Quantum computing with differentiable quantum transforms

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We present a framework for differentiable quantum transforms. Such transforms are metaprograms capable of manipulating quantum programs in a way that preserves their differentiability. We highlight their potential with a set of relevant examples across quantum computing (gradient computation, circuit compilation, and error mitigation), and implement them using the transform framework of PennyLane, a software library for differentiable quantum programming. In this framework, the transforms themselves are differentiable and can be parametrized and optimized, which opens up the possibility of improved quantum resource requirements across a spectrum of tasks.

I. INTRODUCTION

Quantum machine learning (QML) is a rapidly-growing area of research with great potential. Tools for designing QML algorithms and applications are increasingly being incorporated into open-source quantum software [1–5]. Some of these integrate with classical machine learning tools such as Autograd [6], PyTorch [7], TensorFlow [8], and JAX [9]. The core functionality provided by all of these libraries is automatic differentiation (autodifferentiation) of mathematical functions, which is used to compute the gradients required for model training. The capabilities provided by these libraries have enabled significant advances to be made in classical machine learning, allowing developers and practitioners to focus more on architectures, data, and algorithms, rather than on the technical implementation of computing derivatives.

Differentiation is a process that maps a function $f(x)$ to another function, $g(x) = \nabla f(x)$, which computes its derivative. Differentiation can thus be viewed as a function transform. Some classical frameworks, such as JAX [9], Dex [10], and functorch [11] make this notion explicit. For example, JAX is branded as a library for transforming numerical functions, and its built-in transforms include just-in-time compilation and automatic vectorization ($\text{vmap}$) in addition to autodifferentiation. The system is extensible and allows users to write their own transforms. Furthermore, these transforms preserve differentiability of whatever they act upon.

There are many processes in quantum computing that rely on the idea of transforming a quantum function, most often represented by a quantum circuit. Such quantum transforms take a circuit as input, and return a new, modified circuit as output. This idea, and the underlying functional programming elements, is perhaps most explicit in the Haskell-based language Quipper [12], which contains a built-in, user-extensible system for monad transformers that can be applied to quantum circuits. Such transforms are used most often in the context of quantum compilation or transpilation, wherein gates in a circuit are rewritten in terms of other gates, reordered, or otherwise optimized. Many multipurpose quantum software libraries such as Qiskit [2] and Cirq [13], and the compiler $\texttt{tket}$ [14], expose such optimization transforms to the user. However, the concept of quantum transforms extends beyond simply turning one quantum circuit into another. A variety of quantum computing tasks can be expressed in the language of transforms, and more specifically, transforms that can preserve the ability to compute quantum gradients automatically.

In this work we formalize and implement differentiable quantum transforms, and discuss three specific applications: gradient computation, quantum compilation, and noise characterization and mitigation. We outline the formal definitions and key features of transforms in Section II A, and give an overview of the relevant examples in Section II B. We then present in Section III an implementation of an extensible transform system using the PennyLane quantum software library [1]. We show how the aforementioned applications can be implemented, and present explicit software examples that demonstrate its advantages. We conclude with ideas for future research and applications. Most notably, the transforms themselves are fully differentiable, so they can be parametrized and trained. This enables us not only to find optimal transform parameters, but gives us the potential to learn new transforms.

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II. DIFFERENTIABLE QUANTUM TRANSFORMS

A. Formalism

At a high level, a differentiable quantum transform is a composable function that takes a differentiable quantum program as input, and returns one or more differentiable quantum programs as output. Let $S$ be a quantum program [15, 16]. A quantum program may prepare the state of one or more qubits, apply quantum operations (or other quantum programs), and terminates with the measurement of one or more qubits. The probabilistic nature of measurement in quantum mechanics means that the output of a quantum program is non-deterministic in nature. In the context of the programs and transforms we discuss here, we will often consider the program output to be the expectation value of some observable taken in the limit of an infinite number of such measurements (shots), so that the output is reproducible.

Operations applied during the course a quantum program may be unitary operations, or quantum channels. An element of the unitary group on $n$ qubits, $U(2^n)$, is parametrized by $2^{2n}$ real values. Many quantum channels (e.g., depolarization, amplitude damping, etc.) are also expressed in terms of some real-valued parameter. Thus, we express a parametrized quantum program as $S(\sigma)$, where $\sigma = (\sigma_1, \ldots, \sigma_m)$ are the parameters [16]. Quantum programs can be differentiated with respect to their parameters; we denote this by $\frac{\partial S}{\partial \sigma_i}$, where it is implicit that the function being differentiated is the mathematical function implemented by the program $S$.

**Definition 1.** Let $S$ be a quantum program with input parameters $\{\sigma_i\}$. $S$ is a differentiable quantum program if $\frac{\partial S}{\partial \sigma_i}$ is defined for all $\sigma_i$.

Many derivatives (including higher-order ones) with respect to program parameters can be computed and evaluated on hardware. This generally involves the use of parameter-shift rules, which evaluate the quantum program at different values of its parameters and compute a function of the output [17–21]. For example, the common two-term shift rule which applies to many single-parameter gates is

$$\frac{\partial S}{\partial \sigma_i} = c [S(a\sigma_i + s) - S(a\sigma_i - s)],$$

where $s$ is the shift parameter, and $a$ and $c$ are gate-dependent constants (by default, $c = 1/2$, and $a = 1$). While this appears similar to a finite-difference method, the value of $s$ is macroscopic (typically $\pi/2$), enabling gradients to be estimated even in a noisy hardware setting where the infinitesimal shift of finite-differences would be completely washed out due to noise.

A quantum transform $T$ is a metaprogram that deterministically maps an input quantum program to one or more output quantum programs, and optionally depends on one or more parameters $\{\tau_i\}$. A differentiable quantum transform (DQT) is a transform that preserves differentiability of the input program with respect to the program parameters, while itself being a differentiable program. As is the case with quantum programs, we denote differentiation of a transform by $\frac{\partial T}{\partial \tau_i}$, where it is implicit that the function being differentiated is the mathematical function implemented by $S$ after it is transformed by $T$.

**Definition 2.** Let $S$ be a differentiable quantum program with inputs $\{\sigma_i\}$. A program $T$ with inputs $\{\tau_i\}$ is a differentiable quantum transform if it maps $S$ to one or more output programs, i.e.,

$$T(S) \rightarrow \{S'_k\}$$

where each $S'_k$ is also a differentiable quantum program with respect to the same inputs $\{\sigma_i\}$, and $\frac{\partial T}{\partial \tau_i}$ is defined for all $\{\tau_i\}$.

Transforms for which $\{\tau_i\} = \emptyset$ are non-parametrized transforms, whereas those with $\{\tau_i\} \neq \emptyset$ are parametrized transforms. We denote transforms mapping one program to a single other, $\{|S'_k\}| = 1$, as single transforms. Transforms mapping one program to many, $\{|S'_k\}| > 1$, are termed batch transforms. Differentiating the output of a batch transform may consist of differentiating the output of each program independently, or a function of those outputs.

We define both single and batch transforms to be mappable over lists of quantum programs, i.e., for single transforms, $T([S_1, \ldots, S_k]) = [T(S_1), \ldots, T(S_k)]$, where in the case of a batch transform, the result is a list of lists of programs. As such, transforms (whether parametrized or not) are composable.

**Corollary 3.** Let $T$, $U$ be two DQTs. DQTs are composable, i.e., $V = U \cdot T$ is also a DQT.

Composability of transforms enables us to construct and apply extensive pipelines of transforms to quantum programs, all the while preserving the differentiability of that program’s input parameters.
B. Applications

1. Gradient computation as transforms

Computation of quantum gradients is a key application of batch transforms. Consider, for example, the parameter-shift rules for computing gradients of parametrized unitaries on quantum hardware. Given a parametrized quantum circuit function

\[ f(\theta) = \langle \psi | U(\theta)^\dagger \hat{B} U(\theta) | \psi \rangle, \]  

where

- \(|\psi\rangle\) is the initial quantum state,
- \(U(\theta) = e^{iG\theta}\) is some parametrized unitary, with generator \(G\) having equidistant eigenvalues,
- and \(\hat{B}\) is an observable we wish to compute the expectation value of,

the parameter-shift rule allows us to compute the partial derivative of the expectation value by executing the same quantum function with (equidistant) shifted values \([21]\):

\[ \frac{\partial}{\partial \theta} f(\theta) = \sum_{\mu=1}^{2R} f \left( \lambda + \frac{2\mu - 1}{2R} \pi \right) \frac{(\pi^{\mu-1})}{4R \sin^2 \left( \frac{2\mu - 1}{4R} \pi \right)}. \]  

(4)

Here, \(R\) is the set of all (unique) pairwise differences of the eigenvalue spectrum of unitary generator \(G\)^1. In essence, we can evaluate the gradient of \(f(\theta)\) with respect to a particular parameter value \(\theta\) by evaluating the circuit at \(2R\) points, and then algebraically combining the results. This could be accomplished by a batch transform which creates a separate quantum program for each term in the sum, and then combines the results according to Equation 4.

Note that for the case where \(R = 1\) (corresponding to single-qubit rotation gates), the above parameter-shift rule reduces to the commonly known two-term rule \([20]\):

\[ \frac{\partial U(\theta)}{\partial \theta} = \frac{1}{2} \left[ U \left( \theta + \frac{\pi}{2} \right) - U \left( \theta - \frac{\pi}{2} \right) \right]. \]  

(5)

This can be easily extrapolated to other types of gradient computation, such as finite-differences, or for gates that permit more complex parameter-shift rules (such as the controlled-rotation gates with four-term shift rules).

2. Differentiable quantum compilation

Quantum compilation is the process of decomposing a high-level specification of a quantum algorithm into a sequence of elementary operations in a format suitable for a particular quantum device. This is an extensive pipeline with numerous components: circuit synthesis, circuit optimization, transpilation, hardware-specific qubit placement and routing, gate scheduling, and optimization of low-level pulse controls.

All these tasks can be naturally viewed as quantum transforms: a circuit is fed in as input, and a modified and/or optimized circuit comes out. Compilation is implemented in this manner in many other quantum software libraries. These often consist of a pipeline of one or more passes through a set of subroutines that transform the circuit. Such subroutines typically manipulate the circuit at the level of its directed acyclic graph (DAG). There is some existing work which provides guidance on how to put together automated pipelines \([22]\). Software tools for compilation such as \(t\text{ket}\) \([14]\), \(staq\) \([23]\), \(quilc\) \([24]\), Qiskit \([2]\), Cirq \([13]\), XACC \([25]\), QCOR \([26, 27]\), Quipper \([12]\), and the transforms in PennyLane, all give the user the flexibility to define pipelines based on a set of available building blocks. In particular, \(t\text{ket}\) explicitly uses a modular transform system in its software. Both \(t\text{ket}\) and pyquil have support for partial or parametric compilation respectively, which makes compilation of parametrized circuits more efficient by first tracing through execution with symbolic variables, and then specifying the numerical parameter values at runtime.

Implementing compilation using differentiable transforms allows for optimization of parametrized circuits without compromising the differentiability of the parameters. For example, consider a single transform that modifies a quantum

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^1 Note that since \(G\) has equidistant eigenvalues, the set \(R\) simply consists of some base frequency multiplied by natural numbers.
program by finding adjacent rotations of the same type on the same qubit, and combining them into a single rotation, e.g., \( RZ(\phi)RZ(\theta) = RZ(\phi + \theta) \). If both \( \phi \) and \( \theta \) are trainable parameters, the sum of these values represents a new trainable parameter, which we call \( \lambda = \phi + \theta \). If implemented in an autodifferentiable manner where operations on parameters are traced during a forward pass, we can compute the gradient of \( \lambda \) alone and use it to extract the gradients of \( \phi \) and \( \theta \). This can be advantageous if, for example, the parameter-shift rule of Equation 5. With only one trainable parameter, we must evaluate the program only twice, rather than four times in the case where each gradient must be computed individually.

3. Transforms and noise

Many common tasks in both noise characterization and error mitigation can be framed and explored in the context of differentiable transforms. The most basic application is to use transforms to add noise; a single parametrized transform may modify a quantum program by inserting applications of a parametrized noise channel after certain types of gates in order to simulate the behaviour of a noisy device. As transforms are composable, such noise models are highly customizable and allow for varying types and amounts of noise to be added.

However, perhaps a more interesting task is to leverage differentiable transforms to characterize noise. One can create a parametrized noise model as described above, and use the results of experiments on a noisy device to learn the values of the noise parameters that most closely match the observed behaviour. Thanks to the autodifferentiability of the transform parameters, this can be done using standard optimization techniques such as gradient descent.

Error mitigation methods are essential when running computations on noisy near-term quantum devices. One such method, zero-noise extrapolation (ZNE), is a technique that estimates a noiseless value of a result by running a circuit for increasing values of some scale factor that adds noise, and then extrapolating the results back to the zero-noise case [28–31]. ZNE naturally incorporates both single and batch transforms: a number of common methods used for addition of noise, such as CNOT pair insertion and unitary folding [32], can be implemented as single transforms; we can then implement a batch transform which uses the single transform to create new programs with different amounts of noise, and then compute a function of the results to obtain the mitigated value.

III. DIFFERENTIABLE QUANTUM TRANSFORMS IN PENNYLANE

Going beyond the theoretical description, we will discuss and showcase quantum transforms in the context of PennyLane. PennyLane, while not a pure functional library, contains a significant proportion of functional elements which enabled the development of the transforms module, \texttt{qml.transforms} (\texttt{qml} is the standard import alias for PennyLane). We begin with an overview of the key aspects of the system, followed by implementations of the applications discussed in Section II B.

A. The transforms module

PennyLane represents (differentiable) quantum programs and quantum circuits using three different types of data structures: quantum functions, quantum nodes, and quantum tapes, as shown in Figure 1. The core component of computation is a quantum function, which is a programmatic representation of a quantum circuit. Quantum functions are regular Python functions that accept arguments as input, apply a sequence of quantum operations, and return one or more quantum measurements.

In order to run a quantum function and obtain measurement results, a quantum function must be bound to a device. Such a binding is accomplished using a higher-level data structure called a quantum node, or \texttt{QNode}. The device may be a simulator, or actual quantum hardware. Once the two are bound, the quantum circuit can be executed by specifying the set of input parameters, and calling the QNode using the same syntax and parameters as one would call the underlying quantum function (this is enabled by the fact that the QNode wrapper is actually a Python \texttt{decorator}).

In order to actually run a QNode with a set of provided parameters, upon invocation, the QNode constructs an internal representation of the quantum function called a quantum tape. A quantum tape is the lowest-level data structure, representing a quantum program as an annotated queue of operations and measurements. Parameter values are assigned upon construction of the tape.

PennyLane contains explicit construction mechanisms for single transforms, batch transforms, and other types of non-composable transforms that can, e.g., be applied to a QNode to extract information about it. In many cases, the transforms can be applied to more than one type of data structure (for example, the \texttt{qml.transforms.insert}
def circuit(theta, phi, omega):
    qml.RX(theta, wires=0)
    qml.RY(phi, wires=1)
    qml.RZ(omega, wires=2)
    qml.CNOT(wires=[0, 1])
    qml.CNOT(wires=[1, 2])
    qml.CNOT(wires=[2, 0])
    return qml.expval(qml.PauliZ(0) @ qml.PauliZ(1))

dev = qml.device("default.qubit", wires=3)
qnode = qml.QNode(circuit, dev)
theta, phi, omega = 0.1, 0.2, 0.3
result = qnode(theta, phi, omega)

FIG. 1. Representations of quantum programs in PennyLane. (a) A standard quantum circuit. (b) A quantum function. (c) A quantum node (QNode), consisting of a quantum function bound to a quantum device on which it can be executed. (d) A quantum tape, a low-level data structure representing the quantum circuit which is constructed by the QNode and then executed on a device.

transform can be applied to quantum functions, QNodes, or even quantum devices, in order to insert gates at specified positions in a quantum circuit).

1. Single-tape and quantum function transforms

Single-tape transforms are the base unit of transforms in PennyLane. These are one-to-one transforms in which elements of a tape may be removed, added, or modified. Furthermore, the transform may accept one or more parameters which affect how the tape is modified. A simple example is presented in Figure 2, wherein all CNOT gates are converted to CZ and Hadamard gates by way of a textbook circuit identity.

FIG. 2. Example of a quantum tape transform. This transform applies the circuit identity $CNOT_{ij} = H_j \cdot CZ_{ij} \cdot H_j$ to all instances of a CNOT from any control qubit $i$ to target qubit $j$ on a quantum tape.

PennyLane tapes contain two lists: one of operations, and one of measurements. The software implementation of a tape transform consists of simply looping through the operations, and in the current context, queuing a new set of modified operations. PennyLane provides convenience decorators to ease the construction of tape transforms and other types of transforms. For example, the transform depicted in Figure 2 would be implemented in PennyLane as
follows:

```python
import pennylane as qml

@qml.single_tape_transform
def convert_cnots(tape):
    for op in tape.operations + tape.measurements:
        if op.name == 'CNOT':
            qml.Hadamard(wires=op.wires[1])
            qml.CZ(wires=[op.wires[0], op.wires[1]])
            qml.Hadamard(wires=op.wires[1])
        else:
            qml.apply(op)
```

One way to invoke the transform is by applying it to a quantum tape directly.

```python
with qml.tape.QuantumTape() as tape:
    qml.CNOT(wires=[0, 1])
    qml.RX(0.1, wires=0)
    qml.CNOT(wires=[1, 2])
    qml.expval(qml.PauliZ(0) @ qml.PauliZ(1))

transformed_tape = convert_cnots(tape)
```

Quantum function transforms (qfunc transforms) are elevated tape transforms, and simply wrap that underlying structure. Quantum tapes themselves are a lower-level data structure, and generally accessed and manipulated internally (e.g., constructed by a QNode prior to execution), rather than being user-facing. Therefore, qfunc transforms enable the same functionality for a user while still being able to work at the abstraction level of functions. They are implemented in essentially the same way, and in fact a tape transform can be converted to a qfunc transform simply by swapping out the top-level decorator.

```python
@qml.qfunc_transform
def convert_cnots(tape):
    for op in tape.operations + tape.measurements:
        if op.name == 'CNOT':
            qml.Hadamard(wires=op.wires[1])
            qml.CZ(wires=[op.wires[0], op.wires[1]])
            qml.Hadamard(wires=op.wires[1])
        else:
            qml.apply(op)
```

The advantage, now, is that the `convert_cnots` transform can be applied directly to quantum functions as a decorator, with no need to consider tapes at all beyond the implementation of the transform itself.

```python
@convert_cnots
def circuit(param):
    qml.CNOT(wires=[0, 1])
    qml.RX(param, wires=0)
    qml.CNOT(wires=[1, 2])
    return qml.expval(qml.PauliZ(0) @ qml.PauliZ(1))
```

This flexibility enables us to easily `compose` single qfunc transforms by chaining functions, or by stacking decorators. Transforms may also contain classical processing which affects the parameter values of operations on tapes. PennyLane includes a special module, `pennylane.math`, which enables manipulation of the parameter values (more generally, tensors) in a way that is agnostic to the underlying classical machine learning framework, and thus preserves differentiability. For example, we can write a single transform that acts on all `qml.RX` rotations and rotates by the square root of the original parameter value:

```python
import pennylane.math as math

@qml.qfunc_transform
def square_root_rx(tape):
    for op in tape.operations + tape.measurements:
        if op.name == 'RX':
            qml.RX(math.sqrt(op.data[0]), wires=op.wires[0])
        else:
            qml.apply(op)
```

We can create a quantum function that applies `qml.RX` rotations, apply the transform, and then compute the gradients with respect to the input parameters in any framework. Below is an example using the PyTorch framework which illustrates this flexibility.
```python
import torch

def apply_rx(x):
    qml.RX(x, wires=0)
    return qml.expval(qml.PauliZ(0))

dev = qml.device('default.qubit', wires=1)
qnode = qml.QNode(apply_rx, dev, interface='torch')
x_orig = torch.tensor(0.3, requires_grad=True)
res = qnode(x_orig)
res.backward()

transformed_qnode = qml.QNode(square_root_rx(apply_rx), dev, interface='torch')
x_transformed = torch.tensor(0.3, requires_grad=True)
res = transformed_qnode(x_transformed)
res.backward()

>>> x_orig.grad
tensor(-0.2955)

>>> x_transformed.grad
tensor(-0.4754)
```

2. Batch transforms

Batch transforms are one-to-many transforms which take one tape as input, and return a collection of tapes as output. Furthermore, in PennyLane, they may also return a classical processing function that acts on the results of the executed quantum tapes to compute a desired quantity (this function should also be differentiable). A key use case of batch transforms is the computation of quantum gradients, which was discussed in Section II B 1 and is shown graphically in Figure 3. The ability to differentiate and compose transforms ensures that we can compute n-th order derivatives without any obstacles.

Batch transforms can also be used to compute the expectation value of a Hamiltonian, also depicted in Figure 3. Let

\[ \hat{H} = \sum_i c_i P_i, \quad P_i \in \mathcal{P}_n, \]

where \( \mathcal{P}_n \) is the n-qubit Pauli group, and let \( U(\theta) \) be a parametrized quantum circuit. We can compute the expectation value of \( \hat{H} \), \( \langle \hat{H} \rangle \), after applying \( U(\theta) \) as a linear combination of the expectation value of all of its terms,

\[ \langle \hat{H} \rangle = \sum_i c_i \langle 0 | U^\dagger(\theta) P_i U(\theta) | 0 \rangle. \]

To compute \( \langle \hat{H} \rangle \) using a batch transform, we first transform the initial tape into multiple tapes, each of which measures the expectation value of an individual \( P_i \) (alternatively, we can partition the terms of \( \hat{H} \) into commuting sets, and compute one expectation value per set). We then execute each of the tapes, and feed the results into a processing function which will evaluate Equation 7. Below we construct the Hamiltonian and tape depicted in Figure 3.

```python
# Hamiltonian in Figure 3 where c_1 = c_2 = c_3 = 1
coeffs = [1, 1, 1]
obs = [
    qml.PauliZ(0) @ qml.PauliZ(1),
    qml.PauliY(0) @ qml.PauliY(1),
    qml.PauliX(0) @ qml.PauliX(1)
]
H = qml.Hamiltonian(coefficients, observables)

with qml.tape.QuantumTape() as tape:
    qml.RY(0.3, wires=0)
    qml.RY(0.4, wires=1)
```
FIG. 3. Visual depiction of two use cases of batch transforms. (a) Given an input tape, a gradient batch transform returns two objects: (1) one or more new, transformed tapes, and (2) a classical function that accepts the results of the executed transformed tapes, and returns a processed value. This particular example computes the gradient of the second parameter on the input tape using the parameter-shift rule of Equation 5. (b) A batch transform being used to evaluate the expectation value of a Hamiltonian $\hat{H} = c_1 ZZ + c_2 YY + c_3 XX$. (1) For each Pauli term (or, group of commuting terms) in the Hamiltonian, a separate tape is created and executed, returning that term’s expectation value. (2) The final expectation value, which is a linear combination of the Hamiltonian coefficients and associated expectation values, is computed by the processing function according to Equation 7 based on the execution results.

```python
qml.CNOT(wires=[0, 1])
qml.CNOT(wires=[1, 0])
qml.expval(H)
```

We can now apply the batch transform (which is built-in to PennyLane as `qml.transforms.hamiltonian_expand`), and use the processing function on the executed results.

```python
tapes, fn = qml.transforms.hamiltonian_expand(tape)
dev = qml.device('default.qubit', wires=2)
res = dev.execute(tape)

>>> fn(res)
array([0.97272928])
```

Batch transforms can also be applied as a decorator directly to QNodes; the outcome of executing the QNode is simply the output of the classical processing function. If both the transform and processing function preserve differentiability of all the parameters, the output of this processing function can be fed as input into other parts of a differentiable quantum program, or itself be differentiated (as will be demonstrated in Section III B 3).

3. Other transforms

The `qml.transforms` module contains two other types of transforms that do not fit the criteria above: device transforms, and information transforms. Device transforms act on PennyLane devices, modify their internal workings, and then return a new device with different behaviour. An example is `qml.transforms.insert`, which can add additional gates at specified points in the circuit, e.g., to add simulated noise at the level of the device.

```python
def circuit(x):
    qml.RX(-2*x, wires=0)
    qml.S(wires=0)
    return qml.probs(wires=0)
```
dev = qml.device('default.mixed', wires=1)
qnode = qml.QNode(circuit, dev)

# Adds amplitude damping after every gate
noisy_dev = qml.transforms.insert(qml.AmplitudeDamping, 0.05, position="all")(dev)
noisy_qnode = qml.QNode(circuit, noisy_dev)

>>> print(qml.draw(qnode, expansion_strategy="device")(0.3))
0: --RX(-0.6) --S-- | Probs
>>> print(qml.draw(noisy_qnode, expansion_strategy="device")(0.3))
0: --RX(-0.6)--AmplitudeDamping(0.05)--S--AmplitudeDamping(0.05)-- | Probs

Information transforms are non-composable, non-differentiable transforms that take a tape, quantum function, or QNode as input, and return a function capable of computing and/or displaying information about that input. Key examples are qml.draw, used in the previous example, and qml.specs, which takes as input a QNode and returns a function that computes its quantum resources.

B. Examples

In this section, we present implementations of the three examples of Section II B using the differentiable transforms implemented in PennyLane. For each example, we detail a specific scenario in which the differentiability yields significant advantages, insights, or enables novel functionality. Unless otherwise noted, all examples below can be implemented in the most recent release of PennyLane (v0.21).

1. Optimizing gradient computation in a noisy setting

While the parameter-shift rule works for a large variety of gates in variational quantum algorithms, we occasionally chance upon unitaries that we wish to train on hardware that do not permit a parameter-shift rule. This could be for a variety of reasons; perhaps the unitary does not satisfy the form $e^{iGx}$, or the eigenvalue spectrum of its generator is unknown.

In such cases, we typically must fall back to numerical methods of differentiation on hardware such as the method of finite-differences. Previous work exploring finite-differences in a noisy setting has shown that the optimal finite-difference step size for first-order forward difference is of the form [33]

$$h^* = \left(\frac{2\sigma_0^2}{N f''(x)^2}\right)^{1/4},$$

where $N$ is the number of shots (samples) used to estimate expectation values, $\sigma_0$ is the single-shot variance of the estimates, and $f''(x)$ is the second derivative of the quantum function at the evaluation point. While for large $N$ we can make the approximation $h^* \approx N^{-0.25},$ for small $N$ on hardware, we must manually compute the second derivative of the quantum function in order to determine a decent estimate for the gradient step-size, which can further introduce error while adding a prohibitive number of additional quantum evaluations required per optimization step. Instead, we can wrap the gradient computation in a quantum transform that learns optimal parameters for the finite-difference step size in the presence of noise.

Consider the following variational quantum circuit:

```python
N = 1000
dev = qml.device("default.qubit", wires=2, shots=N)

@qml.qnode(dev, max_diff=2)
def circuit(x):
    qml.Hadamard(wires=0)
    qml.Hadamard(wires=1)
    qml.SingleExcitation(x, wires=[0, 1])
    H = qml.PauliX(0) @ qml.PauliX(1)
    return qml.expval(H)
```

Here, circuit is the cost function we would like to optimize on a noisy device using first-order forward finite-differences, and 1000 shots. Rather than hard-coding in a constant finite-difference step size, we can include the variance of the single-shot gradient as a quantity to minimize in the cost function by using the qml.gradients.finite_diff quantum transform:
def cost_and_grad(x, h):
    """Return the cost function to minimize, and the quantum gradient""
    g1 = qml.gradients.finite_diff(circuit, h=h)(x, shots=[(1, N)])
    return circuit(x) + np.var(g1) / N + h, np.mean(g1)

def cost(x, h):
    """Convenience function to return just the cost to minimize""
    return cost_and_grad(x, h)[0]

Starting with \( x = 0.1 \) and \( h = 10^{-7} \) (the default step size value of the `finite_diff` transform) we can now write an optimization loop that:

1. Computes the cost value \( f(x, h) \) and an estimate of the quantum gradient \( \partial_x f(x, h) \) using single-shot finite differences with step-size \( h \) (implemented together in `cost_and_grad`).

2. Using autodifferentiation, computes the partial derivative of the cost value with respect to the step size, \( \partial_h f(x, h) \).

3. Applies a gradient descent step for both parameters \( x \) and \( h \).

    opt = qml.GradientDescentOptimizer(stepsize=0.05)

    # PennyLane contains a wrapped version of NumPy which allows
    # for specification of trainable parameters using `requires_grad`
    h = np.array(1e-7, requires_grad=True)
    x = np.array(0.1, requires_grad=True)

    h_track = []
    cost_track = []

    for i in range(300):
        h = np.clip(h, 0, 5)
        x = np.clip(x, 0, 2 * np.pi)

        h_track.append(h)
        cost_track.append(circuit(x))

        # as the cost function depends on the gradient of
        # the circuit wrt x, we return it alongside the loss value to
        # avoid additional computations
        loss, x_grad = cost_and_grad(x, h)

        # compute the gradient of the cost function wrt h
        h_grad = qml.grad(cost, argnum=1)(x, h)

        x, h = opt.apply_grad([x_grad, h_grad], (x, h))

The results of this 'adaptive step-size finite-difference' optimization is compared to both a naïve finite-difference optimization (using the default step size of \( h = 10^{-7} \)) and the optimal finite-difference optimization (by computing Equation 8 at every step) in Figure 4. It can be seen that the naïve finite-difference optimization fails to converge to the minimum at all; a stepsize of \( 10^{-7} \) results in a very large quantum gradient variance (as can be verified from Equation 8). The adaptive finite difference, as well as the optimum finite difference, by contrast, are both able to converge to the minimum — the optimum variant converging particularly quickly, as would be expected.

Nevertheless, the results show that knowing the underlying theoretical characteristics of a system (such as in the optimal case) are not required. By simply encoding the quantity we wish to minimize — the expectation value and the gradient variance — the use of differentiable quantum transforms allow us to train the model hyperparameters to minimize error during gradient descent. Such approaches may also be viable in more complex models, where optimal or error-minimizing hyperparameter values are not known in advance.

2. Augmenting differentiable compilation transforms with JIT compilation

The core difference between circuit compilation in PennyLane and other quantum software libraries is its compilation routines are quantum transforms, nearly all of which preserve differentiability\(^2\). This enables the computation of

\(^2\) At the time of writing, the two-qubit unitary decomposition remains non-differentiable due to it involving non-differentiable library functions such as eigensystem computation.
FIG. 4. Minimizing a two-qubit variational circuit cost function in a noisy setting, where expectation values must be approximated through sampling with 1000 samples. Gradient descent is utilized for the optimization, with three different methods of computing the gradient at each optimization step: (a) first-order finite difference where the step size $h$ has been optimized alongside the cost function (blue, solid), (b) finite-difference optimization where the optimal step size $h^*$ Equation 8 is computed at each iteration (orange, dashed), and (c) first-order finite differences with a constant step size of $h = 10^{-7}$ (black, dotted).

gradients of compiled circuits using a preferred autodifferentiation framework. Furthermore, such gradient computation is also less resource intensive because the autodifferentiation framework keeps track of the changes in variables and can produce circuits with a reduced number of parameters.

All compilation transforms in PennyLane are implemented as `qml.transforms`, and as such, manipulate a circuit at the level of its tape. Transforms include rotation merging, single-qubit gate fusion, inverse cancellation, and moving single-qubit gates through control/target qubits of controlled operations.

A top-level `qml.compile` transform is made available to the user to facilitate creation of custom compilation pipelines. For example, the following code shows a pipeline consisting of pushing commuting gates left through controls and targets of two-qubit gates, and then fusing all sequences adjacent of single-qubit gates into a single `qml.Rot` (general parametrized unitary) operation.

```python
pipeline = [
    qml.transforms.commute_controlled(direction='left'),
    qml.transforms.single_qubit_fusion
]

dev = qml.device('default.qubit', wires=3)

@qml.qnode(dev)
@qml.compile(pipeline=pipeline)
def circuit(x, y, z):
    qml.CNOT(wires=[0, 1])
    qml.RX(x, wires=1)
    qml.RY(y, wires=1)
    qml.S(wires=1)
    qml.CNOT(wires=[1, 2])
    qml.Hadamard(wires=2)
    qml.CNOT(wires=[2, 0])
    qml.RZ(z, wires=2)
    return qml.expval(qml.PauliZ(1))
```

Figure 5 depicts the original and compiled circuit obtained when running with input parameters (0.1, 0.2, 0.3). Furthermore, the compiled circuit remains fully differentiable with respect to the input arguments, even though they may not appear directly as the arguments in any of the gates of the compiled circuit.

```python
>>> params = np.array([0.1, 0.2, 0.3], requires_grad=True)
>>> grad_fn = qml.grad(circuit)
>>> grad_fn(*params)
(array(-0.0978434), array(-0.19767681), array(1.33356867e-17))
```
A disadvantage of applying transforms in this way is that every circuit execution involves feeding the quantum function through the transform pipeline. For large circuits and multistep pipelines that involve more mathematically complex operations such as full fusion of single-qubit gates, this could lead to significant temporal overhead. This is especially undesirable for gradient computations, as these by nature involve multiple executions of a quantum circuit.

Most of PennyLane’s circuit compilation transforms have been written in a way that will remain differentiable even after applying just-in-time (JIT) compilation. This yields benefits in both the classical and quantum aspects of running an algorithm. The classical preprocessing, which involves applying the quantum transforms, becomes significantly faster after the first jitted evaluation. We can then run the optimized circuit on quantum devices, which will typically have lower depth and fewer operations, without additional overhead. Furthermore, the same can be done for computation of gradients: not only may the number of quantum evaluations be reduced as a result of compiling the circuit, but the jitted gradient, after the first execution, will run significantly faster than the original.

Here we show an explicit example using the JAX interface and jax.jit. Consider the following circuit:

```python
def circuit(x, weights):
    for wire in range(5):
        qml.RX(x[wire], wires=wire)
        qml.Hadamard(wires=wire)
        qml.Rot(*weights[wire, :], wires=wire)

    for wire in range(5):
        qml.CNOT(wires=[wire, (wire + 1) % 5])

    return qml.expval(qml.PauliY(0) @ qml.PauliY(1) @ qml.PauliY(2) @ qml.PauliY(3) @ qml.PauliY(4))
```

This circuit performs 3 layers of single-qubit gates, followed by a ring of CNOTs. On a 5-qubit device, there are 20 total parameters. If we use jax.grad to evaluate the gradient with the parameter-shift rules, we expect to see 41 device executions (two per parameter, plus one for the initial forward pass).

```
import jax
from jax import numpy as jnp

dev = qml.device('default.qubit', wires=5)
x = jnp.array([0.1, 0.2, 0.3, 0.4, 0.5])
weights = jnp.array([[-0.28371043, 0.93681631, -1.00500712],
                     [1.41650132, 1.05433029, 0.91081303],
                     [-0.42656701, 0.98618842, -0.55753227]],
                     3 The two-qubit unitary decomposition is currently non-jittable due to use of conditional statements that determine the particular form of the decomposed circuit.
4 The functionality required to enable jit with JAX is not available in v0.21 of PennyLane; it will be included in the next release. These results can be reproduced using the code on the open PR #1894.
original_qnode = qml.QNode(
    circuit, dev, interface="jax", diff_method="parameter-shift"
)

with qml.Tracker(dev) as tracker:
    jax=grad(original_qnode, argnums=(0, 1))(x, weights)

>>> tracker.totals
{'executions': 41, 'batches': 2, 'batch_len': 41}
>>> %timeit ...
70 ms ± 2.15 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

The time was obtained from running in a Jupyter notebook cell on an Intel i7 3.40GHz processor. We can run the same circuit, but now compile using the qml.transforms.single_qubit_fusion transform, which will merge all adjacent single-qubit gates. This means our original 20-parameter circuit now has effectively 15 parameters, as well as lower circuit depth (expanding the rotations gives an original depth of 10, and compiled depth of 8).

dev = qml.device('default.qubit', wires=5)

compiled_qnode = qml.QNode(
    qml.transforms.single_qubit_fusion()(circuit),
    dev,
    interface="jax",
    diff_method="parameter-shift"
)

with qml.Tracker(dev) as tracker:
    jax=grad(compiled_qnode, argnums=(0, 1))(x, weights)

>>> tracker.totals
{'executions': 31, 'batches': 2, 'batch_len': 31}
>>> %timeit ...
1.79 s ± 3.2 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

Even though the number of quantum evaluations is lower, the application of transforms adds significant time overhead. But now, we can run jit on both the original and compiled gradient functions to speed up the computation. The first execution of the jitted function is typically longer (in this case, roughly 0.4s for the original, and 16s for the compiled case), however subsequent evaluations are markedly faster:

jitted_original_grad = jax.jit(jax.grad(original_qnode, argnums=(0, 1)))
jitted_compiled_grad = jax.jit(jax.grad(compiled_qnode, argnums=(0, 1)))

>>> jitted_original_grad(x, weights) # Run once
>>> %timeit ...
24.7 ms ± 170 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
>>> jitted_compiled_grad(x, weights)
>>> %timeit ...
14.4 ms ± 50.4 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)

New values of the parameters can be passed to the jitted and compiled gradient function without needing to run jit again. In variational algorithms, where a circuit and its gradient are evaluated on the order of thousands of times with different parameters over the course of the optimization process, this would lead to a substantial speedup. While this is only a small example, it demonstrates that ensuring compilation transforms preserve differentiability of the input parameters can lead to benefits both when executing on a quantum device and on a simulator.

3. Differentiable error mitigation

In this section we will implement fully differentiable ZNE with linear extrapolation (i.e., the extrapolated value is itself differentiable with respect to the input circuit parameters). We demonstrate this using the technique of unitary
folding [32]. In this method, a circuit $U$ is first applied, followed by repetitions of $U^\dagger U$. Following the example of the error-mitigation library mitiq [31], the number of such folds $n_f$ is computed based on a scale factor $\lambda$ according to the expression $n_f = (\lambda - 1)/2$, rounded to the nearest integer. A single transform implementing this is shown below:

```python
@qml.qfunc_transform
def unitary_folding(tape, scale_factor):
    for op in tape.operations:
        qml.apply(op)
    num_folds = math.round((scale_factor - 1.0) / 2.0)
    for _ in range(int(num_folds)):
        for op in tape.operations[::-1]:
            op.adjoint()
    for op in tape.operations:
        qml.apply(op)
    for m in tape.measurements:
        qml.apply(m)
```

ZNE fits perfectly into PennyLane’s batch transform system. A batch transform creates and returns multiple versions of the initial tape with different amounts of folding, and returns a function `fit_zne` which performs the noise extrapolation on the results of executing those tapes. We perform the extrapolation by hand-coding a simple linear regression (as we will soon demonstrate, we do so to ensure that differentiability with respect to circuit input parameters is preserved).

```python
from pennylane.tape import stop_recording
from functools import partial
def fit_zne(scale_factors, energies):
    scale_factors = math.stack(scale_factors)
    unwrapped_energies = math.stack(energies).ravel()
    N = len(energies)
    sum_scales = math.sum(scale_factors)
    sum_energies = math.sum(unwrapped_energies)
    numerator = N * math.sum(
        math.multiply(scale_factors, unwrapped_energies)
    ) - sum_scales * sum_energies
    denominator = N * math.sum(scale_factors ** 2) - sum_scales ** 2
    slope = numerator / denominator
    intercept = (sum_energies - slope * sum_scales) / N
    return intercept
```

```python
@qml.batch_transform
def zne(tape, mitigation_transform, scale_factors):
    with stop_recording():
        tapes = [mitigation_transform.tape_fn(tape, scale) for scale in scale_factors]
        processing_fn = partial(fit_zne, scale_factors)
    return tapes, processing_fn
```

The `zne` batch transform can now be applied either to a quantum tape to obtain the transformed tapes and processing function, or to a QNode to directly obtain the mitigated value. In fact once defined, a user can receive error-mitigated results simply by adding a single line to their code: the `@zne` decorator. This is demonstrated below, facilitated by the PennyLane-Qiskit plugin to import and apply a noise model to a device. We design a simple circuit which computes the expectation value of a multi-term Hamiltonian, as would be the case in near-term algorithms running on noisy devices, such as the variational eigensolver.

```python
from qiskit.test.mock import FakeVigo
from qiskit.providers.aer import QasmSimulator
from qiskit.providers.aer.noise import NoiseModel
```
device = QasmSimulator.from_backend(FakeVigo())
noise_model = NoiseModel.from_backend(device)
noisy_dev = qml.device(
    "qiskit.aer", backend='qasm_simulator', wires=3, shots=10000, noise_model=noise_model
)
noisy_dev.set_transpile_args(**{"optimization_level" : 0})

H = qml.Hamiltonian(
    coeffs=[1.0, 2.0, 3.0],
    observables=[
        qml.PauliZ(0) @ qml.PauliZ(1),
        qml.PauliZ(1) @ qml.PauliZ(2),
        qml.PauliX(0) @ qml.PauliX(1) @ qml.PauliX(2)
    ]
)

@zne(unitary_folding, [1.0, 3.0, 5.0, 7.0, 9.0])
@qml.qnode(noisy_dev, diff_method='parameter-shift')
def circuit(params):
    qml.RX(params[0], wires=0)
    qml.CNOT(wires=[0, 1])
    qml.RY(params[1], wires=1)
    qml.CNOT(wires=[1, 2])
    qml.RZ(params[2], wires=2)
    qml.CNOT(wires=[2, 0])
    return qml.expval(H)

params = np.array([0.5, 0.1, -0.2], requires_grad=True)

>>> circuit(params)
2.9115300000000004

Recall that we have programmed the linear regression manually using the qml.math module. This ensures that we can take the gradient of the mitigated value:

>>> qml.grad(circuit)(params)
array([-0.54936 , 1.971385 , 0.021725])

In addition to using the qml.transforms module functionality to build ZNE methods from scratch, PennyLane includes a batch transform, mitigate_with_zne, that integrates directly with mitiq. However, computing gradients is not currently supported when using the mitiq backend.

4. Learning noise parameters with transforms

The trainability of transform parameters can be leveraged for performing characterization tasks, such as learning parameters of noise. Suppose we have a simple noisy device where every single-qubit gate is depolarized by the same qubit-dependent amount. We can simulate this noise using a transform that applies an appropriate depolarization channel after every single-qubit gate.

@qml.qfunc_transform
def apply_depolarizing_noise(tape, p):
    for op in tape.operations:
        qml.apply(op)
        if len(op.wires) == 1:
            qml.DepolarizingChannel(p[int(op.wires[0])], wires=op.wires[0])

    for m in tape.measurements:
        qml.apply(m)

Suppose the set of true depolarization parameters is \( p = [0.05, 0.02] \), i.e., \( p = 0.05 \) for the first qubit, and \( p = 0.02 \) for the second. By choosing a suitable circuit for experimentation, we can set up an optimization loop that will use the transform to learn both depolarization parameters. For instance, let us create the following circuit:

def circuit(angles):
    qml.RX(angles[0], wires=0)
    qml.RY(angles[1], wires=1)
    return qml.expval(qml.PauliZ(0)), qml.expval(qml.PauliZ(1))
We first set up a representation of our noisy device, by creating a QNode and applying the depolarization transform that uses the true depolarization parameters. We set the device to use 10000 shots. Note that this step is merely for simulation purposes, and can simply be replaced by a noisy device that does not apply any transforms at all.

\[
\text{true_deps} = \text{np.array([0.05, 0.02])}
\]

\[
\text{noisy_dev} = \text{qml.device('default.mixed', wires=2, shots=10000)}
\]

\[
\text{noisy_circuit} = \text{apply_depolarizing_noise(true_deps)(circuit)}
\]

\[
\text{noisy_qnode} = \text{qml.QNode(noisy_circuit, noisy_dev)}
\]

Now, we construct an optimization loop to learn these depolarization parameters. We use a simple least-squares loss for the cost, and compute the difference between the output of a transformed QNode whose transform parameters we are trying to learn (which is running on an ideal, simulated device), and the noisy QNode (which is running on a device with the true amount of depolarization noise). Note that here, we can evaluate the QNodes at arbitrary angular parameters. We also must set initial values for the trainable parameters; we choose something relatively high, and we will clip the values to between 0 and 1, to maintain validity of the values as parameters for a depolarization channel.

\[
\text{angles} = \text{np.array([0.2, 0.3], requires_grad=False)}
\]

\[
\text{ideal_dev} = \text{qml.device('default.mixed', wires=2)}
\]

\[
\text{def cost(learn_eps):}
\]
\[
\quad \text{training_qnode} = \text{qml.QNode(apply_depolarizing_noise(learn_eps)(circuit), ideal_dev)}
\]
\[
\quad \text{return sum((training_qnode(angles) - noisy_qnode(angles)) ** 2)}
\]

\[
\text{opt} = \text{qml.GradientDescentOptimizer(stepsize=0.05)}
\]

\[
\text{correction_eps} = \text{np.array([0.1, 0.1], requires_grad=True)}
\]

\[
\text{np.random.seed(0) # For reproducibility}
\]

\[
\text{for } \text{r in range(100):}
\]
\[
\quad \text{correction_eps = np.clip(correction_eps, 0, 1)}
\]
\[
\quad \text{correction_eps = opt.step(cost, correction_eps)}
\]

\[
\text{>>> print(correction_eps)}
\]
\[
\text{tensor([0.04973839, 0.02163015], requires_grad=True)}
\]

The learned parameters are close to the true values. While this is a simple example, it could be generalized to more complex noise models, such as gate- and qubit-dependent noise, other types of noise such as gate over-rotation, as well as composition of noise channels.

### IV. CONCLUSIONS

Differentiable quantum transforms, and their implementation in PennyLane, are a flexible and highly-extensible tool for developing quantum algorithms. The examples shown here only scratch the surface of what transforms can enable in the future.

For example, transforms for quantum gradients can be augmented to ensure that all hyperparameters themselves are trainable. Like we did for finite-differences, similar approaches can be applied to analytic gradient methods such as the parameter-shift formula and the Hadamard test. Without needing to delve into deep characterization, the gradient hyperparameters can be included in the cost function to be minimized, allowing the classical optimization loop to find optimal hyperparameter values to mitigate hardware error and improve convergence.

Recent work [34] demonstrated the advantage of a variational approach to error mitigation: this could be implemented and extended with transforms to perform similar tasks that can optimize parameters of an error mitigation protocol that uses a trainable transform concurrently with the optimization of parameters of a variational algorithm. The example in Section III B 4 in particular could be used as a starting point for exploration into data-driven approaches to characterizing devices in order to create adaptive, more realistic simulations of hardware. Such simulated devices could then be used as resources to learn recovery transforms to undo noise, and develop improved error-mitigation techniques, without the overhead of needing to simulate on actual hardware.

Finally, this unlocks, in all domains, the possibility for learning new transforms. This would be of particular interest for applications in compilation and circuit optimization. Methods for, e.g., variational compilation [35] and differentiable architecture search [36] have been investigated, and parametrized transforms would enable similar methods to be seamlessly integrated into algorithmic pipelines.
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