Towards a geodesic algorithm for optimizing parametrized quantum circuits

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Introduction

Currently, most optimization algorithms for updating the parameters of variational circuits rely on the gradient descent algorithm. Recently, a modification of this algorithm was proposed to include information about the geometry of the quantum state, known as Quantum Natural Gradient [1]. This method involves using the Fubini-Study metric tensor, obtained by taking the real part of the Quantum Geometric Tensor (QGT), which serves as a metric in the projected Hilbert space. We propose a method based on the least action principle in a parameter space with a Fubini-Study metric, that naturally leads to a geodesic path during the optimization of a variational circuit, thus leading to a faster optimization in parameter space. The result is an algorithm that follows a geodesic evolution of the parameters, reducing optimization time. It iteratively adjusts the initial velocity according to the gradient of the cost function to identify the direction in which the cost function decreases. The algorithm was successfully tested on a toy model of one qubit to find the ground state of the Hamiltonian σ_Z.

Parametrized Quantum Systems

Given a $\boldsymbol{\theta} \in \mathbb{R}^d$.

Pure states: $|\psi(\boldsymbol{\theta})\rangle$.

A common parametric family of unitaries in variational quantum algorithms is a product of L non-commuting layers of unitaries:

$$|\psi(\boldsymbol{\theta})\rangle = U_L(\boldsymbol{\theta})\,|\psi_0\rangle\,,$$

where $U_L(\boldsymbol{\theta})$:

$$U_L(\theta) := V_L(\theta_L)W_L ... V_1(\theta_1)W_1.$$

Fubini-Study metric tensor

The Fubini-Study metric tensor is defined as $g(\boldsymbol{\theta}) = Re[G(\boldsymbol{\theta})]$, where:

$$G_{ij}(\boldsymbol{\theta}) = \left\langle \frac{\partial \psi_\theta}{\partial \theta_i}, \frac{\partial \psi_\theta}{\partial \theta_j} \right\rangle - \left\langle \frac{\partial \psi_\theta}{\partial \theta_i}, \psi_\theta \right\rangle \left\langle \psi_\theta, \frac{\partial \psi_\theta}{\partial \theta_j} \right\rangle.$$

Quantum Natural Gradient

The update rule for standard Gradient Descent:

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta \nabla C(\boldsymbol{\theta_k}).$$

Update rule for Quantum Natural Gradient:

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta g^{-1}(\boldsymbol{\theta_k}) \nabla C(\boldsymbol{\theta_k}).$$

Geodesic equation under a potential

The geodesic equation for a particle under a potential can be derived using the principle of least action:

$$S = \frac{1}{2} \int \left(g_{ij}(\theta) \frac{d\theta^i}{dt}\frac{d\theta^j}{dt} - 2C(\theta) \right) dt \longrightarrow \frac{d^2\theta^i}{dt^2} + \Gamma^i_{jk} \frac{d\theta^j}{dt}\frac{d\theta^k}{dt} = -g^{ij}\frac{\partial C}{\partial \theta^j}.$$

Where the Christoffel symbols are defined as:

$$\Gamma^i_{jk} := \frac{1}{2} g^{il} \left(\frac{\partial g_{lj}}{\partial \theta^k} + \frac{\partial g_{lk}}{\partial \theta^j} - \frac{\partial g_{jk}}{\partial \theta^l} \right).$$

Geodesic optimization algorithm

Inspired by the geodesic equation for a particle under a potential and Quantum Natural Gradient, we propose an **optimization algorithm whose update rule is given by the solution of the geodesic equation**.

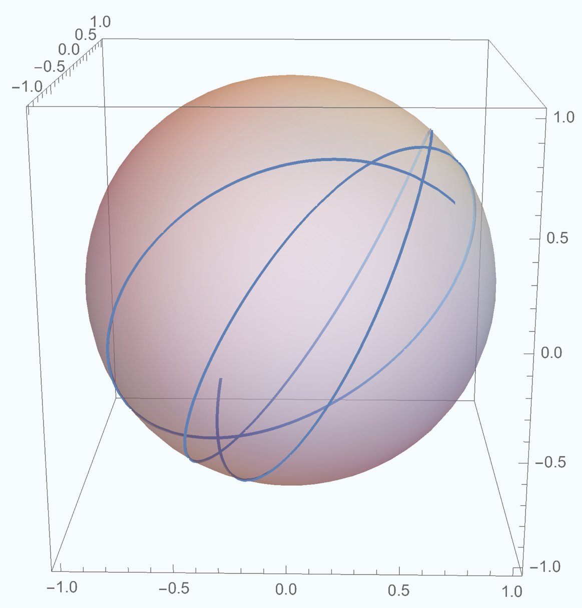
Differences between Quantum Natural Gradient and geodesic equation:

QNG	Geodesic Equation
1st order differential equation	2nd order differential equation
Requires only $\boldsymbol{\theta_0}$	Requires $\boldsymbol{\theta_0}$ and $\dot{\boldsymbol{\theta}}_0$
Guaranteed convergence to local minimum	No convergence, only evolution of parameters

The geodesic optimization algorithm combines both approaches, the update rule is given by the solution of the geodesic equation but we update the initial velocity by

$$\dot{\boldsymbol{\theta}}_0 = -g^{-1}(\boldsymbol{\theta})\nabla C(\boldsymbol{\theta}).$$

Example of Geodesic Evolution on 1-qubit



Numerical experiments on 1 qubit

Task: find ground state of the Hamiltonian $\boldsymbol{\sigma_z}$.
This corresponds to the south pole of the Bloch sphere.

Parametric model:

$$|0\rangle - \boxed{R_y(\theta_1)} - \boxed{R_z(\theta_2)} - |\psi(\theta_1, \theta_2)\rangle$$

Cost function:

$$C(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | \boldsymbol{\sigma_z} | \psi(\boldsymbol{\theta}) \rangle$$

Fubini-Study metric tensor:

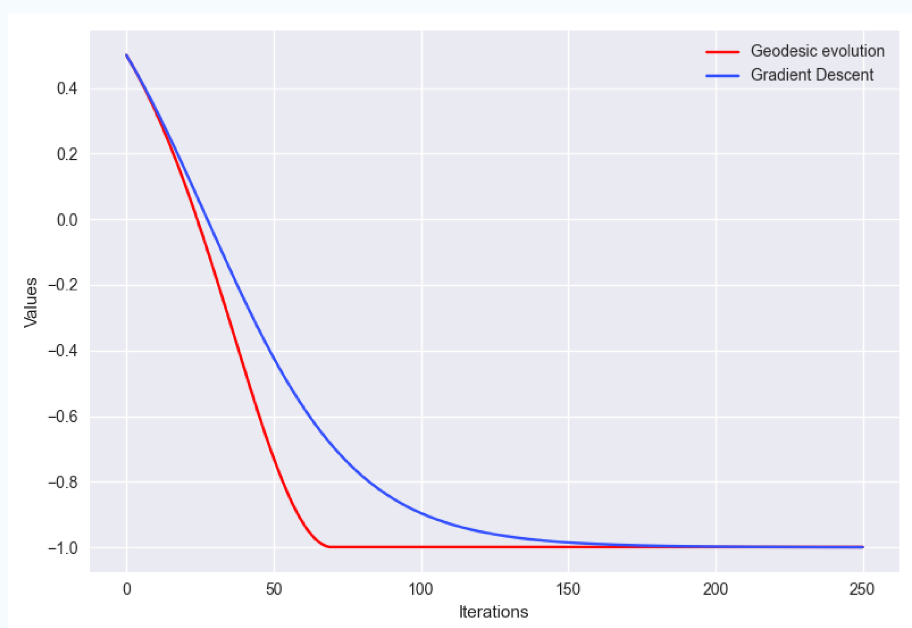
$$g(\boldsymbol{\theta}) = \frac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & \sin^2(\theta_1) \end{pmatrix}$$

Geodesic equations:

$$\frac{d^2\theta_1}{dt^2} - \sin(\theta_1)\cos(\theta_1)\left(\frac{d\theta_2}{dt}\right)^2 = -\sin(\theta_1),$$
$$\frac{d^2\theta_2}{dt^2} + 2\frac{\cos(\theta_1)}{\sin(\theta_1)}\frac{d\theta_1}{dt}\frac{d\theta_2}{dt} = 0.$$

Solve equations numerically using **Runge-Kutta** method.

Geodesic evolution vs Gradient Descent



References

1. J. Stokes, J. Izaac, N. Killoran, and G. Carleo, "Quantum natural gradient," Quantum 4, 269 (2020) doi: 10.22331/q-2020-05-25-269.
2. R. Cheng, "Quantum geometric tensor (Fubini-Study metric) in simple quantum system: a pedagogical introduction," arXiv:1012.1337 (2013).
3. R. Gómez-Lurbe, A. Pérez, "Towards a geodesic algorithm for optimizing parametrized quantum circuits", In preparation.