Chapter 1

Introduction

1.1 Introduction

In recent years, there has been a rise in public concern regarding the environment and its impact on society. Numerous regulations include air, noise and water pollution, management of waste, and preservation of flora and fauna. Environmental authorities have been ordered to improve their current pollution prevention strategies as a result of these directives. As water is vital for existence, the issues of water pollution and waste water management are of particular importance. It is utilised extensively by society for industrial and domestic purposes, most notably in manufacturing, sanitation, heating, drinking, and bathing. In addition, marine and river environments must be considered in terms of fish and mollusk habitats. Coastal waters are also essential, especially in tourist areas where their contamination is detrimental. To this end, there are strict rules governing how waste water must be treated and where sewage can be discharged.

Hydrogeology, an interdisciplinary branch of science and engineering, has made the transport of solutes through the groundwater an important research topic.

The word hydrogeology is composed of three separate words: hydro, which means water, geo, which means earth, and logy, which means study. This branch of science is a combination of two distinct branches, namely hydrology and geology, which study water and the earth, respectively. Hydrology focuses primarily on the movement, distribution, and composition of water on Earth and other planets. This branch also subdivides into many subdivisions like chemical hydrology, echo hydrology, surface hydrology, hydrogeology, hydro informatics, hydro meteorology and isotope hydrology. Geology is the study of the earth's subsurface structure, the rocks that compose it, and the mechanisms by which these change over time. This provides us with information regarding the age of the earth, its history, and the composition and properties of its constituent materials. Practically speaking, geology is essential for the exploration and exploitation of minerals and hydrocarbons, the evaluation of water resources, the comprehension of natural hazards, the remediation of environmental problems, and the understanding of past climate change. Both hydrology and geology possess a unique historical context. Hydrogeology focuses primarily on the subsurface water and solute movement. The water that travels beneath the surface of the earth is known as groundwater, and the region where it moves is known as an aquifer.

1.2 Contamination of Groundwater

Water is one of the essential elements for life on Earth. It exists in two forms, surface water and groundwater, and only 2.5% of it is pure water. The glacier and ice sheets cover more than two-thirds of this freshwater. Ninety-seven percent of the freshwater is sourced from the earth. Therefore, groundwater is one of the most significant sources of freshwater for meeting fundamental requirements such as

agriculture and industry, and as an essential source of drinking water in both urban and rural areas.

As groundwater is the primary source of drinking water, its contamination poses a serious threat to living creatures. Groundwater contamination is extremely detrimental to the environment, human health, and wildlife populations. It may not instantaneously harm human and animal health, but long-term exposure can be hazardous. The contamination of groundwater by septic tank refuse can have detrimental effects on human health. Groundwater is contaminated by a wide range of artificial chemicals and microbes. Drinking water can spread bacteria and viruses that can cause cholera, hepatitis, and other illnesses. It can also cause methemoglobinemia or blue baby syndrome due to its high nitrate content. Different nations are implementing a variety of remediation strategies for surface and groundwater. Groundwater contamination is more difficult to eliminate than surface water contamination because it can travel considerable distances through unseen aquifers. Obtaining pure groundwater after contamination is costly.

After being released into the environment, contaminants travel within an aquifer similarly to groundwater. These materials move from areas of high concentration to areas of low concentration in an aquifer together with the groundwater flow. The contamination of groundwater can result from natural sources or diverse human activities. Residential, municipal, commercial, industrial, and agricultural activities degrade its quality. Surface water and groundwater are connected. Contaminants enter groundwater through porous medium as a result of activities on the land surface, such as the release of industrial wastes that have been stored, contaminated recharge water, septic system source leaks, underground storage system leaks, etc. This type of environmental degradation occurs when contaminants are discharged directly or tangentially into water bodies. The natural contamination of

groundwater depends on the material through which it travels. During movement, it may acquire a variety of compounds, including magnesium, calcium, and chlorides, among others. The presence of naturally occurring minerals and metallic deposits in rock and sediment can also contaminate groundwater. It is contaminated by various point and non-point sources, including storage tanks, disposal sites, industrial refuse disposal sites, accidental spills, leaking petrol, landfills, fertilisers, pesticides and herbicides, as a result of population growth. [9, 10, 11, 12, 13, 14, 15].

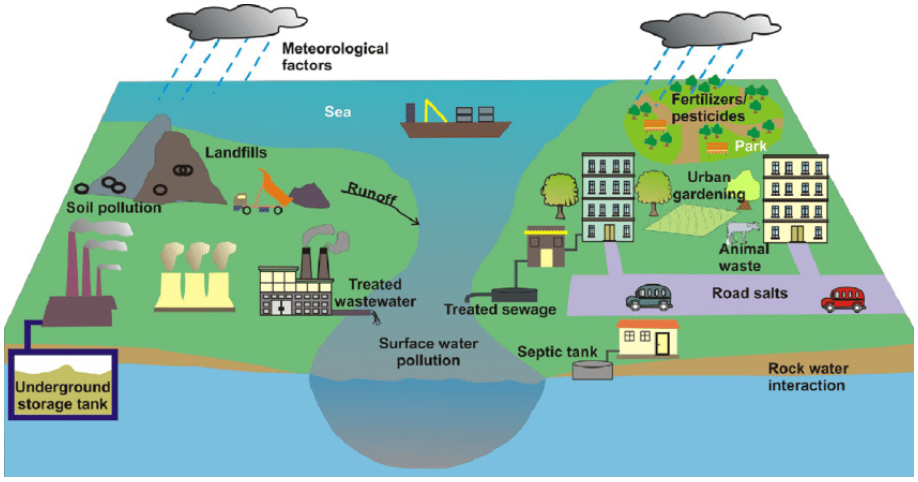

Figure 1.1: Sources of groundwater contamination

Over-pumping an aquifer close to the shore can create a vacuum that is quickly filled with salty seawater, rendering the water supply unfit for cultivation and perhaps undrinkable. Pumping groundwater has surpassed replenishment rate. In the nation, human activities such the disposal of waste, sewage, pesticides, fertilizers, industrial discharges, and toxic waste are to blame for groundwater contamination. According to the National Water Policy (1987), improper management of groundwater resources is another significant factor contributing to the rise in the drinking water crisis. As a result, the water level is rapidly dropping in numerous areas of India due to excessive groundwater extraction. Compared to point-source materials,

non-point source materials are used over a larger region and have a greater impact on water quality of an aquifer.

In the event that groundwater is generally contaminated, rehabilitation is thought to be too costly and laborious, and it may become unusable for many years. Then, even though it is quite unlikely, the only course of action is to look for another supply of water. Therefore, creating a mathematical model that forecasts the flow of solutes in aquifers and their impact on the environment and human health is crucial. In order to do this, it is first required to have a solid understanding of the physical, chemical, and biological mechanisms that govern the solute's movement in groundwater. When developing numerical groundwater models for field situations, careful consideration should be given to describing the problem domain, model parameters and boundary conditions.

1.3 Reaction-advection-diffusion equation

Since most groundwater-moving structures are of the porous variety, there is a great deal of room for research into solute transport in artificial [16, 17] and natural porous media. A significant field of study that use a variety of potent methods to address current contamination issues is mathematical modeling of solute transport in groundwater. Through tests and theoretical research, numerous scientists and engineers have anticipated the solute's flow in the groundwater system.

Within an aquifer, the pollution creates a contaminated plume that disperses over a wide area due to water movement. A transport model known as the solute transport model can be used for calculating the mobility of the plume known as a plume front. It is possible to predict the solute concentration in aquifers, rivers,

lakes, and streams by using solute transport modeling. There are numerous mathematical models for solute transport in groundwater that have been developed by scientists and engineers [9, 18**?**]. Hydrologists and other researchers have mainly used groundwater modeling to assess resource potential and predict future environmental effects under different scenarios. Anderson *et al.* [10] outlined in their monograph the applied groundwater models, flow simulation, and advective transport. Charbeneau [11] stated in his work the mechanics of groundwater and the movement of pollutants. Kehew [12] demonstrated the applied chemical hydrology. In [19] Rausch (2005) provided an analytical answer in addition to describing the solute transport modeling. These investigations have all improved our understanding of solute transport patterns in porous media and raised questions about possible pollution of the subsurface environment.

Partial differential equations (PDEs) can be used to showcase a wide range of natural systems, including thermal pollution of river systems, smoke and dust-induced air pollution, and groundwater pollution. The velocities of the transport medium are determined by solving the equations describing flows in porous media. Diffusion and advection are the primary variables, regardless of the nonlinearity of the flow equations.

The **advection-diffusion equation** (ADE) describes solute transport when advection and diffusion act together. **Reaction-advection-diffusion equation** (RADE) is a different form of the chemical equation that occurs with reaction term if the substance passing through the soil is reactive. RADEs are widely used in many fields, including biology, heat transport, chemical engineering, mechanical engineering, environmental engineering, petroleum engineering, and medical science.

The advection-diffusion equation can be used to explain a variety of real-world situations, including heat transmission in draining films [20], contaminant

dispersion in shallow lakes [21], flow in porous media [22], pollution transport in the atmosphere [23], pollution spread in rivers and steams [24], and flow in oil reservoirs [25].

Voutilainen *et al.* [26] has studied the diffusion process by which tracer molecules diffuse within a rock matrix with both heterogeneous and homogeneous porosities using numerical time-domain diffusion simulations. When solving advection-dispersion-reaction equations, Sun *et al.* [27] proposed a numerical method that improves a reliable technique called operator splitting in terms of both computing efficiency and simulation accuracy. Baltean *et al.* [28] developed a macroscopic model that depicted how convection and diffusion work in a heterogeneous medium to move a passive solute. Parlange *et al.* [29] formerly offered a general approximation for the one-dimensional nonlinear diffusion equation's solution, which was applicable to any soil parameters and boundary conditions.

One of the challenging equations to forecast the movement of a contaminant in a body of water is the reaction-advection-diffusion equation. The general solute transport model is reaction-advection-diffusion equation given by

$$\frac{\partial u}{\partial t} = \nabla.(D.\nabla u) - V.\nabla u + \lambda f(u), \tag{1.1}$$

where u is the transport dependent variable, D is the diffusivity tensor, V is the advective velocity vector. λ is rate coefficient and $f(u)$ is reaction term.

Considering the constant parameters of transportation concerning location and timing, RADE provides explicit closed form solution by using suitable numerical methods. The concentration of the solute (pollutant) as a function of distance and time from the source of contamination is obtained by solving the equation. The final steps in solving the equations are to consider the groundwater velocity, rate of

chemical reactions, coefficients of dispersion, boundary conditions, initial concentration of solutes in the aquifer and the physical boundaries of the groundwater flow system.

1.4 Fractional calculus

The differentiation and integration of integer order to any order is extended to the fractional calculus. It is crucial for explaining a wide range of chemical and physical events that can be represented as fractional-order differential equations in many scientific and engineering domains. The fractional-order RADE is among the most significant fractional-order differential equations. The field of fractional calculus has grown significantly from the contributions of well-known mathematicians such as J. Liouville, G. W. Leibniz, H. Weyl, B. Riemann, A. K. Grünwald, J. Caputo and A.V. Letnikov. When describing memory and genetic properties of different materials and processes, fractional calculus offers a very useful method [30].Fractional derivatives are shown to be highly useful for solving physical issues including fluid mechanics, rheology, and diffusion processes, among others. Because of its numerous applications in practical science and engineering—which are represented theoretically by fractional-order partial differential equations (FPDE)—fractional calculus [31] has gained significant attention in recent decades. Although there isn't now a valid geometrical or physical interpretation for the mathematical model, experts from all around the world are actively working to investigate it. Fractional space derivatives are utilized in the fractional differential equation to simulate anomalous diffusion or dispersion. The literature review reveals that Fick's second law is insufficient to explain the associated transport behavior in some diffusion processes. Anomalous

diffusion is the term used to describe a phenomena when the mean square displacement of a diffusion particle grows nonlinearly with time.

1.4.1 History of Fractional Calculus

A specific day has been named by numerous authors as the "birthdate" of "fractional calculus." L'Hopital asked G.W. Leibniz on a specific notation he was using in his work for the nth-derivative of the linear function $f(x) = x, D^n x/Dx^n$ in a letter dated September 30, 1695. L'Hopital's posed the question to Leibniz, what would the result be if $n = 1/2$. Leibniz's response: "An apparent paradox, from which one-day useful consequences will be drawn." Fractional calculus was created in these words. This letter indicates that the derivatives of fractional and integer orders were almost created simultaneously.

Numerous further letters were written about this topic after the 1695 letter. In 1697, G.W. Leibniz sent letter to J. Bernoulli and J. Wallis mentioning the possibility of fractional-order differentiation, that for non-integer value of n is

$$\frac{d^n e^{ax}}{dx^n} = a^n e^{ax}.$$

Several additional authors focused on this topic after Leibniz passed away. Leonard Euler made a contribution to the expansion of fractional differential calculus in this series. The factorial approach $n!$ to non-integer values was generalized by Daniel Bernoulli, which is called Gamma function $\Gamma(\cdot)$.

Between 1810 and 1819, Sylvestre Francois Lacroix, the French mathematician used Euler's derivation for his textbook 'Traite du Calcul Diferentiel et du Calcul Integer' [32]. Lacroix generalized the derivative from integer-order to

arbitrary order α of x^β as

$$\frac{d^\alpha x^\beta}{dx^\alpha} = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)} x^{\beta-\alpha}. \tag{1.2}$$

In 1822, Joseph Fourier generalized the notion of differentiation for arbitrary function through his book [33]. Until 1822, there were no attempts to describe physical phenomena of generalized arbitrary derivatives like integer-order derivatives only interest was on to set the basis of fractional differential calculus.

Fractional differential calculus was used by Niels Henrik Abel in 1823 to solve the tautochrone problem [34]. J. Liouville gave two distinct definitions of fractional derivatives later in 1832 [35].The first definition is based on a series that means he expanded the function $f(x)$ in the series

$$f(x) = \sum_{n=0}^{\infty} C_n e^{a_n x}, \tag{1.3}$$

then arbitrary α order derivative to be

$$D^\alpha f(x) = \sum_{n=0}^{\infty} C_n \, a_n^\alpha \, e^{a_n x}, \tag{1.4}$$

which is restricted a series that depends on the order of differentiation to be convergent. According to the second definition of fractional derivative, it was applied to the function of the form x^{-a} with $a > 0$. He considered $I = \int_0^\infty u^{a-1} e^{-xu} \, du$. Transformation $xu = t$ gives

$$x^{-a} = \frac{1}{\Gamma(a)} . I.$$

Applying the derivative operator D^{α} on both sides of the equation and using equation (1.2), we get

$$D^{\alpha}x^{-a} = \frac{(-1)^{\alpha}\Gamma(a+\alpha)}{\Gamma a}x^{-a-\alpha}. \tag{1.5}$$

The disadvantage of second definition is that it is not suitable to a wide class of function.

The main difference between Lacroix and Liouville definitions on fractional derivative is that according to Lacroix definition fractional derivative of constant gives a non-zero value, while other one gives zero. This sparks an interesting debate on whose definition was right in the $19th$ century. The next well-known mathematician to provide a definition for the fractional derivative was B. Riemann, who came after the timeframe. The idea of Liouvill's influenced, Riemann with his memoirs in which Liouville wrote the ordinary differential equation $\frac{d^n y(x)}{dx^n} = 0$ has the complementary solution

$$y_c = c_0 + c_1 x + c_2 x^2 + \cdots + c_{n-1}x^{n-1}.$$

Thus Riemann tried to find the solution $y(x)$ of $\frac{d^n y(x)}{dx^n} = f(x)$, where $f(x) \in C[d, e]$ by setting $y^{(k)}(a) = 0$, $a \in (d, e)$ with $0 \leq k \leq n-1$. The solution obtained is unique and given by

$$y(x) = \frac{1}{(n-1)!}\int_a^x (x-t)^{n-1} f(t)dt.$$

By extending this to non-integer order α we have Riemann-Liouville definition of fractional order integral as

$$y(x) = J_x^\alpha f(x) = \frac{1}{\Gamma\alpha}\int_a^x (x-t)^{\alpha-1} f(t)dt, \quad \alpha \geq 0,$$

and the fractional order derivative be

$$aD_x^\alpha f(x) = \frac{d^n}{dx^n} aJ_x^{(n-\alpha)} f(x).$$

Consequently, In 1892, Hadamard [36] had given definition for both fractional order integral and derivative. In 1917, Weyl [37] had formulated similar definition to the Riemann-Liouvill definition, but with different Kernel function $(t-x)^{\alpha-1}$ and different terminals of integration. Grunwald [38] and Post [39] had formulated fractional derivative as the limit of a sum, with the help of classical definition of a derivative. In 1927, Marchaud [40] suggested a comparable fractional derivative with any order.

An important role was played by Mittage-Leffler for the function for the generalization of e^x in fractional calculus which was given in 1903. Erdelyi-Kober fractional integral was presented by Erdeyi [41] and Kober [42], which was generalized the Riemann fractional integral and the Weyl integral. Riesz also formulated fractional integral which was successfully used in potential theory. The term "Caputo fractional derivative" was first used by M. Caputo in 1967. It is derived by computing the fractional integral first, then the ordinary derivative.

There are many other definitions exist in the literature [43]. In 1927, Davis [44] shows the benifits from using fractional calculus for functional equations. In 1938, [45] used the Riemann-Liouville and Weyl integral to develop the fractional version of the integration by parts. E. Love came up with explicit solutions for two integral equations [46] in 1967. She also demonstrated the presence of necessary and

sufficient conditions as well as the uniqueness of the solution. [47] He expanded the real order fractional calculus's features to the complex order later in 1971.

B. Ross deserves recognition for organizing and editing the inaugural conference on fractional calculus at the University of New Haven in June 1974, not long after completing his doctoral dissertation on the subject. One of the important papers was by Campos [48], where a generalization of both the Weyl and Cauchy integrals had been devised. The monograph by S. Sanko, A. Kilbas, and O. Marichev, initially published in Russian in 1987 and then translated into English in 1993, was referred to as an "encyclopedia" of fractional calculus. The number of books, journals, and texts available now that cover fractional calculus and its applications are predicted to increase even further in the years to come. But what is the importance of fractional calculus in physical phenomena until recent days, this was regarded as a secret mathematical theory without application of fractional calculus, however, there have been a lot of study done in the recent few decades on the applications of fractional calculus to a wide range of closely related scientific domains, such as control systems, finance, and economics, as well as the physics of diffusion and advection processes. In fact, there are currently a number of applications for fractional calculus, including fractional control of engineering systems, the development of calculus of variations, optimal control to fractional dynamic systems, fundamental investigations into the constitutive relations of mechanical, electrical, and thermal systems, and a variety of engineering materials, including viscoelastic polymers, foams, gels, and animal tissues, and their applications in science and engineering. Other applications include plasma physics, bio-engineering systems, such as brakes and machine tools, as well as image and signal processing, among other areas.

1.5 Fractional-order reaction-advection- diffusion equation

Not much study has been done on the RADE's fractional-order form thus far. The author's primary focus in this thesis is on the numerical solutions of the fractional-order reaction-advection-dispersion equation (FRADE) and the analysis of the problem's solution profile. Researchers have taken up this exercise because of the growing interest in FRADE due to its practical applications in fields such as material science, electro chemistry, acoustics, robotics and controls, and electro magnetism. The FRADE has promises in providing a precise depiction of solute transportation in intricate media, including permeable aquifers. Because fractional order derivatives are non-local, FRADE has wide-ranging real-world applications in engineering, physics, economics, and other fields. This feature makes FRADE far more memory-efficient than integer-order RADE. Many physical and engineering problems, including anomalous diffusion, medicine, biology, solute transport, random and disordered media, control, signal processing, and so on, have been described by FRADEs in time, space, and time-space. Time, space, and time-space FRADEs are key components to characterize and comprehend the dispersion phenomena, and they have attracted a lot of attention lately. Due to its higher model flexibility, non-local behavior, and eventual convergence to the integer-order system, researchers and engineers are actively working to find the solution of RADE in fractional-order systems. Few techniques, including the variable transformation method, the Green function method, the implicit and explicit difference methods, and the Adomian decomposition approach, are discovered through the literature review to solve FRADE.

Fractional calculus has been the subject of extensive study in recent years due to its numerous applications in the disciplines of chemical, physical, biological, geological,

and financial systems. For example, the mathematical model on fractional diffusion describes nondiffusive transport in plasma turbulence [49] and a nonlinear fractional diffusion model for capillary flow through porous media [50]. More accurate models of the systems under discussion can be obtained with fractional calculus. Both business and academia are paying more and more attention to the use of fractional derivative as a mathematical tool to construct more robust mathematical models in specific reservoir engineering domains. By substituting a fractional order derivative for an integer order, it is possible to create a realistic model of a physical phenomenon that is dependent on both the past and present times. Specifically, the microscopic behaviors of mass transport in porous media are intricate, and the physical events exhibit peculiar kinetics that the classical diffusion equation is unable to describe. In contrast, the microscopic dynamics of these phenomena are explained by the fractional diffusion equation.

Fractured porous medium is regarded as a fractal because of its intricate structure. The particles migrate along the pore channel fractures, which act as complex motion, causing the force field to become stochastically scattered fracture. Consequently, the anomalous diffusion equation and the diffusion equation in porous media will behave similarly. Nigmatullin [51, 52] first derived the fractional diffusion equation for the medium of fractal geometry in an effort to create more accurate mathematical representations of practical issues. This research on the anomalous contamination migration from fracture into porous rock matrix is available [53]. The transport equations of fractional order included within Liouville equations have been considered in [54]. Uchaikin and Sibatov [55] had solved the transport equation for fractional order in disordered semiconductors. Later, Kadem and Baleanu [56] have studied the fractional order transport equation's solution. Additionally, the fractional order transport equations based on Levy stable processes are provided [57].

While the fractional diffusion equation explains the microscopic dynamics of mass transportation in porous media, the classical diffusion equation is unable to describe the complicated microscopic behaviors of mass transportation and the physical phenomena' peculiar kinetics. The groundwater flow problem is represented in fractional order form in, [58, 59] where the classical Darcy law is generalized by considering the water flow as a function of a non-integer derivative of the piezometric head. Benson *et al.* [60] have clarified that the advection-diffusion equation's fractional order form is helpful for understanding the flow of contaminants in heterogeneous porous media and on earth surfaces like natural rivers.

The influence of different force fields on different motions enables elementary particles to conduct complicated motion; thus, the trajectories of the particles recreate geometrical objects with complex structures. It will never follow a Gaussian distribution in this situation, thus the diffusion equation cannot be modeled using the conventional Fick's law. Different approaches have been used to deviate from the conventional Darcy's law; the continuous time random walk (CTRW) technique is the most practical where the mean squared displacement of the particles is described by the nonlinear power law $\langle x^2(t)\rangle \approx t^{\alpha}, 0 < \alpha \leq 1$. By using $\alpha = 1$, the usual relation for the standard order process of diffusion may be obtained.

1.6 Mathematical preliminaries

Some definitions and notations used in the thesis, are provided in this section.

1.6.1 Riemann–Liouville operator

Definition: The Riemann–Liouville fractional integral operator of order $\alpha > 0$ of a function $f(x) \in [a, b]$ is defined by [61, 62]

$$J_x^\alpha f(x) = \frac{1}{\Gamma\alpha} \int_0^x (x-\xi)^{\alpha-1} f(\xi) d\xi, \alpha > 0, x > 0,$$
$$J_x^0 f(x) = f(x).$$

The Riemann-Liouville fractional derivative operator is denoted by $D_x^\alpha f(x)$ and defined by

$$D_x^\alpha f(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_a^x \frac{f(\xi)}{(x-\xi)^\alpha} dx, \alpha \in (0, 1). \tag{1.6}$$

In general,

$$D_x^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_0^x \frac{f(\xi)}{(x-\xi)^{\alpha-n+1}} d\xi.$$

Properties of Riemann–Liouville operator

1. $J_x^\alpha J_x^\beta f(x) = J_x^\beta J_x^\alpha f(x)$.
2. $J_x^\alpha J_x^\beta f(x) = J_x^{\alpha+\beta} f(x)$.
3. $J_x^0 f(x) = f(x)$.
4. $J_x^\alpha x^p = \frac{\Gamma(p+1)}{\Gamma(\alpha+p+1)} x^{\alpha+p}$.

1.6.2 Caputo fractional derivative

Definition: The Caputo fractional derivative, which is commonly seen in the literature on porous media, is defined as [61]

$$D^{\alpha}f(x) = \begin{cases} \dfrac{1}{\Gamma(n-\alpha)} \int_0^x \frac{f^{(n)}(t)}{(x-t)^{\alpha+1-n}} dt, & \text{if } n-1 < \alpha < n, \\ \dfrac{d^n f(x)}{dx^n}, & \text{if } \alpha = n \in N. \end{cases} \tag{1.7}$$

Also $D^{\alpha}C = 0$, for a constant C.

Therefore, it follows that

$$D^{\alpha}x^{\beta} = \begin{cases} 0, & \text{if } \beta \in N_0 \text{ and } \beta < \lceil \alpha \rceil, \\ \dfrac{\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha)} x^{\beta-\alpha}, & \text{if } \beta \in N_0 \text{and} \beta \geq \lceil \alpha \rceil \text{ or } \beta \notin N \text{and} \beta > \lfloor \alpha \rfloor, \end{cases} \tag{1.8}$$

where $\lfloor \alpha \rfloor$ is floor function and $\lceil \alpha \rceil$ is ceiling function, which are well known.

Properties of Caputo fractional derivative

1. Let $f \in C_{-1}^{n}, n \in N \cup 0$ then $D^{\alpha}f(x), 0 \leq \alpha \leq n$ is well defined and $D^{\alpha}f(x) \in C_{-1}$.

2. If $n-1 \leq \alpha, n \in N$ and $f(t) \in C_m^n, m \geq -1$, then $(J_x^{\alpha} D^{\alpha})f(x) = f(x) - \sum_{k=0}^{n-1} f^k(0+) \dfrac{x^k}{k!}, x \geq 0$.

1.6.3 Variable order Caputo derivative

The fractional order $\alpha(x,t)$ partial derivative of a function $u(x,t)$, with respect to x, in the Caputo sense ([63], [64], [65], [66]) is defined as [67]

$$ {}_0^cD_x^\alpha u(x,t) = \begin{cases} \dfrac{1}{\Gamma(r-\alpha)} \int_0^x (x-\xi)^{r-\alpha-1} \dfrac{\partial^r u(\xi,t)}{\partial \xi^r} d\xi, & \text{if } r-1 < \alpha < r, \\ \dfrac{\partial^r u(x,t)}{dx^r}, & \text{if } \alpha = r \in N. \end{cases} \tag{1.9} $$

Similarly, with respect to t the fractional order $\alpha(x,t)$ partial derivative of a function $u(x,t)$ in the Caputo sense is

$$ {}_0^cD_t^\alpha u(x,t) = \begin{cases} \dfrac{1}{\Gamma(s-\alpha)} \int_0^t (t-\tau)^{s-\alpha-1} \dfrac{\partial^s u(x,\tau)}{\partial \tau^s} d\tau, & \text{if } s-1 < \alpha < s, \\ \dfrac{\partial^s u(x,t)}{dt^s}, & \text{if } \alpha = s \in N, \end{cases} \tag{1.10} $$

where $\alpha(x,t)$ represents a function of two variable x and t.

1.6.4 Laplace transformation

Definition: Let $f(t)$ is a piecewise continuous function on every finite interval on semi-axis $(t \geq 0)$ and there exist some constants M and p such that $|f(x)| < M\, e^{p\,t}$, for all $t \geq 0$, then Laplace transformation $F(s) = L[f(t)]$ exists for all $s > 0$ and is defined by [68]

$$ L[f(t)] = \int_0^\infty f(t)\, e^{-st} dt. $$

1.6.4.1 Corollary

The Caputo derivative of VO-FD implies the following [67]

$$ {}_0^c D_x^{\alpha} x^{\beta} = \begin{cases} \dfrac{\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha)} x^{\beta-\alpha}, & \text{if } \beta \in N_0 \; and \; \beta \geq r, \; or \beta \notin N_0 \; and \; \beta > r, \\ 0, & \text{if } \beta \in N_0 \; and \; \beta < r, \end{cases} \tag{1.11} $$

where $r-1 < \alpha(x,t) \leq r$ and N_0 is the set of non-negative integers.

1.6.5 The Legendre wavelets

This section consists of definitions of one-dimensional Legendre wavelets. The Legendre wavelets $\psi_{n,m}(t) = \psi^L(k,n,m,t)$ depend on four arguments, where $n = 1, 2, ..., 2^{k-1}$, $k \in N$, $m = 0, 1, ..., (M-1)$, where m is the order of Legendre Polynomial and t is the normalised time. Legendre wavelets on interval [0,1] can be defined as

$$ \psi_{n,m}(t) = \begin{cases} \sqrt{m+\dfrac{1}{2}} 2^{k/2} L_m(2^k t - 2n + 1), & \text{if } \dfrac{n-1}{2^{k-1}} \leq t \leq \dfrac{n}{2^{k-1}}, \\ 0, & \text{Otherwise}, \end{cases} \tag{1.12} $$

where

$$ L_0(t) = 1, $$

$$ L_1(t) = t, $$

and

$$ L_{m+1}(t) = \frac{(2m+1)}{(m+1)} t L_m(t) - \frac{(m)}{(m+1)} L_{m-1}(t), m = 1, 2, 3, \cdots . $$

1.6.6 Approximation of a function

Approximation of a function $u(x,t) \in L^2[0,1] \times [0,1]$ can be done as

$$u(x,t) \approx \Psi_{k,M}^T(t) U \Psi_{k_1,M_1}(x), \tag{1.13}$$

where

$$\Psi_{k,M} = [\psi_{1,0}, ..., \psi_{1,M-1}, \psi_{2,0}, ..., \psi_{2,M-1}, ..., \psi_{2^{(k-1)},0}, ..., \psi_{2^{(k-1)},M-1}]^T,$$

$$\Psi_{k_1,M_1} = [\psi_{1,0}, ..., \psi_{1,M_1-1}, \psi_{2,0}, ..., \psi_{2,M_1-1}, ..., \psi_{2^{(k_1-1)},0}, ..., \psi_{2^{(k_1-1)},M_1-1}]^T,$$

and U is a $2^{k-1}M \times 2^{k_1-1}M_1$ coefficient matrix with entries as

$$u_{n,m,n_1,m_1} = \int_0^1 \psi_{n,m}(x) (\int_0^1 u(x,t) \psi_{n_1,m_1}(t) dt) dx. \tag{1.14}$$

1.6.7 Floor and Ceiling functions

The Floor of a real number α, denoted by $\lfloor \alpha \rfloor$, is the largest integer that is less than or equal to α. It is expressed express in the following way

$$\lfloor \alpha \rfloor = \max\{n : n \in Z, n \leq \alpha\}.$$

The Ceiling of a real number α, denoted by $\lceil \alpha \rceil$, is the smallest integer that is greater than or equal to α. It is expressed as

$$\lceil \alpha \rceil = \min\{n : n \in Z, n \geq \alpha\}.$$

1.6.8 Kronecker product

Definition: Let two matrices P of order $m \times n$ and Q of order $p \times q$ then the Kronecker product of P and Q is denoted as $P \otimes Q$ and defined as [69]

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ p_{m1} & a_{m2} & \cdots & p_{mn} \end{pmatrix}, Q = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ q_{m1} & q_{m2} & \cdots & q_{mn} \end{pmatrix},$$

which is the $mp \times nq$ matrix having the following block structure

$$P \otimes Q = \begin{pmatrix} p_{11}Q & p_{12}Q & \cdots & p_{1n}Q \\ p_{21}Q & p_{22}Q & \cdots & p_{2n}Q \\ \vdots & \vdots & \vdots & \vdots \\ p_{m1}Q & a_{m2}Q & \cdots & p_{mn}Q \end{pmatrix}. \tag{1.15}$$

1.6.9 The Riesz fractional operator

The Riesz fractional operator [70] for $n \in N$ and $n-1 < \alpha < n$, on a finite interval $a \leq x \leq b$ is defined as

$$\frac{\partial^\alpha u}{\partial |x|^\alpha} = D^\alpha u = -c_\alpha ({}_aD_x^\alpha u + {}_x D_b^\alpha u), \tag{1.16}$$

where $c_\alpha = \dfrac{1}{2cos(\alpha\pi/2)}; \alpha \neq 1$ and $u \in C^n[0,1]$.

Now

$${}_aD_x^\alpha u = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial |x|^n} \int_a^x \frac{u(\xi, y, t)}{(x-\xi)^{\alpha+1-n}} d\xi, \; n-1 < \alpha < n, \tag{1.17}$$

$$ {}_xD_b^\alpha u = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial |x|^n} \int_x^b \frac{u(\xi, y, t)}{(x-\xi)^{\alpha+1-n}} d\xi, \; n-1 < \alpha < n, \tag{1.18} $$

are the left-side and right-side Riemann–Liouville fractional derivatives, respectively [71], where $\Gamma(\cdot)$ denotes the Gamma function. In particular when $\alpha = 2$, ${}_0D_x^\alpha u(x,t) = {}_xD_L^\alpha u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2}$.

1.6.10 Grünwald-Letnikov derivative

The left and right Grünwald-Letnikov derivatives [1] with order $\alpha > 0$ of the given function $f(t)$ are defined by

$$ {}_{GL}D_{a,t}^\alpha f(t) = \lim_{h \to 0, Nh = t-a} h^{-\alpha} \sum_{j=0}^{N} (-1)^j ({}^\alpha U_j) f(t - jh), \tag{1.19} $$

and

$$ {}_{GL}D_{t,b}^\alpha f(t) = \lim_{h \to 0, Nh = b-t} h^{-\alpha} \sum_{j=0}^{N} (-1)^j ({}^\alpha U_j) f(t + jh). \tag{1.20} $$

1.6.11 Grünwald-Letnikov approximation [1]

To approximate the left and right Riemann Liouville derivatives, the right and left shifted Grünwald-Letnikov formulas are represented by ${}_{RL}D_{t_0,t}^\alpha$ and ${}_{RL}D_{t,T}^\alpha$, respectively and can be approximated by

$$ {}_{RL}D_{t_0,t}^\alpha u(t_k) \approx \Delta t^{-\alpha} \sum_{j=0}^{k} \nu_j^\alpha u(t_{k-j}), \tag{1.21} $$

and

$$ {}_{RL}D_{t,T}^\alpha u(t_k) \approx \Delta t^{-\alpha} \sum_{j=0}^{n_T - k} \nu_j^\alpha u(t_{k+j}), \tag{1.22} $$

where $\nu_j^\alpha = (-1)^j({}^\alpha U_j)$. For one shift, the left and right Riemann Liouville derivatives are approximated as

$$ {}_{RL}D^\alpha_{t_0,t}u(t_k) \approx \Delta t^{-\alpha} \sum_{j=0}^{k+1} \nu_j^\alpha u(t_{k-j+1}), \tag{1.23}$$

and

$$ {}_{RL}D^\alpha_{t,T}u(t_k) \approx \Delta t^{-\alpha} \sum_{j=0}^{n_T-k+1} \nu_j^\alpha u(t_{k+j-1}). \tag{1.24}$$

1.7 operational matrices

1.7.1 The operational matrix for VO-FD

Let $\Phi(t)$ be a $2^{k_1-1}M_1$-dimensional column vector as

$$ \Phi(t) = [\phi_1(t), \phi_2(t), ..., \phi_{2^{k_1-1}M_1}(t)]^T, \tag{1.25}$$

where $\phi_i(t) = t^{i-1}$, $i = 1, 2, ..., 2^{k_1-1}M_1$.

Then $\Phi(t)$ and the LWs vector $\Psi_{k_1,M_1}(t)$ are related as

$$ \Phi(t) = R\Psi_{k_1,M_1}, \tag{1.26}$$

where $R_{i,j} = < \phi_i(t), \psi_j(t) >$.

1.7.1.1 Lemma

[72] Suppose $\Phi(t)$ be defined as in equation (1.25) and $\alpha(x,t)$ $(0 < \alpha(x,t) \leq 1)$ be a positive real-valued function defined on R^2. Then the Caputo VO derivative of the

order $\alpha(x,t)$ of $\Phi(t)$ can be represented as

$$ {}_0^cD_t^{\alpha(x,t)}\Phi(t) = F_t^{\alpha(x,t)}\Phi(t), \tag{1.27}$$

where $F_t^{\alpha(x,t)}$ is an OM of order $2^{k_1-1}M_1 \times 2^{k_1-1}M_1$, given by

$$F_t^{\alpha(x,t)} = \frac{1}{t^{\alpha(x,t)}} \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & \dfrac{\Gamma(2)}{\Gamma(2-\alpha(x,t))} & \dots & 0 \\ 0 & 0 & \dots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & \dfrac{\Gamma(2^{k_1-1}M_1)}{\Gamma(2^{k_1-1}M_1-\alpha(x,t))} \end{pmatrix}. \tag{1.28}$$

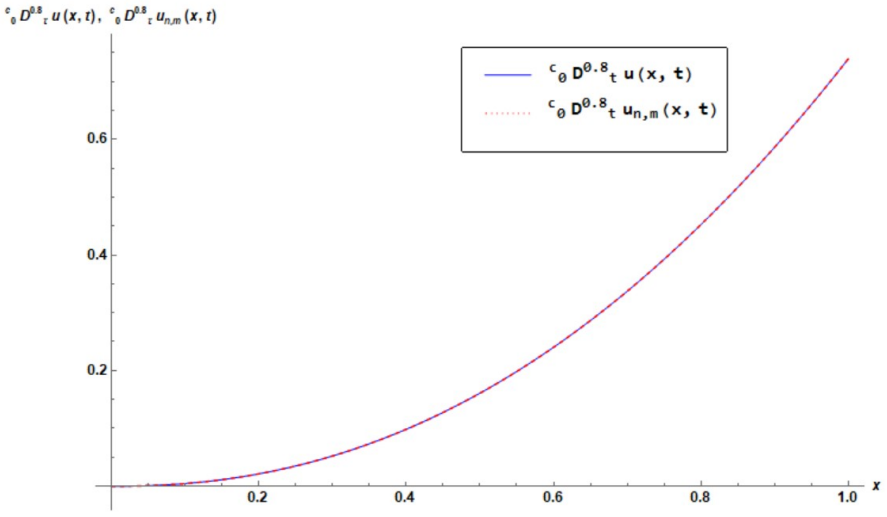

Figure 1.2: Plots of exact ${}_0^cD_t^{0.8}u(x,t)$ and approximate ${}_0^cD_t^{0.8}u_{n,m}(x,t)$ *vs.* x at fixed $k = k_1 = 1$, $M = M_1 = 8$ and $t = 0.5$.

1.7.1.2 Theorem

[72] Suppose $\Omega = [0,1] \times [0,1]$ and $\alpha(x,t)$ is a real valued function with domain Ω. The Caputo variable order fractional derivative of Ψ_{k_1,M_1} of order $\alpha(x,t)$ is

$$ {}_0^c D_t^{\alpha(x,t)} \Psi_{k_1,M_1}(t) = (Q^{(\alpha(x,t))}) \Psi_{k_1,M_1}(t), \tag{1.29}$$

where $Q^{(\alpha(x,t))} = R^{-1} F_t^{\alpha(x,t)} R$, R is $2^{k_1-1}M_1 \times 2^{k_1-1}M_1$ matrix defined in (1.26) and $F_t^{\alpha(x,t)}$ is an $2^{k_1-1}M_1 \times 2^{k_1-1}M_1$ operational matrix defined in (1.28).
Hence to find the approximate variable order fractional derivative in Caputo sense of a function $u(x,t)$, first find the approximation of the function $u(x,t)$ defined in (1.13) as

$$u(x,t) \approx \Psi_{k,M}^T(t) U \Psi_{k_1,M_1}(x) = u_{n,m}(x,t).$$

Now the approximation of variable order derivative in Caputo sense using (1.29) can be calculated as

$$\begin{aligned} {}_0^c D_t^{\alpha(x,t)} u(x,t) &\approx {}_0^c D_t^{\alpha(x,t)} u_{n,m}(x,t) \\ &= Q^{(\alpha(x,t))} \Psi_{k,M}^T(t) F \Psi_{k_1,M_1}(x) \\ &= (R^{-1} F_t^{\alpha(x,t)} R) \Psi_{k,M}^T(t) F \Psi_{k_1,M_1}(x), \end{aligned} \tag{1.30}$$

Now let us verify the exact variable order Caputo derivative defined in (1.10) with the approximated variable ordered Caputo derivative defined in (1.30). Figure 1.2 depicts the comparison of the exact with the approximated variable ordered Caputo derivative of a function $u(x,t) = (xt)^{2.2}$ for order $\alpha(x,t) = 0.8$ at fixed $t = 0.5$.

1.7.2 The operational matrix for partial derivative

Let $u_{n,m}(x,t)$ be the approximation of $u(x,t)$ as defined in section 1.6.6, where $\Psi_{k_1,M_1}(t)$ is the Legendre wavelet column vector, then

$$u_{n,m}(x,t) = \Psi_{k,M}^T(t) U \Psi_{k_1,M_1}(x), \tag{1.31}$$

where U is an unknown $2^{k_1-1}M_1 \times 2^{k_1-1}M_1$ order matrix. The derivatives can be approximated as [73]

$$\frac{\partial u_{n,m}(x,t)}{\partial x} = \Psi_{k,M}^T(t) U D \Psi_{k_1,M_1}(x), \tag{1.32}$$

where D is a $2^{k_1-1}M_1 \times 2^{k_1-1}M_1$ order operational matrix for derivative which is

$$D = \begin{pmatrix} F & 0 & 0 & \dots & 0 & 0 \\ 0 & F & 0 & \dots & 0 & 0 \\ 0 & 0 & F & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & F & 0 \\ 0 & 0 & 0 & \dots & 0 & F \end{pmatrix}, \tag{1.33}$$

in which F is a $M_1 \times M_1$ matrix with components

$$F_{r,s} = \begin{cases} 2^k \sqrt{(2r-1)(2s-1)}, & \text{if } r = 2,3,\dots, M_1,\ s = 1,\dots, r-1, \text{ and } (r+s) \text{ is odd} \\ 0, & \text{otherwise .} \end{cases} \tag{1.34}$$

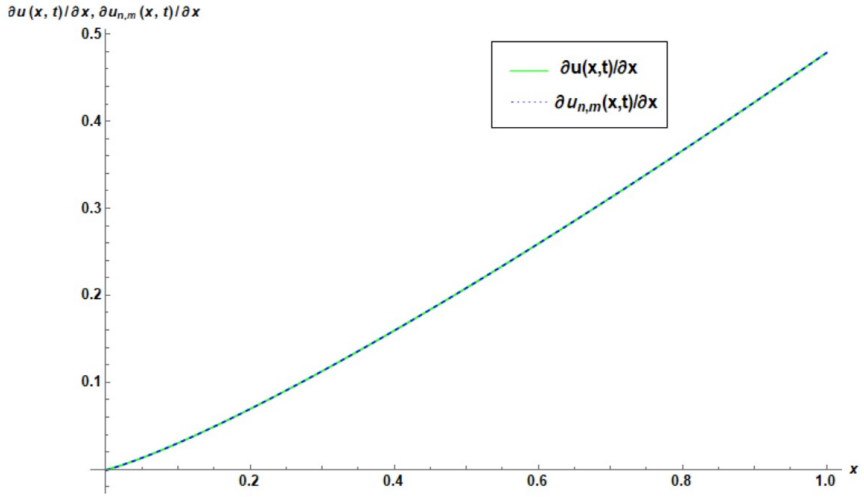

Figure 1.3: Plots of exact $\partial u(x,t)/\partial t$ and approximated $\partial u_{n,m}(x,t)/\partial t$ *vs.* x at fixed $k = k_1$=1, $M = M_1$=8 and $t = 0.5$.

For first order derivative,

$$\frac{\partial u_{n,m}(x,t)}{\partial t} = \Psi_{k,M}^T(t) D^T U \Psi_{k_1,M_1}(x), \tag{1.35}$$

and for higher order derivatives,

$$\frac{\partial^n u_{n,m}(x,t)}{\partial x^n} = \Psi_{k,M}^T(t) U D^n \Psi_{k_1,M_1}(x), \tag{1.36}$$

and

$$\frac{\partial^n u_{n,m}(x,t)}{\partial t^n} = \Psi_{k,M}^T(t) (D^T)^n U \Psi_{k_1,M_1}(x). \tag{1.37}$$

The verification of the approximated first order partial derivative defined in (1.35) with the exact first order partial derivative of a function $u(x,t)$ with respect to x is given in Figure 1.3 taking the function as $u(x,t) = (xt)^{2.2}$ at fixed $t = 0.5$.

1.7.3 Integral operational matrix

Let $\Psi_{k_1,M_1}(t)$ be the Legendre wavelet column vector defined in the section 1.6.6, then the integration of $\Psi_{k_1,M_1}(t)$ with respect to t can be defined as [74]

$$\int_0^t \Psi_{k_1,M_1}(\tau)d\tau = P\Psi_{k_1,M_1}(t), \tag{1.38}$$

where P is a $2^{k_1-1}M_1 \times 2^{k_1-1}M_1$ ordered matrix given by

$$P = \frac{1}{2^{k_1}} \begin{pmatrix} H & G & G & \dots & G & G \\ 0 & H & G & \dots & G & G \\ 0 & 0 & H & \dots & G & G \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & H & G \\ 0 & 0 & 0 & \dots & 0 & H \end{pmatrix}, \tag{1.39}$$

where G and H are $M_1 \times M_1$ ordered matrices given below :

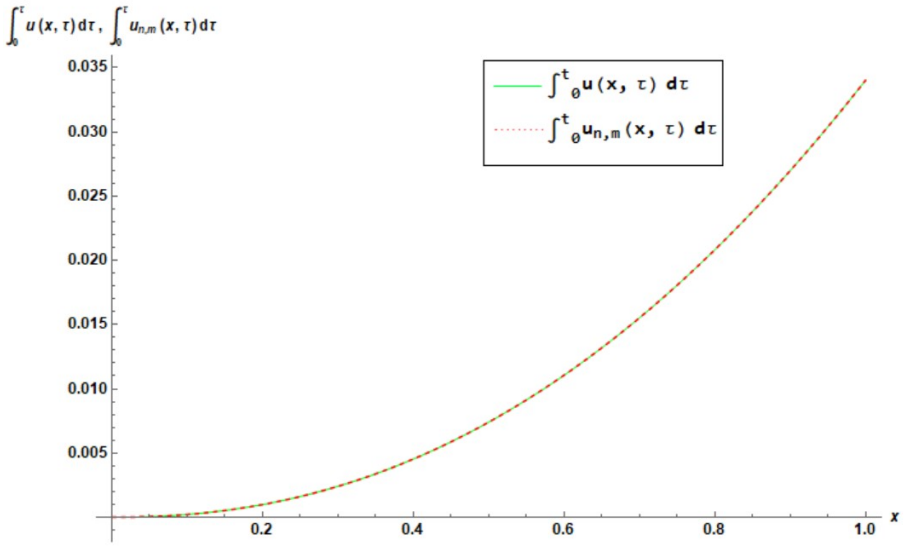

Figure 1.4: Plots of exact $\int_0^t u(x,\tau)d\tau$ and approximated $\int_0^t u_{n,m}(x,\tau)d\tau$ *vs.* x at fixed $k = k_1$=1, $M = M_1$=8 and $t = 0.5$.

$$G = \begin{pmatrix} 2 & 0 & 0 & ... & 0 & 0 \\ 0 & 0 & 0 & ... & 0 & 0 \\ 0 & 0 & 0 & ... & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & ... & 0 & 0 \\ 0 & 0 & 0 & ... & 0 & 0 \end{pmatrix}, \tag{1.40}$$

and

$$H = \begin{pmatrix} 1 & \frac{1}{3^{1/2}} & ... & 0 & 0 \\ -\frac{3^{1/2}}{3} & 0 & ... & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & .. & 0 & \frac{(2M_1-3)^{1/2}}{(2M_1-3)(2M_1-1)^{1/2}} \\ 0 & 0 & ... & -\frac{(2M_1-1)^{1/2}}{(2M_1-1)(2M_1-3)^{1/2}} & 0 \end{pmatrix}. \tag{1.41}$$

Hence, we can define integration of function $u(x,t)$ as

$$\int_0^t u_{n,m}(x,\tau)d\tau = \Psi_{k,M}^T(t)(P^T)U\Psi_{k_1,M_1}(x). \tag{1.42}$$

The verification of the approximated integration defined in (1.42) with the exact integration of a function $u(x,t)$ with respect to t is given in Figure 1.4 taking the function as $u(x,t) = (xt)^{2.2}$ at fixed $t = 0.5$.

1.7.4 Approximation of a function using Shifted Legendre polynomial

The recursive relations define Legendre polynomials on $[-1, 1]$ as

$$l_0(x) = 0,$$

$$l_1(x) = x,$$

$$l_{m+1}(x) = \frac{2m+1}{m+1} x l_m(x) - \frac{m}{m+1} l_{m-1}(x), m = 1, 2, 3, \cdots .$$

The transformation $t = \frac{x+1}{2}$ can be used to convert a Legendre polynomial to a shifted Legendre polynomial. This will change the range $[-1, 1]$ to $[0, 1]$, and the shifted Legendre polynomial will become

$$L_m(t) = \sum_{k=0}^{m} (-1)^{m+k} \frac{(m+k)!}{(m-k)!} \frac{t^k}{(k!)^2}, m = 0, 1, 2, \cdots .$$

The shifted Legendre polynomial of degree i on the interval $[0, X]$ is therefore given by the explicit analytical form

$$L_{X,i}(x) = \sum_{s=0}^{i} \frac{(-1)^{i+s}(i+s)!}{(i-s)!} \frac{x^s}{X^s (s!)^2}, i = 0, 1, 2, ...; \tag{1.43}$$

and the boundary values of $L_{X,i}(x)$ are

$$L_{X,i}(0) = (-1)^i,$$

$$L_{X,i}(X) = 1.$$

1.7.4.1 One Dimensional Space

In one dimension, the orthogonality condition of the Shifted Legendre polynomial $L_n(x)$ is

$$\int_0^1 L_i(x)L_j(x)dx = \begin{cases} \dfrac{1}{2i+1}, & \text{if } i = j, \\ 0, & \text{otherwise .} \end{cases}$$

Consider a function $c(x) \in C[0,1]$, which is approximated as [75]

$$c(x) \approx \sum_{k=0}^{n} a_k L_k(x), \tag{1.44}$$

where

$$a_k = (2k+1)\int_0^1 u(x)L_k(x)dx.$$

In matrix notation, this approximation of $c(x)$ will be

$$c(x) \approx A^T\psi(x),$$

where order of coefficient matrix A and the matrix $\psi(x)$ is $(n+1)\times 1$, which are determined as

$$A = [a_0, a_1, a_2, ..., a_n]^T.$$

and

$$\psi(x) = [L_0(x), L_1(x), L_2(x), ..., L_n(x)]^T,$$

1.7.4.2 Two Dimensional Space

The shifted Legendre polynomial of order $(n+1)$ can also be expressed as follows to extend approximation in two-dimensional space.

$$L_m(x,y) = L_i(x)L_j(y),$$

where $m = (n+1)i + j + 1$ and $i = 0, 1, 2, ..., n$, $j = 0, 1, 2, ..., n$.

Here, the orthogonality condition for $L_m(x,y)$ is

$$\int_0^1 \int_0^1 L_{i_1}(x)L_{j_1}(y)L_{i_2}(x)L_{j_2}(y)dxdy = \begin{cases} \dfrac{1}{(2i_1+1)(2j_1+1)}, & \text{if } i_1 = i_2, j_1 = j_2, \\ 0, & \text{otherwise .} \end{cases}$$

A function $c(x,y) \in C[0,1] \times C[0,1]$ can be approximated as [75]

$$c(x,y) \approx \sum_{k=0}^{(n+1)^2} b_k L_k(x,y) = B(\psi_n(x) \otimes \psi_n(y)), \tag{1.45}$$

where the order of the coefficient matrix B is $1 \times (n+1)^2$ and the order of the Kronecker product $\psi_n(x) \otimes \psi_n(y)$ of matrices $\psi_n(x)$ and $\psi_n(y)$ is $(n+1)^2 \times 1$ defined as

$$\begin{aligned} \psi_n(x) \otimes \psi_n(y) =& [L_0(x)L_0(y), ..., L_0(x)L_n(y), L_1(x)L_0(y), ..., L_1(x)L_n(y), ... \\ & ,L_n(x)L_0(y), ..., L_n(x)L_n(y)]^T. \end{aligned}$$

and

$$B = [b_0, b_1, b_2, ..., b_{(n+1)^2}]^T.$$

The characteristics of the Kronecker product and its uses are listed in [76] and [69].

1.7.4.3 (2+1) Dimensional Space

The approximation in (2+1)-dimensional space is extended by using the above definitions. The orthogonality condition of the Shifted Legendre polynomial in this case is given by

$$\int_0^1 \int_0^1 \int_0^1 L_{i_1}(x)L_{j_1}(y)L_{k_1}(t)L_{i_2}(x)L_{j_2}(y)L_{k_2}(t)dxdydt$$
$$= \begin{cases} \dfrac{1}{(2i_1+1)(2j_1+1)(2k_1+1)}, & \text{if } i_1 = i_2, j_1 = j_2, \\ & k_1 = k_2, \\ 0, & \text{otherwise .} \end{cases} \tag{1.46}$$

A function $c(x, y, t) \in C[0, 1] \times C[0, 1] \times C[0, 1]$ can be approximated as [75]

$$c(x, y, t) \approx c_{n,n,n}(x, y, t) = \sum_{i,j,k=0}^{n} c_{i,j,k} L_{i,j,k}(x, y, t) = (\psi_n(t))^T C(\psi_n(x) \otimes \psi_n(y)), \tag{1.47}$$

where the order of the coefficient matrix C is $(n + 1) \times (n + 1)^2$, the order of matrices $\psi_n(x)$ and $\psi_n(y)$ both is $(n+1) \times 1$ and the order of the Kronecker product $\psi_n(x) \otimes \psi_n(y)$ of matrices $\psi_n(x)$ and $\psi_n(y)$ is $(n + 1)^2 \times 1$ as defined by

$$\psi_n(x) \otimes \psi_n(y) = [L_0(x)L_0(y), ..., L_0(x)L_n(y), L_1(x)L_0(y), ..., L_1(x)L_n(y), ...$$
$$, L_n(x)L_0(y), ..., L_n(x)L_n(y)]^T.$$

1.7.4.4 Operational matrices for Shifted Legendre fractional ordered derivative

The operational matrix of the fractional order derivative of the vector $\psi_n(x)$ using Shifted Legendre is defined in this section as $\frac{\partial^\alpha \psi_n(x)}{\partial x^\alpha} \approx D^{(\alpha)}\psi_n(x)$, where $D^{(\alpha)}$ is given by [77]

$$D^{(\alpha)} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 0 \\ \sum_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} \zeta_{\lceil\alpha\rceil,0,k} & \sum_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} \zeta_{\lceil\alpha\rceil,1,k} & \cdots & \sum_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} \zeta_{\lceil\alpha\rceil,n,k} \\ \vdots & \vdots & & \vdots \\ \sum_{k=\lceil\alpha\rceil}^{i} \zeta_{i,0,k} & \sum_{k=\lceil\alpha\rceil}^{i} \zeta_{i,1,k} & \cdots & \sum_{k=\lceil\alpha\rceil}^{i} \zeta_{i,n,k} \\ \vdots & \vdots & & \vdots \\ \sum_{k=\lceil\alpha\rceil}^{n} \zeta_{n,0,k} & \sum_{k=\lceil\alpha\rceil}^{n} \zeta_{n,1,k} & \cdots & \sum_{k=\lceil\alpha\rceil}^{n} \zeta_{n,n,k} \end{pmatrix}, \tag{1.48}$$

where

$$\zeta_{i,j,k} = \frac{2j+1}{h^k} \sum_{p=0}^{j} \frac{(-1)^{i+p+j+k}(k+i)!\,(p+j)!}{k!\,(i-k)!\,\Gamma(k-\alpha+1)(j-p)!\,(p!\,)^2(k+p-\alpha+1)}.$$

The first $\lceil\alpha\rceil$ rows of $D^{(\alpha)}$ are zero.

The fractional partial order derivative of order $\alpha > 0$ of the Kronecker product $\psi_n(x)\otimes\psi_n(y)$ with respect to x can be calculated using the aforementioned definition

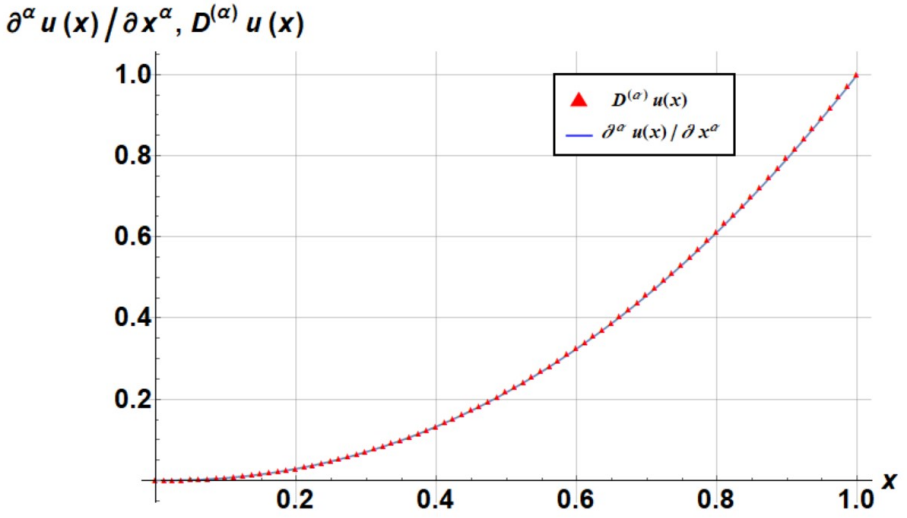

Figure 1.5: Plots of comparison between exact and approximate values of Caputo fractional order derivative for $u(x) = x^{2.2}$ at $\alpha = 0.7$.

and the results of the article of [76] are as follows:

$$\begin{aligned}\frac{\partial^\alpha}{\partial x^\alpha}(\psi_n(x) \otimes \psi_n(y)) =& \frac{\partial^\alpha \psi_n(x)}{\partial x^\alpha} \otimes \psi_n(y) + \psi_n(x) \otimes \frac{\partial^\alpha \psi_n(y)}{\partial x^\alpha} \qquad (1.49)\\ =& \frac{\partial^\alpha \psi_n(x)}{\partial x^\alpha} \otimes \psi_n(y)\\ \approx& (D^{(\alpha)}\psi_n(x)) \otimes (I\psi_n(y))\\ \approx& (D^{(\alpha)} \otimes I)(\psi_n(x) \otimes \psi_n(y)). \qquad (1.50)\end{aligned}$$

The fractional derivative with respect to y in the same manner leads to

$$\frac{\partial^\alpha}{\partial y^\alpha}(\psi_n(x) \otimes \psi_n(y)) \approx (I \otimes D^{(\alpha)})(\psi_n(x) \otimes \psi_n(y)), \qquad (1.51)$$

where the order of both the identity matrix I and operational matrix $D^{(\alpha)}$ of fractional order derivative, is $(n+1) \times (n+1)$.

The comparison of the Caputo fractional order derivative of the function $u(x) = x^{2.2}$ calculated using the formula and the operational matrix of the Caputo

fractional order derivative given in equations (1.49) - (1.51), is displayed in Figure 1.5.

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