Quantum Numerical Gradient Estimation - Jordan's Algorithm

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Abstract

Given a function $f : \mathbb{R}^d \to \mathbb{R}$, which is known to be continuously differentiable, one wants to estimate its gradient, ∇f at a given point $\mathbf{x} = (x_1, x_2, \ldots x_d)$ with n bits of precision. Classical algorithms require a minimum of $d^i + 1$ queries to the function for the i^{th} differential, whereas a quantum computer can be shown to require 2^{i-1} queries, i.e. the number of queries is independent of the size of the input, d, of $\mathbf{x}$.

1 Introduction

Numerical gradient estimation is a ubiquitous part of many problems, ranging from neural networks, to dynamical systems, to computational fluid dynamics. For some of these, the objective functions are amongst the most computationally time consuming parts of the solution. In context of such numerical calculations, the query complexity of a function is a natural measure of its time complexity [1]. Thus, an efficient algorithm is one which makes the fewest function evaluations; and our the number of such evaluation calls will define our time complexity.

The Qiskit implementation of the algorithm included with this report, is for the case of $d = 1$, and demonstrates the first differential ($i = 1$) of two simple functions, $\sin(x)$ and $10x + e^x + x^2$. The implementation utilizes quantum phase estimation as a subroutine and a modified *unitary matrix*, which is further elaborated upon within the presentation. This report discusses the original algorithm and a few of the algorithms derived from it.

2 Solution Summary

The simple algorithm leverages the fact that, in the vicinity of a point $\mathbf{x} = (x_1, x_2, \ldots x_d)$, $e^{2\pi\iota\lambda f(\mathbf{x})}$ is periodic, the period is parallel, and inversely proportional to the gradient $\nabla f(\mathbf{x})$. A superposition state is created by discretizing a infinitesimal hyper-rectangle around the domain point, evaluating the function, rotating the phase in proportion to the value of the function, reversing the oracle call and applying a multidimensional quantum Fourier transform to the bits encoding the aforementioned hyper-rectangle [3].

3 Analysis

Traditionally, for the 1D case, i.e. $d = 1$, gradients are estimated either analytically, or by using the finite difference method. To calculate the first and other higher derivatives, should they exist, the procedure is as follows

$$f'(x) = \lim_{h \to \infty} \frac{f(x+h) - f(x)}{h} \tag{1}$$

For the 1st gradient we need $d + 1$ calls to the function $f(x)$.

$$f''(x) = \lim_{h \to \infty} \frac{f(x) - 2f(x-h) + f(x-2h)}{h^2} \tag{2}$$

For the 2st gradient we need $2d + 1$ calls to the function $f(x)$.
Remember:

1. I should be able to understand your entire paper without consulting the article you read. This means you need to define every technical term that you will use and build my (the reader's) intuition about the topic by giving simple examples, etc.

2. Use both in-line equations such as $x^2 - x = 0$ as well as centered equations like
$$(a - b)(c - d)(e - f)(g - h) = 0.$$

4 Conclusion

Sum up the most important points you want to make about the article. Restate your overall evaluation. Tell whether the article increase your understanding of the subject or not. Why? Why not? Mention question you were expecting to be answered by the article that were not answered. Finally would you recommend others to read the article? Why?

References

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