Quantum Algorithm for Nonlinear Differential Equations

Dongwei Shi
ISE department Lehigh University
dos222@lehigh.com

December 16, 2024

Abstract

This paper is not a research article and does not propose any new perspectives or algorithms. Instead, it provides a concise summary of existing studies on using quantum computing techniques to address general nonlinear differential equations. In particular, it includes background information on two widely used mathematical concepts in this field: the Koopman operator and Carleman linearization. The aim is to offer an accessible overview and inspire further interest in this promising area of research.

1 Introduction

1.1 Literature Review

Differential equations find extensive applications in diverse fields such as fluid dynamics, biology, and finance. For instance, in fluid dynamics, the Navier-Stokes equations serve as fundamental tools for modeling fluid behavior [1]. In epidemiology, ordinary differential equations, such as those based on the Susceptible-Infectious-Recovered (SIR) model, are indispensable for analyzing the spread of infectious diseases [2]. Additionally, in finance, the Black-Scholes model relies on differential equations to facilitate option pricing [3].However, computing solutions for high-dimensional differential equations—where the state space has hundreds or even thousands of dimensions—presents a significant challenge. This challenge arises from the curse of dimensionality, wherein traditional numerical methods entail discretizing equations at grid points. As the dimension of equations increases, the number of grid points grows exponentially. Consequently, even basic linear algebra computations within these numerical algorithms become prohibitively computationally expensive.

A promising strategy for mitigating this complexity involves using quantum computing techniques since quantum computing leverages unique features such as quantum entanglement and superposition, enabling exponential speedups in specific computational tasks. As previous research has pointed out, replacing the linear systems solvers in classical numerical methods with their quantum counterparts, the Quantum Linear Systems Algorithm (QLSA),[4] can yield provably efficient quantum algorithms for solving linear Ordinary Differential Equations (ODEs)[5, 6, 7, 8] and linear Paritial Differential Equations (PDEs)[7, 9, 10, 11]. Additionally, quantum algorithms based on Hamiltonian simulation, rather than the QLSA, have also been shown theoretically to solve efficiently computational problems involving linear differential equations, whether for the standard Hamiltionian Simulation or non-Hermitian Hamiltionian Simulation[12].

However, despite a series of theoretical successes in developing quantum algorithms for linear differential equations, addressing nonlinear cases remains an open problem. Early attempts[13] to directly integrate QLSA with nonlinear ODEs proved to have poor scaling with evolution time. Recently, Liu et al.[14] demonstrated significant improvements by introducing Carleman linearization to certain nonlinear ODEs. Using QLSA on the linearized differential equations greatly enhanced the complexity bound with respect to the evolution time. This approach has motivated many researchers to consider first employing linearization techniques, such as Carleman Linearization[15, 16, 17], Koopman von Neumann linearization[18, 19, 20] and the level-set method[21], to approximate or represent low-dimensional nonlinear differential equations with high-dimensional linear ones, and then use quantum algorithms designed for linear differential equations to solve these problems. In contrast to this approach, another study proposed a different method for solving nonlinear ODEs [22], inspired by the connection between Koopman Operator Theory and the discrete Fourier transform. Based on the quantum Fourier algorithm, this method

offers an alternative perspective. However, its applicability is significantly limited by overly restrictive assumptions.

In this paper, we do not aim to propose or address any new research problems. Instead, our intention is to provide a summary of the current state of research on quantum algorithms for nonlinear differential equations. Specifically, we focus on a series of studies that design quantum algorithms based on Koopman Operator Theory, aiming to spark the interest of readers in this emerging area.

1.2 Background

In this section, I will introduce two key techniques commonly used in quantum algorithms for nonlinear ordinary differential equations: Carleman Linearization and the Koopman Operator. Both methods share a similar underlying principle: approximating nonlinear differential equations with high-dimensional linear ODEs. By leveraging such linearization transformations, they enable quantum computers, which are inherently designed for linear operations, to address nonlinear problems effectively.

1.2.1 Carleman Linearization

Carleman Linearization provides a systematic methodology for deriving the corresponding lifted dynamics from an initial value problem with $t \in [t_0, T]$ defined as follows [23]

$$\frac{d\boldsymbol{x}}{dt} = B_1\boldsymbol{x} + B_2\boldsymbol{x}^{\otimes 2} + ... + B_k\boldsymbol{x}^{\otimes k} \quad \text{with} \quad \boldsymbol{x}_0 = \boldsymbol{x}(t_0). \tag{1}$$

Here, the matrices $B_i \in \mathcal{R}^{d\times d^i}$ are time-independent, k is the degree of the polynomial ODE and $\boldsymbol{x}^{\otimes i}$ denotes the i-fold tensor product for each positive integer i from 1 to k, $\boldsymbol{x}_0$ means the inital value of given ODE. We define an infinite-dimensional vector $\boldsymbol{y} = (\boldsymbol{y_1}, \boldsymbol{y_2}, \boldsymbol{y_3}, ...)^T$ with $\boldsymbol{y_i} = \boldsymbol{x}^{\otimes i}$, and formulate matrices A^i_{i+j-1}

$$A^i_{i+j-1} = \sum_{v=1}^{i} \otimes_i B_j. \tag{2}$$

Where $\otimes_i B = I \otimes I \otimes I \otimes ... \otimes B \otimes ... \otimes I$ with B at $(d-i+1)$-th position. Further, formula (2) lead to the following equation

$$\frac{d\boldsymbol{y_i}}{dt} = \sum_{j=1}^{k} A^i_{i+j-1}\boldsymbol{y_{i+j-1}}. \tag{3}$$

Formally, this can be represented as an infinite-dimensional ordinary differential equation

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{\mathcal{A}}\boldsymbol{y} \qquad \text{with} \quad \boldsymbol{y_i}(t_0) = \boldsymbol{x}(t_0)^{\otimes i}, \tag{4}$$

where $\boldsymbol{\mathcal{A}}$ is an infinite-dimensional matrix defined as:

$$\boldsymbol{\mathcal{A}} = \begin{bmatrix} A^1_1 & A^1_2 & A^1_3 & ... & A^1_k & 0 & 0 & ... \\ 0 & A^2_2 & A^2_3 & ... & A^2_k & A^2_{k+1} & 0 & ... \\ 0 & 0 & A^3_3 & ... & A^3_k & A^3_{k+1} & A^3_{k+2} & ... \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \end{bmatrix}. \tag{5}$$

In practice, the system is often truncated at a certain order N. Here is an illustrative example [23] of Carleman Linearization applied to the following system

$$\frac{dx}{dt} = x^2. \tag{6}$$

Carleman Linearization procedure can derive a linear ode-like

$$\frac{d}{dt}\begin{bmatrix} x \\ x^2 \\ x^3 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & ... \\ 0 & 0 & 2 & 0 & 0 & ... \\ 0 & 0 & 0 & 3 & 0 & ... \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{bmatrix}\begin{bmatrix} x \\ x^2 \\ x^3 \\ \vdots \end{bmatrix}. \tag{7}$$

1.2.2 Koopman Operator

Firstly, consider a d-dimensional (i.e., $\boldsymbol{x} \in X \subset \mathbb{R}^d$) dynamical system described by a first-order autonomous order ordinary differential equations with $t \in [t_0, T]$ and

$$\frac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{f}(\boldsymbol{x}(t)). \tag{8}$$

where $\boldsymbol{x} = (x_1, x_2, ..., x_d)^T$ belongs to a space X and this dynamics $\boldsymbol{f}$ is also a d-dimensional vector valued function with $f = (f_1, f_2, ..., f_d)^T$. Then we introduce observables or measurement functions, represented by the function $g : X \to \mathbb{R}$. Note this is a function on $\mathcal{G}(X)$ (e.g., an $\mathcal{L}^2$ Hilbert space). The flow map F_t represents the evolution of the system dynamics as a mapping on X.

$$F_t : \boldsymbol{x}(t_0) \to \boldsymbol{x}(t + t_0). \tag{9}$$

The Koopman operator family, denoted as $\{\mathcal{K}_t\}$, is defined as

$$\mathcal{K}_t : g(\boldsymbol{x}(t_0)) \to g(F_t(\boldsymbol{x}(t_0))) = g(\boldsymbol{x}(t_0 + t)) \tag{10}$$

Alternatively, we can express $\mathcal{K}_t$ as a composition of functions

$$\mathcal{K}_t : g \to g \circ F_t. \tag{11}$$

It is crucial to note that the Koopman operator is linear, owing to the linearity of the function space $\mathcal{G}(X)$. Further, we can define the generator of the Koopman family as $\mathcal{K}$ with

$$\mathcal{K}g := \lim_{t \to 0} \frac{\mathcal{K}_t g - g}{t} = \frac{\partial g}{\partial t}. \tag{12}$$

Based on the chain rule, the generator can explicitly formulate as

$$\mathcal{K}g = \frac{\partial g}{\partial t} = \nabla g(\boldsymbol{x}) \frac{d\boldsymbol{x}}{dt} = \nabla g(\boldsymbol{x}) \cdot \boldsymbol{f}(\boldsymbol{x}). \tag{13}$$

The transformation of representing it in the form of an operator can be further extended as

$$\mathcal{K} = \nabla \cdot \boldsymbol{f}(\boldsymbol{x}) = \sum_{i=1}^{d} f_i(x) \frac{\partial}{\partial x_i}. \tag{14}$$

As a trade-off to address nonlinearity, we convert a nonlinear mapping on the variable x into a linear operator on the variable g, which leads to an infinite-dimensional space.

In Koopman Operator Theory, eigenvalues and eigenfunctions (or eigenpairs for brevity) are employed for practical numerical computations[24, 25]. Suppose $(\lambda, \phi(\boldsymbol{x}))$ is an eigenpair for the generator of Koopman family $\mathcal{K}$. By definition of eigenpairs

$$\mathcal{K}\phi(\boldsymbol{x}(t + t_0)) = \frac{d\phi(\boldsymbol{x}(t + t_0))}{dt} = \lambda\phi(\boldsymbol{x}(t + t_0)). \tag{15}$$

Based on the ODE in equation (15), we can derive the following outcomes for any $t \in [t_0, T]$

$$\phi(\boldsymbol{x}(t + t_0)) = \phi(\boldsymbol{x}(t_0))e^{\lambda t}. \tag{16}$$

Actually, $\phi(\boldsymbol{x})$ is also an eigen-function for $\mathcal{K}_t$, this can be observed from

$$\mathcal{K}_t\phi(\boldsymbol{x}(t + t_0)) = \phi(\boldsymbol{x}(t_0 + 2t)) = e^{\lambda t}\phi(\boldsymbol{x}(t_0 + t)). \tag{17}$$

In practice people often denote $e^{\lambda t}$ as μ, based on this notation $(\mu, \phi) = (e^{\lambda t}, \phi)$ is an eigenpair for $\mathcal{K}_t$.

If $g \in \mathcal{G}(X) \subset Span\{\phi_k\}$, then even nonlinear observable can be represented as a linear combination of eigenfunctions. This can be formulated as $g = \sum_j c_j\phi_j$, where $c_j \in \mathbb{R}$ is the corresponding coefficient of g concerning ϕ_j. Further, as pointed out in [24], the evolution of the observable can also be represented as a linear combination of eigenpairs which is derived from

$$\mathcal{K}_t g(\boldsymbol{x}(t + t_0)) = \mathcal{K}_t(\sum_{j=1}^{\infty} c_j\phi_j(\boldsymbol{x}(t_0 + t))) = \sum_{j=1}^{\infty} c_j e^{\lambda_j t}\phi_j(\boldsymbol{x}(t_0 + t)) = \sum_{j=1}^{\infty} c_j\mu_j\phi_j(\boldsymbol{x}(t_0 + t)). \tag{18}$$

Hence, we can infer

$$g(\boldsymbol{x}(t+t_0)) = \sum_{j=1}^{\infty} c_j e^{\lambda_j t} \phi_j(\boldsymbol{x}(t_0)). \tag{19}$$

Multi-dimensional observables are based in the same manner. Just consider vector-valued c_j with the same dimension of the observable. The value of c_j is also known as j-th Koopman mode [26].

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