Understanding Quantum Algorithms Through Riemannian Optimisation

NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

Andres Arcia Lopez   Nanyang Technological Institute - SPMS

Co-Authors: Professor Cyrus Mostajeran   Dr. Marek Gluza

Introduction

The design of new quantum algorithms remains an unintuitive and elusive area that has lagged behind the rest of the developments of quantum computing[6]. Despite decades of research, we have developed very few quantum techniques, in part due to the lack of a unifying framework to aid our understanding of existing quantum algorithms and to facilitate the design of new ones.

The community still only relies on a small number of fundamental primitives. These primitives all fall within three classes.

- **Periodicity finding** - like Shor's factoring algorithm.
- **Searching** - algorithms providing a quadratic improvement to optimisation or search problems, like Grover's algorithm.
- **Quantum Physics Simulations** - Feynman's procedure for speeding up quantum simulations using a quantum computer.

Since 1995, no new classes of quantum algorithms have been discovered

Grover's algorithm plays a central role for unstructured search, serving as a building block for many modern quantum techniques within this class. Developing a unifying framework to understand the success of algorithms in this class, or others, and to discover new ones, would therefore be highly valuable.

Grover's Algorithm Overview

Suppose we have a set of $N = 2^n$ objects labelled by a unique binary string of length N. Let $\mathcal{B}$ be the set of objects we are intersted in finding anbd let $f(x)$ act as a quantum oracle such that

$$f(x) = \begin{cases} 0 & x \notin \mathcal{B} \\ 1 & x \in \mathcal{B} \end{cases}.$$

Start by preparing an initial state $|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |x\rangle$.

Define the operatos $D(\alpha) = e^{i\alpha\psi_0}$ and $U_f(\beta) = e^{i\beta H_f}$, where $\alpha, \beta \in \mathbb{R}$ and

$$\psi_0 = |\psi_0\rangle\langle\psi_0|,\ H_f = \sum_{x\in\mathcal{B}} |x\rangle$$

The state we wish to obtain is

$$|\psi^*\rangle = \frac{1}{\sqrt{|\mathcal{B}|}} \sum_{x\in\mathcal{B}} |x\rangle.$$

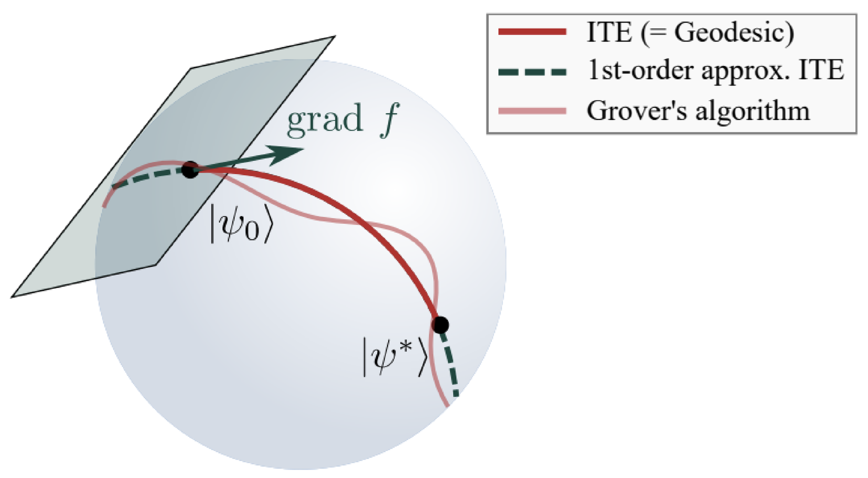
Grover's algorithm achieves an approximation to $|\psi^*\rangle$ by $\mathcal{N}$ applications of $G_k(\alpha_k, \beta_k) = -D(\alpha_k)U_f(\beta_k)$. Namely, we get

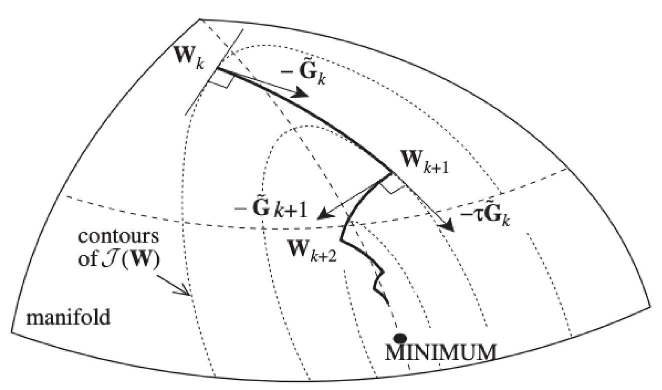
$$\prod_{k=1}^{\mathcal{N}} G_k(\alpha_k, \beta_k)|\psi_0\rangle \approx |\psi^*\rangle.$$

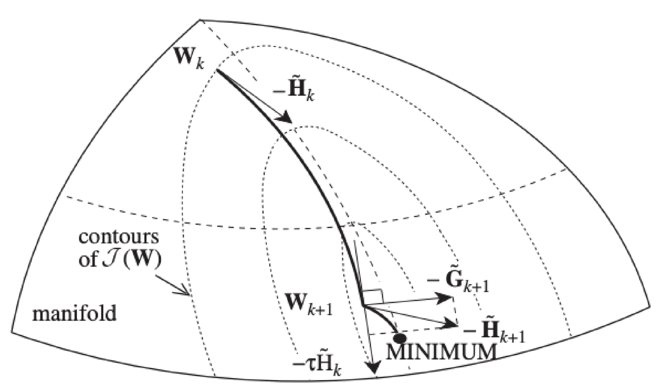
Different choices of α_k, β_k correspond ot different ways of implementing Grover's algorithm. Originally, Grover used $\alpha_k = \pi = \beta_k$[5], but other more optimal choices have been found since.

A diiferent Perspective to Grover's Algorithm

A natural framework to understand Grover's search algorithm is provided by optimisation on Riemannian manifolds. More specifically, we can show that Grover explicitly arises by optimising a least-squares cost function on the unitary manifold via a Riemannian steepest descent algorithm.







As H_f is a projector operator, we can obtain our solution state $|\psi^*\rangle$ using imaginary-time evolution (ITE).

$$|\psi^*\rangle = \lim_{\tau\to\infty} \frac{e^{\tau H_f}|\psi_0\rangle}{\left|e^{\tau H_f}|\psi_0\rangle\right|}$$

The novel framework of Double Bracket Quantum Algorithms (DBQAs)[4] allows us uncover in more detail how Grover's algorithm relates to ITE. This framework first recognises that ITE is a solution to

$$\frac{\partial\Psi(\tau)}{\partial\tau} = \left[\left[\Psi(\tau), H_f\right], \Psi(\tau)\right],$$

where $\Psi(\tau) = |\Psi(\tau)\rangle\langle\Psi(\tau)|$. By discretising the differential equation, we obtain the first order approximation $|\psi_s\rangle = e^{s[H_f,\psi_0]}|\psi_0\rangle + \mathcal{O}(s^2)$.

As H_f is a projector, we can show that there exists s_τ, for any τ, such that

$$\frac{e^{\tau H_f}|\psi_0\rangle}{\left|e^{\tau H_f}|\psi_0\rangle\right|} = e^{s_\tau[H_f,\psi_0]}|\psi_0\rangle.$$

By employing a product formula approximation[3] for the exponentiation of the commutator, $e^{s[H_f,\psi_0]} = e^{it_{2\mathcal{N}}\psi_0}\dots e^{it_3H_f}e^{it_2\psi_0}e^{it_1H_f} + \mathcal{O}(s^{m/2})$, for a certain $m \in \mathbb{Z}_+$ and $t_k = c_k\sqrt{s}$. It follows that, we recover Grover's algorithm up to a factor of $(-1)^{\mathcal{N}}$.

$$e^{s[H_f,\psi_0]}|\psi_0\rangle \approx (-1)^{\mathcal{N}} \prod_{k=1}^{\mathcal{N}} G_k(t_{2k}, t_{2k-1})\psi_0\rangle$$

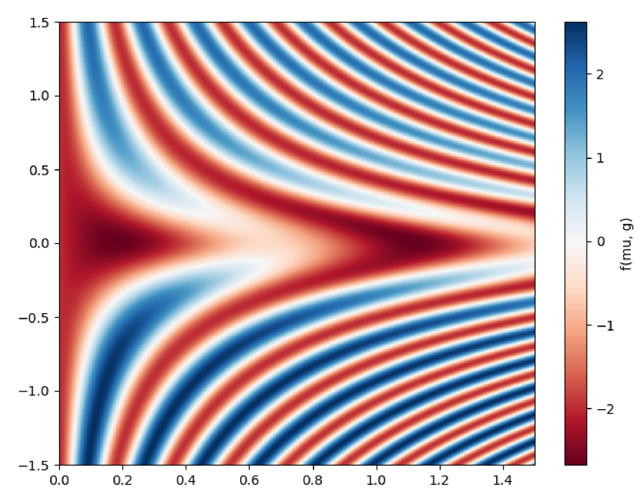
Grover's Link to Riemannian Optimisation

From the previous section we can see that Grover's algorithm arises by approximating $e^{s[H_f,\psi_0]}$. This expression corresponds to the steepest descent direction of the cost function $f : U(n) \to \mathbb{R}$ defined as

$$f(W) = \langle\psi_0|W^\dagger H_f W|\psi_0\rangle.$$

Taking into account that ITE traces a geodesic on $U(n)$ between $|\psi_0\rangle$ and $|\psi^*\rangle$, we can interpret Grover a product formula approximation of the geodesic. This geometric interpretation allows us to recover key properties of Grover's algorithm, such as its query complexity.

A question that arises is whether optimising the cost function through other Riemannian optimisation algorithms can uncover more details about current quantum algorithms or even help us design new ones. A natural next step is to consider a conjugate gradient algorithm.



Starting at, say, $W_0 = I$ and choosing an initial state $|\psi_0\rangle$, we keep updating the state via $|\psi_{k+1}\rangle = e^{-\mu S_k}|\psi_0\rangle$, where we choose μ such that $f(e^{-\mu S_k})$ is minimised and S_k corresponds to the algorithm's search direction.

Steepest Descent (SD): $S_k = [H_f, \psi_k]$.

Conjugate Gradient (CG): $S_k = [H_f, \psi_k] + \gamma_k S_{k-1}$, where it is interesting to consider different choices for γ_k.

Currently, the focus is on determining benchmark properties such as in what cases is CG better than SD and whether, as is the case for Nesterov acceleration for optimisation problems on $\mathbb{R}^n$[2], an optimal algorithm exists on $U(n)$.

References

[1] Traian Abrudan, Jan Eriksson, and Visa Koivunen. Conjugate gradient algorithm for optimization under unitary matrix constraint. *Signal Processing*, 89(9):1704–1714, September 2009.

[2] Jean François Aujol, Charles Dossal, and Aude Rondepierre. Optimal convergence rates for Nesterov acceleration, July 2019.

[3] Andrew M. Childs and Nathan Wiebe. Product formulas for exponentials of commutators. *Journal of Mathematical Physics*, 54(6):062202, June 2013.

[4] Marek Gluza. Double-bracket quantum algorithms for diagonalization. *Quantum*, 8:1316, April 2024.

[5] Lov K. Grover. A fast quantum mechanical algorithm for database search. In *Proceedings of the Twenty-Eighth Annual ACM Symposium on Theory of Computing*, STOC '96, pages 212–219, New York, NY, USA, July 1996. Association for Computing Machinery.

[6] Peter W. Shor. Why haven't more quantum algorithms been found? *J. ACM*, 50(1):87–90, January 2003.

[7] Yudai Suzuki, Marek Gluza, Jeongrak Son, Bi Hong Tiang, Nelly H. Y. Ng, and Zoë Holmes. Grover's algorithm is an approximation of imaginary-time evolution, September 2025.