lambda(\vec{\alpha})$ that may depend on the parameters. To find the optimal parameter count we are hence interested in finding a reduction that uses the minimal number of parameters. We conjecture that with no restrictions on f this will be a hard problem. In any case, when considering circuits for variational algorithms it makes sense to restrict to f that are at least continuous. We will make a stronger assumption and assume that for $f = (f_1, \ldots, f_l)$ each f_j is an analytic function of the unit circle $\mathbb{R}_{\text{mod } 2\pi}$. We then show the following.

Proposition. If f is a function used in a reduction and consists of analytic functions of the unit circle, then $f(\vec{\alpha}) = M\vec{\alpha} + \vec{c}$ where M is a matrix of integers, and \vec{c} is some constant set of phases.

This then gives us the notion of an affine reduction $C_1[\vec{\alpha}] = \lambda(\vec{\alpha})C_2[M\vec{\alpha} + \vec{c}]$. It is this notion of reduction between parametrised circuits that we use in the paper. In particular, we wish to restrict to just the circuits containing each parameter once, so that we require the affine reduction to be 'no-cloning' and not copy a parameter onto multiple places. We call such a reduction *parsimonious*. We can then state our main result formally.

Theorem. The parameter optimisation algorithm of [17] (which we also describe in the accompanying paper) is optimal: the circuits it produces do not parsimoniously affinely reduce to any other circuit with fewer parameters.

The algorithm of [17] is based on the ZX-calculus [8, 9], and so is our proof. Our result actually applies to any parametrised Clifford ZX-diagram with *non-trivial* parameters (a mild condition specifying that a parameter actually affects the linear map), and so we also see that for instance allowing post-selections or ancillae does not allow for lower parameter counts. In particular, we can use the correspondence between ZX-diagrams and measurement patterns [5] to show that we can find one-way model measurement-based computations [21] with a minimal number of non-Clifford measurements.

Theorem. The simplification strategy for measurement patterns with gflow of [5] produces a measurement pattern that has a minimal number of parametrised measurements amongst those patterns that it parsimoniously affinely reduces to.

The ZX-calculus has a standard set of rewrite rules that suffice to prove any equality between Clifford circuits [4]. We show that this same set of rewrite rules in fact suffices to prove any equality between parametrised Clifford circuits:

Theorem. Let D_1 and D_2 be two parametrised diagrams with the same number of parameters and where all the parameters of D_1 are non-trivial, such that $D_1[\vec{\alpha}] = \lambda(\vec{\alpha})D_2[\vec{\alpha}]$ for all $\vec{\alpha}$ for some scalar function $\lambda(\vec{\alpha}) \in \mathbb{C}$. Then $D_1 = C \otimes D_2$ for some Clifford scalar C and we can uniformly rewrite $D_1[\vec{\alpha}]$ into $C \otimes D_2[\vec{\alpha}]$ using the ZX-calculus. This result reinforces why the optimisation algorithm is optimal: any equation between parametrised Clifford circuits follows from the same rules that suffice for proving Clifford equality. Hence, there are no non-trivial equations between parametrised circuits. This matches what was found for diagonal CNOT+Z-phase circuits in [3] where they show that only phases that are dyadic rational multiples of π have non-trivial identities.

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