Methods and Algorithms for Solving Inverse Problems for Fractional Advection-Dispersion Equations

Thesis by
Abeer Aldoghaither

In Partial Fulfillment of the Requirements
for the Degree of
Doctor of Philosophy

King Abdullah University of Science and Technology, Thuwal,
Kingdom of Saudi Arabia

(October, 2015)
The thesis of Abeer Aldoghaither is approved by the examination committee

Committee Member: David Ketcheson

Committee Member: Tadeusz Patzek

Committee Member: Yalchin Refendiev

Committee Member: Ying Wu

Committee Chairperson: Taous-Meriem Laleg-Kirati
Methods and Algorithms for Solving Inverse Problems for Fractional Advection-Dispersion Equations

Abeer Aldoghaither

Fractional calculus has been introduced as an efficient tool for modeling physical phenomena, thanks to its memory and hereditary properties. For example, fractional models have been successfully used to describe anomalous diffusion processes such as contaminant transport in soil, oil flow in porous media, and groundwater flow. These models capture important features of particle transport such as particles with velocity variations and long-rest periods.

Mathematical modeling of physical phenomena requires the identification of parameters and variables from available measurements. This is referred to as an inverse problem.

In this work, we are interested in studying theoretically and numerically inverse problems for space Fractional Advection-Dispersion Equation (FADE), which is used to model solute transport in porous media. Identifying parameters for such an equation is important to understand how chemical or biological contaminants are transported throughout surface aquifer systems. For instance, an estimate of the differentiation order in groundwater contaminant transport model can provide information about soil properties, such as the heterogeneity of the medium.

Our main contribution is to propose a novel efficient algorithm based on modulat-
ing functions to estimate the coefficients and the differentiation order for space FADE, which can be extended to general fractional Partial Differential Equation (PDE). We also show how the method can be applied to the source inverse problem.

This work is divided into two parts: In part I, the proposed method is described and studied through an extensive numerical analysis. The local convergence of the proposed two-stage algorithm is proven for 1D space FADE. The properties of this method are studied along with its limitations. Then, the algorithm is generalized to the 2D FADE.

In part II, we analyze direct and inverse source problems for a space FADE. The problem consists of recovering the source term using final observations. An analytic solution for the non-homogeneous case is derived and existence and uniqueness of the solution are established. In addition, the uniqueness and stability of the inverse problem is studied. Moreover, the modulating functions-based method is used to solve the problem and it is compared to a standard Tikhono-based optimization technique.
ACKNOWLEDGEMENTS

I am so grateful to all who in one way or another contributed in the completion of this thesis. First, I would like to express my sincere thank to my advisor, Prof. Taous-Meriem Laleg-Kirati for her continuous support, motivation, encouragement, and guidance. I would also like to thank our formal post doctor, Da-Yan Liu who was always willing to help and give his best suggestions and insightful comments. Finally, I thank my parents for their non-stopping support and my husband for his understanding and patience.
# TABLE OF CONTENTS

Examination Committee Approval ........................................... 2

Copyright ........................................................................... 3

Abstract ............................................................................ 4

Acknowledgements ............................................................... 6

List of Abbreviations ............................................................ 10

List of Symbols ................................................................... 11

List of Figures ....................................................................... 12

List of Tables ......................................................................... 15

1 Introduction ........................................................................ 16
   1.1 Objectives and Contributions ........................................... 20

2 Preliminaries ........................................................................ 21
   2.1 Basic Functions ............................................................. 21
      2.1.1 Gamma Function ..................................................... 21
      2.1.2 Shifted Jacobi Orthogonal Polynomial ....................... 22
   2.2 Fractional Derivatives ..................................................... 22
      2.2.1 Historical Overview ............................................... 22
      2.2.2 Definitions ............................................................. 23
      2.2.3 Relation between the Grünwald-Letnikov, Riemann-Liouville,
           and Caputo ............................................................... 27
      2.2.4 Properties of Fractional Derivatives ......................... 27
   2.3 Inverse Problems ........................................................... 32
      2.3.1 Definitions and Properties ....................................... 33
      2.3.2 Solving Inverse Problems ....................................... 34
2.4 Chapter Summary ................................................. 38

3 Fractional Advection-Dispersion Equation .......................... 40
  3.1 Introduction .................................................... 40
  3.2 Fractional Advection-Dispersion Equations ....................... 40
    3.2.1 Classification of Fractional Advection-Dispersion Equations 42
    3.2.2 Derivation of the Space-Fractional Advection-Dispersion Equation 43
  3.3 Direct Problem .................................................. 44
    3.3.1 Analytic Solution .......................................... 45
    3.3.2 Numerical Simulations ...................................... 50
  3.4 Inverse Problems Formulation .................................. 53
  3.5 Chapter Summary ................................................ 54

4 Modulating Functions Based Algorithm to Estimate the Coefficients and the Differentiation Order ................. 57
  4.1 Introduction .................................................... 57
  4.2 Definitions and Properties ..................................... 58
    4.2.1 Modulating Functions Method for Identification .......... 61
  4.3 Modulating Functions Method for Estimating the Average Velocity and the Dispersion Coefficient ..................... 61
  4.4 Parameters and Differentiation Order Estimation ............... 65
    4.4.1 Combined Newton’s and Modulating Functions Method to Estimate d, \( \nu \), and \( \alpha \) .......... 66
    4.4.2 Two-Stage Algorithm ....................................... 70
    4.4.3 Convergence of the Algorithm ............................ 71
  4.5 Numerical Simulations .......................................... 80
  4.6 Estimating the Coefficients \( \nu \) and \( d \) in Case Flux Measurements are Not Available ...................... 95
    4.6.1 Numerical Simulations ..................................... 96
  4.7 Discussion ..................................................... 97
  4.8 Chapter Summary ................................................ 100

5 Parameters and Differentiation Order Estimation for a 2D Space FADE .................................. 102
  5.1 Introduction .................................................... 102
  5.2 Problem Statement ............................................... 103
<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.3</td>
<td>Modulating Functions Method for Estimating the Coefficients</td>
<td>104</td>
</tr>
<tr>
<td>5.4</td>
<td>Parameters and Differentiation Order Estimation</td>
<td>107</td>
</tr>
<tr>
<td>5.4.1</td>
<td>Combined Newton’s and Modulating Functions Method to Estimate the Coefficients and the Differentiation Orders</td>
<td>108</td>
</tr>
<tr>
<td>5.4.2</td>
<td>Two-Stage Algorithm</td>
<td>114</td>
</tr>
<tr>
<td>5.5</td>
<td>Numerical Results</td>
<td>114</td>
</tr>
<tr>
<td>5.6</td>
<td>Chapter Summary</td>
<td>118</td>
</tr>
<tr>
<td>6</td>
<td>Inverse Source Problem for the Space FADE</td>
<td>120</td>
</tr>
<tr>
<td>6.1</td>
<td>Introduction</td>
<td>120</td>
</tr>
<tr>
<td>6.2</td>
<td>Inverse Source Problem</td>
<td>121</td>
</tr>
<tr>
<td>6.2.1</td>
<td>Uniqueness</td>
<td>122</td>
</tr>
<tr>
<td>6.2.2</td>
<td>Stability</td>
<td>124</td>
</tr>
<tr>
<td>6.3</td>
<td>Numerical Analysis</td>
<td>125</td>
</tr>
<tr>
<td>6.3.1</td>
<td>Numerical Simulations</td>
<td>126</td>
</tr>
<tr>
<td>6.4</td>
<td>Chapter Summary</td>
<td>131</td>
</tr>
<tr>
<td>7</td>
<td>Inverse Source Problem Using Modulating Functions</td>
<td>132</td>
</tr>
<tr>
<td>7.1</td>
<td>Introduction</td>
<td>132</td>
</tr>
<tr>
<td>7.2</td>
<td>Problem Statement</td>
<td>132</td>
</tr>
<tr>
<td>7.2.1</td>
<td>Modulating Function Method to Estimate (r(x))</td>
<td>133</td>
</tr>
<tr>
<td>7.2.2</td>
<td>Optimization Methods: Tikhonov Regularization</td>
<td>137</td>
</tr>
<tr>
<td>7.2.3</td>
<td>Numerical Simulations</td>
<td>141</td>
</tr>
<tr>
<td>7.3</td>
<td>Chapter Summary</td>
<td>147</td>
</tr>
<tr>
<td>8</td>
<td>Concluding Remarks</td>
<td>148</td>
</tr>
<tr>
<td>8.1</td>
<td>Conclusion</td>
<td>148</td>
</tr>
<tr>
<td>8.2</td>
<td>Future Research Work</td>
<td>149</td>
</tr>
<tr>
<td>References</td>
<td></td>
<td>151</td>
</tr>
<tr>
<td>A.1</td>
<td>Journal Papers</td>
<td>158</td>
</tr>
<tr>
<td>A.2</td>
<td>Conference Papers</td>
<td>158</td>
</tr>
<tr>
<td>A.3</td>
<td>Presentations</td>
<td>159</td>
</tr>
<tr>
<td>A.4</td>
<td>Posters</td>
<td>159</td>
</tr>
</tbody>
</table>
LIST OF ABBREVIATIONS

ADE    Advection-Dispersion Equation
FADE   Fractional Advection-Dispersion Equation
GCV    Generalized Cross Validations
ISP    Inverse Source Problem
PDE    Partial Differential Equation
LIST OF SYMBOLS

\( \alpha \) fractional differentiation order
\( \beta \) fractional differentiation order
\( c \) solute concentration
\( d \) dispersion coefficient
\( M \) number of modulating functions
\( r \) source term
\( \Delta t \) time step size
\( \nu \) average velocity
\( \Delta x \) space step size
\( \zeta \) white Gaussian noise
LIST OF FIGURES

2.1 (a) The usual derivative is local, (b) The fractional derivative is non-local and depends on the behavior of the entire functions. .................................................. 30
2.2 (a) The function \( f(x) = x^2 \) and its 0.2, 0.4, 0.6, 0.8 and the 1\(^{st}\) derivatives. (b) The 1\(^{st}\), 1.2, 1.4, 1.6, 1.8, and 2\(^{nd}\) derivatives of \( f(x) = x^2 \) .......................................................... 31
2.3 Inverse problem via direct problem ................................................................. 32
2.4 Behavior of the total error .................................................................................. 36
2.5 The L-curve for Tikhonov regularization ............................................................ 39
3.1 Comparison of the solution in space to integer order and fractional ADE. .......... 41
3.2 Numerical solution of the direct problem .......................................................... 53
4.1 Two-stage algorithm to estimate \( \nu, d, \) and \( \alpha \) .............................................. 70
4.2 Exact and estimated \( \nu \) with different numbers of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1), d(x) = 0.7x \) and \( \Delta x = \frac{1}{2100} \) ........................................... 82
4.3 Exact and estimated \( d \) with different numbers of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1), d(x) = 0.7x \) and \( \Delta x = \frac{1}{2100} \) ........................................... 82
4.4 Exact and estimated \( \nu \) with different number of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1), d(x) = 0.7x \) with 2\% noise where \( L_1 = 2 \) and \( \Delta x = \frac{1}{2100} \) ................................................................. 83
4.5 Exact and estimated \( d \) with different number of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1), d(x) = 0.7x \) with 2\% noise where \( L_1 = 2, \Delta x = \frac{1}{2100} \) ................................................................. 83
4.6 Exact and estimated \( \nu \) with different number of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1) \) and \( d(x) = 5 \exp(-4x) \) with 2\% noise where \( L_1 = 2, \Delta x = \frac{1}{2100} \) ................................................................. 84
4.7 Exact and estimated \( d \) with different number of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1) \) and \( d(x) = 5 \exp(-4x) \) with 2\% noise where \( L_1 = 2, \Delta x = \frac{1}{2100} \) ................................................................. 84
4.8 The estimated $d$ and $\nu$ in noise-free case with different values of $L_1$ when $d = 1.1, \nu = 0.4, \alpha = 1.8, \Delta x = \frac{1}{2100}$. .......................... 85
4.9 The relative errors of $\nu$ and $d$ in noise-free case with different values of $L_1$ when $d = 1.1, \nu = 0.4, \alpha = 1.8, \Delta x = \frac{1}{2100}$. .......................... 85
4.10 The estimated $d$ and $\nu$ with 3% noise with different values of $L_1$ when $d = 1.1, \nu = 0.4, \alpha = 1.8, \Delta x = \frac{1}{2100}$. .......................... 86
4.11 The relative errors of $\nu$ and $d$ with 3% noise with different values of $L_1$ when $d = 1.1, \nu = 0.4, \alpha = 1.8, \Delta x = \frac{1}{2100}$. .......................... 86
4.12 The relative errors of the estimated parameters with different numbers of modulating functions .......................... 87
4.13 The estimated parameters obtained with 5 modulating functions and different noise levels. .......................... 88
4.14 The estimated $\nu$ and $d$ with different values of $L_1$ and $\Delta x = \frac{1}{2000}$. .......................... 89
4.15 The relative errors of $\nu$ and $d$ with different values of $L_1$ and $\Delta x = \frac{1}{2000}$ .......................... 89
4.16 The relative errors of the estimated parameters with different numbers of modulating functions .......................... 90
4.17 The exact and the estimated $\nu$ with 3% noise with different values and $\Delta x = \frac{1}{2000}$. .......................... 91
4.18 The exact and the estimated $d$ with 3% noise with different values and $\Delta x = \frac{1}{2000}$. .......................... 91
4.19 The estimated parameters obtained with five modulating functions and different noise levels. .......................... 92
4.20 The relative errors for the estimated parameters with five modulating functions with different noise levels. .......................... 92
4.21 The estimated $d$ and $\nu$ with 2% noise with different values of $L_1$ when $d = 1.1, \nu = 0.3, \alpha = 1.3, \Delta x = \frac{1}{3000}$. .......................... 94
4.22 The relative errors of $\nu$ and $d$ with 2% noise with different values of $L_1$ when $d = 1.1, \nu = 0.3, \alpha = 1.3, \Delta x = \frac{1}{3000}$. .......................... 94
4.23 The relative errors of the estimated parameters obtained with 4 modulating functions and different noise levels. .......................... 95
4.24 The exact and the approximated parameters with different integration intervals $L_1$ when adding 3.2% noise with $\Delta x = \frac{1}{100}$ .......................... 98
4.25 The relative errors when adding 3.2% noise with $\Delta x = \frac{1}{100}$ .......................... 98
4.26 The relative errors of $\nu$. .......................... 99
4.27 The relative errors of $d$. .......................... 99
5.1 Two-stage algorithm to estimate $\nu_1, \nu_2, d_1, d_2, \alpha$ and $\beta$. ............ 115
5.2 The estimated parameters with 2\% stationary noise case with $\Delta x = \frac{1}{50}$ 117
5.3 Relative errors for different integration interval ......................... 117

6.1 Numerical solution of the direct problem. ......................... 127
6.2 Solution of the inverse problem without noise. ......................... 127
6.3 Solution of the inverse problem with and without regularization with 5\% noisy measurements. ............................... 128
6.4 The exact and the regularized solution with different noise levels. .. 128
6.5 Exact solution and the regularization solution with 5\% noisy measurement. ........................................... 130
6.6 The exact and the regularized solution with different noise levels. .. 130

7.1 The exact and the estimated sources using the modulating functions method with different noise levels. ......................... 143
7.2 The relative errors with different numbers of modulating functions. .. 143
7.3 The exact source and the estimated source using 15 polynomial modulating functions and the Tikhonov regularization with 3\% noise levels. 144
7.4 The exact and the approximated source different number of modulating functions with 3\% noise. ......................... 145
7.5 Comparison between the Tik and the modulating functions method when M=6 with 3\% noise. ......................... 146
7.6 The exact and the approximated source with 5 basis in noise free case with $\Delta x = \frac{1}{15}$ ........................................... 146
7.7 The exact and the approximated source with 5 basis with 3\% noise with $\Delta x = \frac{1}{15}$ ........................................... 147
## LIST OF TABLES

4.1 Relative errors of $\nu$ and $d$, where $\nu(x) = 2(\sin(\pi x) + 1)$, $d(x) = 0.7x$, $\alpha = 1.8$ and $\Delta x = \frac{1}{2100}$ in noise-free case. .............................................. 82
4.2 Relative errors of $\nu = \frac{||\nu - \nu^0||_2}{||\nu||_2}$, where $\nu(x) = 2(\sin(\pi x) + 1)$, $d(x) = 0.7x$, $\alpha = 1.8$ and $\Delta x = \frac{1}{2100}$ with different noise levels. ............................................. 83
4.3 Relative errors of $d(x) = \frac{||d - d^0||_2}{||d||_2}$, where $\nu(x) = 2(\sin(\pi x) + 1)$, $d(x) = 0.7x$, $\alpha = 1.8$ and $\Delta x = \frac{1}{2100}$ with different noise levels. ............................................. 84
4.4 Relative errors of $\nu$ and $d$, where $\nu(x) = 2(\sin(\pi x) + 1)$, $d(x) = 5\exp(-4x)$, $\alpha = 1.8$ and $\Delta x = \frac{1}{2100}$ with 2% noise. ............................................. 84
4.5 $d = 1.1$, $\alpha = 1.8$, $\nu = 0.4$, and $\Delta x = \frac{1}{2100}$, 3% noise. ............................................... 88
4.6 $d = 1$, $\alpha = 1.6$, $\nu = 0.5$, and $\Delta x = \frac{1}{2000}$, 1% noise. ............................................... 91
4.7 $d = 1.1$, $\alpha = 1.8$, $\nu = 0.4$, and $\Delta x = \frac{1}{2000}$, 2% noise. ............................................... 91
4.8 $d = 1.1$, $\alpha = 1.3$, $\nu = 0.3$, and $\Delta x = \frac{1}{3000}$, 2% noise. ............................................... 94
4.9 $d = 1.1$, $\alpha = 1.3$, $\nu = 0.3$, and $\Delta x = \frac{1}{3000}$, 2% noise. ............................................... 94
4.10 Estimating $d$ when the exact values are $d = 1.1$, $\alpha = 1.8$, $\nu = 0.4$, and $\Delta x = \frac{1}{2100}$, 3% noise on both measurements. .................................................. 99
4.11 Estimating $v$ when the exact values are $d = 1$, $\alpha = 1.8$, $\nu = 0.5$, and $\Delta x = \frac{1}{2100}$, 2% noise on both measurements. .................................................. 100
4.12 When estimating all parameters $d = 1.1$, $\alpha = 1.8$, $\nu = 0.4$, and $\Delta x = \frac{1}{2100}$, 2% noise on both measurements. .................................................. 100
5.1 $\nu_1 = 0.5$, $\nu_2 = 0.3$, $d_1 = 1$, $d_2 = 0.8$, $\alpha = 1.5$, $\beta = 1.6$, and $\Delta x = \frac{1}{50}$, $\sigma = 0.05$ ................................................................. 117
6.1 The relative errors with different stabilizing functional $\Omega(R)$ when: $N = 100$, $\theta = 0.5$. ................................................................. 129
7.1 The relative errors using the modulating functions method. ........................................ 143
7.2 The relative errors $\frac{||r - r^0||_2}{||r||_2}$ with different noise levels. ........................................ 144
Chapter 1

Introduction

The term "fractional calculus" refers to the generalization of integer-order derivatives and integrals to rational order, which was first introduced in 1695 by L’Hopital and Leibniz [1].

Fractional derivatives and integer order derivatives are both linear operators. However, the integer order derivatives are local operators, while fractional derivatives incorporate nonlocal and system memory effects, which means that at a given point the fractional derivative of a function depends on the characteristics of the function across the entire domain [2]. Therefore, fractional derivative based models are able to describe phenomena across multiple space and time scales without partitioning the problem into smaller compartments [1, 3]. For this reason, when modeling real physical phenomena, fractional derivatives can provide more accurate results than integer order derivatives [4, 5].

Fractional calculus has been used recently in various application fields, such as physics, chemistry, biology, mechanical engineering, signal processing and systems identification, electrical engineering, control theory, finance, and fractional dynamics [1, 6]. For instance, it has been used to model the electrode cardiac tissue interface of a pacemaker, thermal transfer in the lungs, and flow of a compressible fluid in fractured wells [7, 8, 9].

Some studies suggested that it is more accurate to use a fractional model when
describing anomalous diffusion [10, 11], since it captures some important features of particle transport, such as particles with velocity variations and long-rest periods [2]. In addition, when modeling with fractional partial differential equations, some studies find that the fractional derivative can replace in a certain way the variation of the parameters [12]. However, for most of the real-world application models, the value of the parameters are often unknown and need to be estimated from available measurements. Estimating coefficients for fractional differential equations is not a trivial problem, especially if the coefficients are not constant. Furthermore, the problem becomes more challenging when it involves the identification of the fractional differentiation order, where standard approaches usually fail [13].

Recently, some progress has been made to solve inverse problems for fractional partial differential equations. However, most of the presented methods and algorithms involve an optimization problem and require a regularization technique to recover stability lost because of ill-posedness of the problem. For instance, Wei et al. [11] considered an inverse source problem for a spatial fractional diffusion equation where they solved the inverse problem numerically by presenting the best perturbation method based on the Tikhonov regularization. Bondarenko et al.[14, 15], obtained an exact analytic solution of an inverse time fractional diffusion equations, where they determined the diffusion coefficient and the derivative order. They also presented the numerical solution by solving a minimization problem by applying the Levenberg-Marquardt algorithm. In addition, Jin et al. [16] proved the uniqueness of the potential term for a time fractional diffusion equation. They also presented a Newton-type method to solve the problem numerically. Based on a modification of the exact kernel, Qian [17] presented a regularization method to determine the boundary temperature for a fractional diffusion problem.

In this thesis the interest is studying inverse problems of the following fractional
advection-dispersion equation describing anomalous diffusion in porous media:

$$\frac{\partial c(x, t)}{\partial t} = -\nu(x) \frac{\partial c(x, t)}{\partial x} + d(x) \frac{\partial^\alpha c(x, t)}{\partial x^\alpha} + r(x, t), \quad 0 < x < L, \quad t > 0, \quad (1.1)$$

with the following initial and Dirichlet boundary conditions:

$$\begin{cases} 
  c(x, 0) = g_0(x), & 0 < x < L, \\
  c(0, t) = 0, & t > 0, \\
  c(L, t) = 0, & t > 0, 
\end{cases} \quad (1.2)$$

where $c$ is the solute concentration, $\nu$ and $d$ are the average velocity and the dispersion coefficient respectively which are supposed positive, fixing the direction of flow, $r$ is the source term, and $\alpha$ is the fractional differentiation order for the space derivative with $1 < \alpha \leq 2$.

For many decades the advection-dispersion equation, which is based on Fick’s law, has been used to model solute transport in heterogeneous porous media. However, it has been proven recently that transport process in heterogeneous media, where a particle plume spreads faster or slower than predicted by the classical models, often cannot be well described by the classical Advection-Dispersion Equation (ADE) while the fractional advection-dispersion equation model is more efficient [10]. The nonlocal operator is capable of modeling the non-Fickian transport, which is primarily caused by heterogeneities. Inverse modeling of such an equation is important, as it can provide an estimate of parameters that in many cases cannot be measured using direct modeling. For instance, to prevent groundwater from further contaminations, useful information on the pollution can only be obtained by inverse modeling.

Unlike the fractional diffusion equation which attracted many researchers, work on fractional advection-dispersion equation is less well covered. Chi et al. [18], considered an inverse problem for a space-fractional advection-dispersion equation where they determined the space-dependent source magnitude from a final observation. They
have solved the inverse problem numerically in the presence and the absence of noise using an optimal perturbation regularization algorithm. However, the stability of the proposed method depends on the initial guess and the choice of some base functions. Zhang et al. [5], have solved this inverse problem using the same optimal perturbation regularization algorithm when the fractional order, the diffusion coefficient and the average velocity are unknown. In spite of its importance, to the best of our knowledge, except [5] there is no published work on the parameter identification problem for the space-fractional advection-dispersion equation in the case where the differentiation order is unknown.

In this research project, inverse problems for FADE are studied both theoretically and numerically. In the next chapter, some definitions and properties of fractional derivatives and the basic concept of inverse problems are recalled. In Chapter 3, the fractional advection-dispersion equation is introduced and the exact analytic solution of the non-homogeneous case is derived. Furthermore, the uniqueness of the solution is proved. In Chapter 4, a new algorithm, based on the so-called modulating functions to estimate the average velocity, the dispersion coefficient, and the differentiation order is proposed. First, the average velocity and the dispersion coefficient are estimated by applying the modulating functions method, where the problem is transferred into solving a linear system of algebraic equations. Further, the modulating functions method combined with a Newton’s iteration algorithm is applied to estimate the coefficients and the differentiation order simultaneously. Then, the local convergence of the proposed method is proved. Numerical examples are presented to illustrate the validity and effectiveness of the proposed method. In Chapter 5, the algorithm presented is generalized to a two-dimensional fractional advection-dispersion equation. To show the effectiveness of the proposed method, some results of numerical simulations are presented. In Chapter 6, an inverse source problem is analyzed mathematically and numerically. The uniqueness and stability of the inverse problem
are studied. In addition, a numerical method based on the Tikhonov regularization is presented. In Chapter 7, the modulating functions algorithm is used to recover the source and compared to an optimization based method.

1.1 Objectives and Contributions

The objective of this thesis is to develop efficient methods for solving inverse problems using techniques that can be applied to some PDE. As an example of PDE, we focused on the fractional advection-dispersion equation used for modeling solute transport in heterogeneous porous media. The contributions of this thesis are as follows:

- A new effective algorithm is developed, where we combined the modulating functions method with a Newton’s method to estimate the coefficients and the differentiation order for the space FADE.
- An analytic form of the gradient is driven and the local convergence of the proposed algorithm is proved.
- The modulating functions method and the combined algorithm is generalized to estimate the coefficients and the differentiation orders for the two-dimensional space FADE.
- An inverse source problem for the space FADE is studied where the uniqueness and the stability of the solution are studied.
- A numerical method based on the Tikhonov regularization is proposed to estimate the source.
- An algorithm based on the modulating functions method is presented to estimate the source.
- The modulating functions method is compared to a standard optimization based technique.
Chapter 2

Preliminaries

In this chapter, we recall useful definitions, concepts and results on fractional derivatives and inverse problem.

2.1 Basic Functions

In this section, we recall definitions of some special functions that we use later in the thesis.

2.1.1 Gamma Function

The Euler’s gamma function $\Gamma(z)$ is one of the basic functions of fractional calculus. It generalizes the factorial $z!$ to take also non-integers and complex values and it is defined as follows

**Definition 2.1.1.** [1] The gamma function $\Gamma(\cdot)$ is defined as: for $z \in \mathbb{C}$ and $\text{Re}(z) > 0$

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} \, dt. \quad (2.1)$$
2.1.2 Shifted Jacobi Orthogonal Polynomial

Definition 2.1.2. [19] The shifted Jacobi orthogonal polynomial \( P_n^{(\mu, \kappa)} \) is defined on \([0,1]\) as follows:

\[
P_n^{(\mu, \kappa)}(x) := \sum_{j=0}^{n} \binom{n + \mu}{j} \binom{n + \kappa}{n - j} (x - 1)^{n-j} x^j,
\]

with \( \mu, \kappa \in ]-1, \infty[. \)

2.2 Fractional Derivatives

2.2.1 Historical Overview

The concept of fractional calculus was introduced around 300 years ago when in 1695 L’Hopital raised a question to Leibnitz ”What does the derivative of order \( \frac{1}{2} \) mean?” Leibnitz’s reply was ”This is an apparent paradox from which, one day, useful consequences will be drawn”. This draws the attention of many mathematicians to focus on this topic. However, nothing much has been done in the field. One of the reasons is that the mathematical tools of fractional calculus were not available. Another reason is the lack of practical applications of this field. Nevertheless, in the nineteenth century interesting developments have been made in the theory of Fractional Calculus. For instance, in 1812 Laplace proposed an integral formulation, which was used later by Lacroix to define derivatives of arbitrary order. In 1823, Abel was the first to investigate an interesting physical problem using techniques from fractional calculus. He solved the integral equation that appears in the solution of the tautochrome problem. Liouville also made several attempts to define fractional derivatives and he was the first to consider the solution of differential equations and the progress continues. By the second half of the twentieth century, most of the mathematical tools to deal
with fractional calculus were available. Therefore, fractional calculus shifted from pure mathematical formulation to applications and it has been used to model many physical phenomena in various fields [20].

2.2.2 Definitions

In the literature, several definitions of the fractional derivatives have been proposed. For instance, the Grünwald-Letnikov, the Riemann-Liouville, the Caputo and the Riesz-Feller [1]. Eventhough they are different, they are all related to each other. The Grünwald-Letnikov is the most obvious approach to define fractional derivatives. It is mainly used for numerical approximation of fractional derivatives. However, dealing with fractional derivatives as a limit of fractional-order difference is not convenient due to the mathematical complexity. Therefore, some studies use the Grünwald-Letnikov numerically, but try to solve the initial problem with other definitions. The Riemann-Liouville played an important role for its application in pure mathematics while Caputo has been introduced to respond to applied problems. Indeed, Caputo derivatives allow the use of physically interpretable initial conditions, which is not permitted by the Riemann-Liouville.

In our study, we will be interested in the Riemann-Liouville for the two-stage algorithm and the modulating functions method given in Chapters 4, 5 and 7. The Riesz Feller definition will be used for the math development given in Chapter 6 and the Grünwald-Letnikov will be used for the numerical studies.

For a function $f(t)$ defined on an interval $[a, b]$, where $a$ and $b$ can be infinity, a left-sided fractional derivative and a right-sided fractional derivative can be defined. The left-sided fractional derivative is an operation that depends on the "past" of $f$, while the right-sided fractional derivative depends on the "future" of $f(t)$. From now on, we will denote by $\alpha \mathcal{D}_t^\alpha f(t)$ the left-sided fractional derivative, by $\mathcal{D}_t^\alpha f(t)$ the right-sided fractional derivative, $\alpha$ the differentiation order, $a$ is a fixed lower
terminal, and $b$ is a fixed upper terminal, with $a, b \in \mathbb{R}$ such that $a < b$.

1. **Grünwald-Letnikov Fractional Derivative:**

   The Grünwald-Letnikov approach is based on the generalization of the $n^{th}$ integer order derivative to a fractional order.

   Consider the first order derivative of a continuous function $f$ defined on $\mathbb{R}$ as:

   \[ f'(t) = \frac{df}{dt} = \lim_{h \to 0} \frac{f(t) - f(t - h)}{h}, \quad (2.2) \]

   and applying this twice will give us the second order derivative as:

   \[ f''(t) = \frac{d^2 f}{dt^2} = \lim_{h \to 0} \frac{f(t) - 2f(t - h) + f(t - 2h)}{h^2}. \quad (2.3) \]

   By induction we get that

   \[ f^{(n)}(t) = \frac{d^n f}{dt^n} = \lim_{h \to 0} \frac{1}{h^n} \sum_{i=0}^{n} (-1)^i \binom{n}{i} f(t - ih). \quad (2.4) \]

   The generalization by allowing $n$ to be an arbitrary real or complex number will lead us to the Grünwald-Letnikov definition of fractional derivatives.

   **Definition 2.2.1.** [1] Let $f$ be a continuous function defined on $\mathbb{R}$; then the Grünwald-Letnikov fractional derivatives are defined as follows: $\forall t, \alpha \in \mathbb{R}$,

   \[ aD_t^\alpha f(t) = \lim_{h \to 0} h^{-\alpha} \sum_{i=0}^{\lfloor \frac{\alpha}{\pi} \rfloor} (-1)^i \binom{\alpha}{i} f(t - ih), \quad a < t, \quad (2.5) \]

   \[ bD_t^\alpha f(t) = \lim_{h \to 0} h^{-\alpha} \sum_{i=0}^{\lfloor \frac{\alpha}{\pi} \rfloor} (-1)^i \binom{\alpha}{i} f(t + ih), \quad b > t, \quad (2.6) \]
where \([x]\) denotes the integer part of \(x\), and

\[
\binom{\alpha}{i} = \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha - i + 1)\Gamma(i + 1)}.
\]

The standard Gr"unwald estimates generally yield unstable finite difference equations regardless of whether the resulting finite difference method is an explicit or an implicit system. In this case a shifted Gr"unwald formula can be used, which is defined as follows \([6, 5]\): \(\forall x \in \mathbb{R}^*_+\),

\[
D_x^\alpha c(x, t) = h^{-\alpha} \sum_{k=0}^{\left\lfloor \frac{x}{h} \right\rfloor} \frac{\Gamma(k - \alpha)}{\Gamma(-\alpha)\Gamma(k + 1)} c(x - (k - 1)h, t). \tag{2.7}
\]

2. Riemann-Liouville Fractional Derivatives:

The Riemann-Liouville approach of the definition of fractional derivative is based on the repeated integration of a continuous function \(f\).

**Definition 2.2.2.** \([1]\) The Riemann-Liouville fractional derivatives of a continuous function \(f\) defined on \(\mathbb{R}\), with \(\alpha \in \mathbb{R}^*_+\) are defined as follow: \(\forall t \in \mathbb{R}\) and \(n \in \mathbb{N}^*\)

\[
aD_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_a^t (t - \tau)^{n-\alpha-1} f(\tau) d\tau, \quad n - 1 \leq \alpha < n, \quad a < t, \tag{2.8}
\]

\[
iD_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \left( -\frac{d}{dt} \right)^n \int_t^b (\tau - t)^{n-\alpha-1} f(\tau) d\tau, \quad n - 1 \leq \alpha < n, \quad b > t, \tag{2.9}
\]

where \(\Gamma(\cdot)\) is the gamma function defined in \((2.1)\).

3. Caputo Fractional Derivatives:

**Definition 2.2.3.** \([1]\) The Caputo fractional derivatives of \(f\), where \(f \in \mathbb{C}^n(\mathbb{R})\)
and $\alpha \in \mathbb{R}_+^*$ are defined as: $\forall t \in \mathbb{R}$ and $n \in \mathbb{N}^*$

\[
\begin{align*}
a D_t^\alpha f(t) &= \frac{1}{\Gamma(n-\alpha)} \int_t^0 (t-\tau)^{n-\alpha-1} f^{(n)}(\tau)d\tau, \quad n - 1 \leq \alpha < n, \quad a < t, \quad (2.10) \\
\end{align*}
\]

\[
\begin{align*}
i D_t^\alpha f(t) &= \frac{(-1)^n}{\Gamma(n-\alpha)} \int_0^t (\tau-t)^{n-\alpha-1} f^{(n)}(\tau)d\tau, \quad n - 1 < \alpha < n, \quad b > t, \quad (2.11) \\
\end{align*}
\]

where $\Gamma(\cdot)$ is the gamma function defined in (2.1).

4. Riesz Fractional Derivative:

The Riesz fractional derivative is a two-sided derivative, which can be defined in terms of a right-sided and a left-sided fractional derivatives. Two-sided fractional derivatives allow the modeling of flow regime impacts from either side of the domain.

The Riesz Riemann-Liouville is defined in terms of the left-sided and the right-sided Riemann-Liouville fractional derivative as follows:

**Definition 2.2.4.** [21] The Riesz fractional derivative of a continuous function $f$ defined on $\mathbb{R}$, with $\alpha > 0$ is given by: $\forall t \in \mathbb{R}$ and $t > a$,

\[
\frac{\partial^\alpha}{\partial |t|^\alpha} f(t) = -\frac{1}{2 \cos \frac{\alpha \pi}{2}} (a D_t^\alpha + i D_b^\alpha) f(t), \quad (2.12)
\]

where $a D_t^\alpha$ and $i D_b^\alpha$ denotes the Riemann-Liouville fractional derivatives.

**Definition 2.2.5.** [22] For a well behaved function $f$, defined on $\mathbb{R}$, the Riesz-Feller fractional derivative is defined by: for $0 < \alpha \leq 2$, and $|\theta| \leq \min\{\alpha, 2-\alpha\}$,

\[
\begin{align*}
D_\theta^\alpha f(t) &= \frac{\Gamma(1+\alpha)}{\pi} \left\{ \sin\left[\frac{(\alpha+\theta)\pi}{2}\right] \int_{-\infty}^{+\infty} f(t+\xi) - f(t) \frac{d\xi}{\xi^{1+\alpha}} \\
&\quad + \sin\left[\frac{(\alpha-\theta)\pi}{2}\right] \int_{-\infty}^{+\infty} f(t-\xi) - f(t) \frac{d\xi}{\xi^{1+\alpha}} \right\}, \quad (2.13)
\end{align*}
\]

where $\theta$ is the skewness.
2.2.3 Relation between the Grünwald-Letnikov, Riemann-Liouville, and Caputo

In this section, we will denote the left-sided Riemann-Liouville fractional derivative by $R_D^\alpha t$ and the left-sided Caputo fractional derivative by $C_D^\alpha t$.

**Proposition 2.2.1.** [1] If $f(t)$ is $n-1$ continuously differentiable in the interval $[a,b]$ and $f^{(m)}(t)$ is integrable in $[a,b]$, then the

$$ R_D^\alpha t f(t) = \sum_{i=0}^{m-1} \frac{f^{(i)}(a)(t-a)^{i-\alpha}}{\Gamma(1+i-\alpha)} + C_D^\alpha t f(t), $$  

(2.14)  

where $m-1 \leq \alpha \leq m < n$ with $m \in \mathbb{N}^*$.

**Proof.** Applying repeatedly integration by parts to the Riemann-Liouville will give us: for $\forall t \in \mathbb{R}$, and $a < t$,

$$ R_D^\alpha t f(t) = \sum_{i=0}^{m-1} \frac{f^{(i)}(a)(t-a)^{i-\alpha}}{\Gamma(1+i-\alpha)} + \frac{1}{\Gamma(m-\alpha)} \int_a^t \frac{f^{(m)}(\tau)d\tau}{(t-\tau)^{\alpha-m+1}}. $$  

(2.15)  

The right hand side of the above equation is equal to the Grünwald-Letnikov derivatives. \hfill \Box

**Proposition 2.2.2.** Let $f(t)$ be $n-1$ continuously differentiable in the interval $[a,b]$ and $f^{(m)}(t)$ be integrable in $[a,b]$. Then, if $f^{(m)}(a) = 0$, for $n = 0, 1, 2, \ldots, m-1$,

$$ R_D^\alpha t f(t) = C_D^\alpha t f(t) \quad \forall t \in \mathbb{R}, $$  

(2.16)  

where $m-1 \leq \alpha \leq m < n$ with $m \in \mathbb{N}^*$.

2.2.4 Properties of Fractional Derivatives

We recall some useful properties of fractional derivatives.
1. **Linearity**

Assuming that the fractional derivatives of $f$ and $g$ exists, then for $\lambda, \mu \in \mathbb{R}$ [1]:

$$D^\alpha(\lambda f(t) + \mu g(t)) = \lambda D^\alpha f(t) + \mu D^\alpha g(t), \quad (2.17)$$

where $D^\alpha$ denotes any of the fractional derivatives we have defined before.

2. **Laplace Transform of Fractional Derivatives**

We assume that the fractional derivative and the Laplace transform of $f$ exists.

Then, the Laplace transform of the Grünwald-Letnikov, Riemann-Liouville and Caputo fractional derivative are defined by [1]: $\forall s \in \mathbb{C}$,

- **Grünwald-Letnikov**
  
  $$\mathcal{L}[0D_t^\alpha f(t)] = s^\alpha \hat{f}(s), \quad (2.18)$$

- **Riemann-Liouville**
  
  $$\mathcal{L}[0D_t^\alpha f(t)] = s^\alpha \hat{f}(s) - \sum_{i=0}^{n-1} s^i[0D_t^{\alpha-i-1} f(t)]_{t=0}, \quad n - 1 \leq \alpha < n \quad (2.19)$$

- **Caputo**
  
  $$\mathcal{L}[0D_t^\alpha f(t)] = s^\alpha \hat{f}(s) - \sum_{i=0}^{n-1} s^{\alpha-i-1} f^{(i)}(0), \quad n - 1 \leq \alpha < n \quad (2.20)$$

where $\hat{f}(\cdot)$ denotes the Laplace transform of $f(\cdot)$, and $s$ is the variable in the frequency domain.

3. **Fourier Transform of Fractional Derivatives**

We assume that the fractional derivative and the Fourier transform of $f$ exists.

Then, the Fourier transform of the Grünwald-Letnikov, Riemann-Liouville, and
the Caputo fractional derivatives are defined by [1]: \( \forall k \in \mathbb{R} \),

\[
\mathcal{F}[\,_{-\infty}D_t^\alpha f(t)] = (-ik)^\alpha \hat{f}(k)
\]  

(2.21)

where \( \,_{-\infty}D_t^\alpha \) denotes any of the mentioned fractional differentiations, \( \hat{f}(\cdot) \) denotes the Fourier transform of \( f(\cdot) \), and \( k \) is the variable in the frequency domain.

While the Fourier transform of the Riesz Feller fractional derivative is defined by [22]:

\[
\mathcal{F}[D_\alpha^\alpha f(t)] = -\psi_\alpha^\alpha(k) \hat{f}(k),
\]  

(2.22)

where \( \psi_\alpha^\alpha(k) = |k|^\alpha e^{i \text{sign}(k) \theta \pi / 2} \).

4. Derivative of the Fractional Operator with Respect to \( \alpha \)

In the next proposition, we present the derivative of the fractional derivative with respect to the fractional order \( \alpha \). We consider the left Riemann-Liouville derivative. However, similar results can be obtained using other definitions.

**Proposition 2.2.3.** If the \( \alpha \)\(^{th} \) order Riemann-Liouville derivative of \( f \) exists where \( n - 1 \leq \alpha < n \), then the derivative of \( \frac{\partial^\alpha f}{\partial x^n} \) with respect to \( \alpha \) is given by

\[
\frac{\partial}{\partial \alpha} \frac{\partial^\alpha f(x)}{\partial x^n} = \psi_0(n-\alpha) \frac{\partial^\alpha f(x)}{\partial x^n} - \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_0^x (x-\tau)^{n-\alpha-1} \ln(x-\tau) f(\tau) \, d\tau,
\]  

(2.23)

where \( \psi_0(n-\alpha) = \frac{\Gamma(n-\alpha)}{\Gamma(n-\alpha)} \).

**Proof.** The result can be obtained by differentiating (2.8) with respect to \( \alpha \). \( \square \)

5. Nonlocality

As shown in Figure 2.1, the integer order derivatives are local operators that is the derivative of a function at a point depends only on the local behavior of
the function. However, the fractional derivatives are nonlocal operators, which means that the value of the fractional derivative at a point depends on the entire behavior of the function [10].

Figure 2.1: (a) The usual derivative is local, (b) The fractional derivative is nonlocal and depends on the behavior of the entire functions.

6. Plots of Fractional Derivatives

The fractional derivatives form a continuum between their integer order counterparts. As an example, the Riemann-Liouville fractional derivative of $f(x) = x^n$ is given by

$$D_x^\alpha(x^n) = \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)} x^{n-\alpha},$$

(2.24)

The plot of $f(x)$ and its fractional derivatives for $n = 1$ is given in Figure 2.2. The figures show the large range behavior that can be covered by fractional derivatives allowing for more flexibility when dealing with problems and offering more appropriate tool for modeling physical phenomena [10].
Figure 2.2: (a) The function $f(x) = x^2$ and its 0.2, 0.4, 0.6, 0.8 and the 1\textsuperscript{st} derivatives. (b) The 1\textsuperscript{st}, 1.2, 1.4, 1.6, 1.8, and 2\textsuperscript{nd} derivatives of $f(x) = x^2$
2.3 Inverse Problems

The field of inverse problems was introduced in the 20th century. It is a mathematical problem that can provide information for many applications in various fields, where it uses available information to recover hidden information for a given system.

Let $X$ and $Y$ be normed spaces, $K : X \to Y$ a (linear or nonlinear) mapping. Then, given the mathematical model

$$K(x) = y,$$  \hspace{1cm} (2.25)

where $x$ is a vector of unknowns and $y$ is a vector of measurements, the direct problem is to find $y$ given $x$, while the inverse problem is to find $x$ given $y$. In practice, the unknown could be parameters in our mathematical model or the source term or boundaries or a combination of these. Solving an inverse problem for the system (2.25) consists in inverting the operator $K$. But, can we invert $K$? and even if we can, is it numerically stable? The answer to these questions will be given in the next sections. We will see in particular that in general direct problems are well-posed while inverse problems are almost always ill-posed [23].
2.3.1 Definitions and Properties

An inverse problem is usually ill-posed, which means that it violates the criteria of a well posed problem that have been introduced by the mathematician Hadamard in 1902 [24].

**Definition 2.3.1.** [24] A partial differential equation is well posed, in the sense of Hadamard, if

- it has a solution,
- the solution is unique,
- the solution depends continuously on the data.

These properties of a well-posed problem can be presented mathematically as follows:

**Definition 2.3.2.** [23] Let $X$ and $Y$ be normed spaces, $K : X \rightarrow Y$ a (linear or nonlinear) mapping. The equation $Kx = y$ is called properly-posed or well-posed if the following holds:

- **Existence:** For every $y \in Y$ there is (at least one) $x \in X$ such that $Kx = y$.
- **Uniqueness:** For every $y \in Y$ there is at most one $x \in X$ such that $Kx = y$.
- **Stability:** The solution $x$ depends continuously on $y$; that is, for every sequence $(x_n) \subseteq X$ with $Kx_n \rightarrow Kx$ ($n \rightarrow \infty$), it follows that $x_n \rightarrow x$ ($n \rightarrow \infty$).

A problem that fails to satisfy any of these properties is called an ill-posed problem.
2.3.2 Solving Inverse Problems

We consider the following linear systems

\[ Kx = y, \]  \hspace{1cm} (2.26)

where \( K : X \rightarrow Y \) is a discrete linear operator, \( x \in X \) is a vector of unknowns and \( y \in Y \) is a vector of measurements.

To solve the system given in (2.26), we require that the problem is well posed. The conditions of existence and uniqueness of a solution can be enforced by expanding the solution space or by adding extra constraints on the solution, but the stability condition is harder to recover.

In practice the exact value of \( y \) is unknown, but a noisy measurement \( y^\delta \) with noise \( \delta > 0 \) such that:

\[ \| y - y^\delta \|_2 \leq \delta \]  \hspace{1cm} (2.27)

will be used to approximate the solution \( x \) of (2.26).

Then, instead of solving (2.26) we will solve the following perturbed equation:

\[ Kx^\delta = y^\delta. \]  \hspace{1cm} (2.28)

Solving (2.28) requires inverting the operator \( K \), which may lead to an unstable problem, that is a small perturbation in the measurements will produce huge errors in the solution. In this situation, the inverse problem for a continuous system is referred to as ill-posed or as ill-conditioned in the case of a discrete system.

In general, inverse problems are solved by minimizing the error between the predicting data and the measured data, which leads to an optimization problem of the form

\[ x = \arg\min J(x) \quad \text{with} \quad J(x) = \| Kx - y \|_p^2. \]  \hspace{1cm} (2.29)
where \( p \geq 1 \).

Due to the ill-posedness regularization techniques maybe required.

(a) **Regularization**

The idea of regularization method is to replace the ill-posed problem by well posed problem, which can be done by introducing a regularized operator which considers available prior information about the exact solution.

**Definition 2.3.3.** A regularization strategy is a family of linear and bounded operators \( R_\lambda : Y \rightarrow X \), where \( \lambda > 0 \) such that [23]:

\[
\lim_{\lambda \to 0} R_\lambda K x = x, \quad \forall x \in X,
\]

\( \lambda \) is called a regularization parameter.

If the regularized solution \( x^{\lambda, \delta} \) of \( K x = y \) is defined as:

\[
x^{\lambda, \delta} := R_\lambda y^\delta,
\]

then the error between the exact and the regularized solution is:

\[
\|x^{\lambda, \delta} - x\|_2 \leq \|R_\lambda y - R_\lambda y\|_2 + \|R_\lambda y - x\|_2 \leq \delta \|R_\lambda\|_2 + \|R_\lambda K x - x\|_2. \quad (2.32)
\]

This means that, the total error is bounded by the error of the measurement and the error of regularization (\( i.e. \) the error depends on \( \lambda \) and \( \delta \)).

The choice of \( \lambda \) is critical, since

- for \( \lambda \) small \( \Rightarrow \) lose stability and gain accuracy.
- for \( \lambda \) large \( \Rightarrow \) lose accuracy and gain stability.
Therefore, to minimize the error, the choice of $\lambda = \lambda(\delta)$ is critical and should depend on $\delta$ that minimizes the following expression as illustrated in Figure (2.4):

$$\delta \| R_\lambda \|_2 + \| R_\lambda K x - x \|_2.$$  

(2.33)

Later in this chapter, we will introduce some methods to obtain the best value of $\lambda$.

There are many methods to define the regularized operator depending on the problem. Examples of regularization techniques are the Tikhonov regularization, Landweber iteration, and Total Variation [23]. The Tikhonov regularization is one of the most commonly used techniques to regularized discrete ill-posed problems.

(b) **Tikhonov Regularization**

The Tikhonov regularization is a technique to determine an approximate solution $x^{\lambda,\delta}$ to the system given in (2.26) by adding a functional $\Omega(x)$ that includes prior information on the problem, such that [25]:

$$\| K x - y \|_2 < \delta \quad and \quad min_x \Omega(x).$$  

(2.34)
The functional $\Omega(x)$ is non-negative, continuous, and defined on a dense subset $X_1$ of $X$. Every solution to the inverse problem belongs to $X_1$ and for all $d > 0$, the subset $X_{1,d} = \{x : \Omega(x) \leq d\}$ is compact.

The regularized solution will be the value of $x$ that minimizes the following Tikhonov functional:

$$J_\lambda(x) = ||Kx - y||_2^2 + \lambda \Omega(x), \quad x \in X. \quad (2.35)$$

The choice of $\Omega(x)$ depends on the prior information we have on the problem. For example, if a reference value $\bar{x}$ is given, then an appropriate choice of $\Omega(x)$ would be

$$\Omega(x) = ||x - \bar{x}||_2^2, \quad \bar{x} \in X, \quad X_1 = X. \quad (2.36)$$

While, if a minimal solution $x$ is required, then

$$\Omega(x) = ||x||^2 \quad (2.37)$$

would be appropriate.

**Theorem 2.3.1.** [23] Let $K : X \to Y$ be a linear and bounded operator between Hilbert spaces and let $\lambda > 0$. Then the Tikhonov functional $J_\lambda$ given in (2.35) has a unique minimum $x^\lambda \in X$, this minimum $x^\lambda$ is the unique solution of the normal equation:

$$\lambda x^\lambda + K^*Kx^\lambda = K^*y, \quad (2.38)$$

where $\Omega(x) = ||x||^2$.

From the previous theorem, since (2.38) has a uniques solution, then $(\lambda I + K^*K)$ is invertible and

$$x^\lambda = (\lambda I + K^*K)^{-1}K^*y, \quad (2.39)$$
is the unique solution to (2.38). In this case, the operator $R_\lambda$ is given by:

$$R_\lambda = (\lambda I + K^*K)^{-1}K.$$  \hspace{1cm} (2.40)

The question now is how can we choose the best value for $\lambda$? In general, there is no systematic way of choosing the parameter $\lambda$. Some of the methods are Discrepancy Principle of Morozov, L-curve, and Generalized Cross Validations (GCV) [23]. In the next section, we will only present the L-curve method and the reader can refer to the suggested references for more details on the other methods.

(c) L-curve Method

The L-curve method is used to find the best possible value for the regularization parameter $\lambda$, based on the Tikhonov regularization. It is a plot, for all possible values of $\lambda$, of the regularized solution norm versus the corresponding residual norm.

As an example, below is the L-curve for the Tikhonov regularization with $\Omega(x) = ||x||^2$. As we can see in Figure (2.5), on one hand, if we over regularize the solution the residual norm will increase. On the other hand, if little regularization is imposed, then the residual norm will be small, but the solution will be too large, therefore, the best value for $\lambda$ is the one at the corner.

2.4 Chapter Summary

In this chapter, we presented some background materials on fractional derivatives. The use of these definitions in a differential equation leads to a fractional differential equation, which is used to model many physical phenomena. Then, we have introduced the concept of inverse problems and some strategies that have been used to
solve inverse problems. Mainly, we focused on the optimization, since it is the commonly used technique. Optimization techniques are usually heavy computationally and require an extensive storage. Moreover, the convergence of the methods depends on the initial guess and the stop condition. Furthermore, when estimating the differentiation order for a fractional equation, the problem becomes more difficult due to the nonlinearity of the operator. There are other several drawbacks that we will overcome by introducing an efficient method that can be used to solve inverse problem for some PDE. As an example, we focused on the space-fractional advection-dispersion equation used for modeling solute transport in heterogeneous porous media. The derivation and the solution of the direct problem for the space FADE will be given in the next chapter.
Chapter 3

Fractional Advection-Dispersion Equation

3.1 Introduction

The fractional advection-dispersion equation is used to describe landscape evolution, which is one of the important problems for earth scientists. For example, understanding how chemical or biological contaminants are transported through subsurface aquifer systems is essential for protection and remediation of groundwater resources. In this chapter, the fractional advection-dispersion equation will be defined and studied. An exact analytic solution for the non-homogeneous case will be derived. Moreover, the uniqueness of the solution will be proved. Finally, a numerical solution of the direct problem will be presented.

3.2 Fractional Advection-Dispersion Equations

For many decades, the classical ADE has been used to model solute transport in porous media. However, experiments showed that usually in porous media the Fick’s law does not lead to the correct description and the classical ADE is inadequate for modeling such a phenomena [3]. Indeed particles, which may be considered as tracers,
Figure 3.1: Comparison of the solution in space to integer order and fractional ADE.

typically have long rest periods and may travel slower or faster than the average motion. In addition, the tracer behavior may be characterized as being nonlocal; that is, their behavior does not depend only on the nearby conditions. Schumer proposed to introduce the fractional operator into the ADE, defining a fractional ADE as an efficient tool to model such a phenomena. This is due to the nonlocality and memory effect of the fractional operator. Moreover, the fractional operator best describes the heavy-tailed behavior of the particles which can not be described by the classical ADE that has a bell-shaped distribution (See figure 3.1) [10]. Therefore, the fractional advection-dispersion equation occurs when replacing the integer order derivative in the classical ADE by a fractional order derivative in time or space. Schumer et al. [2], derived the general fractional advection-dispersion equation to describe particle transport on the Earth surface using the Eulerian approach as follows:

$$\frac{\partial^\beta c(x, t)}{\partial^\beta t} = -\nu(x) \frac{\partial c(x, t)}{\partial x} + d(x) \frac{\partial^\alpha c(x, t)}{\partial x^\alpha} + f(x, t), \quad (3.1)$$

where $c$ is the concentration, $\nu$ is the average velocity, $d$ the is dispersion coefficient, $f(x, t)$ is the source term, $\beta$ is a fractional order for the time derivative and $\alpha$ for the
space derivative with $0 < \beta \leq 1$ and $1 < \alpha \leq 2$.

### 3.2.1 Classification of Fractional Advection-Dispersion Equations

According to Schumer [10], we can classify the fractional advection-dispersion equation into space-fractional ADE’s ($\beta = 1$ and $1 < \alpha \leq 2$), time fractional ADE’s ($\alpha = 1$ and $0 < \beta \leq 1$), and time-space fractional ADE’s ($0 < \beta \leq 1$ and $1 < \alpha \leq 2$). Space-fractional ADE’s are used to model particles with velocity variation, while time fractional ADE’s are used to model particles with long rest period. Schumer et al. [10], developed a fractional advection-dispersion equations using both the Lagrangian and the Eulerian approach. Below are three cases of fractional advection-dispersion equation discussed by Schumer [10]:

- **Space-fractional advection-dispersion equation**
  \[
  \frac{\partial c(x, t)}{\partial t} = -\nu \frac{\partial c(x, t)}{\partial x} + d \frac{\partial^\alpha c(x, t)}{\partial x^\alpha}, \quad 1 < \alpha \leq 2. \tag{3.2}
  \]

- **Time fractional advection-dispersion equation**
  \[
  \frac{\partial^\beta c(x, t)}{\partial^\beta t} = -\nu \frac{\partial c(x, t)}{\partial x} + d \frac{\partial^2 c(x, t)}{\partial x^2}, \quad 0 < \beta \leq 1. \tag{3.3}
  \]

- **Space-time fractional advection-dispersion equation**
  \[
  \frac{\partial^\beta c(x, t)}{\partial^\beta t} = -\nu \frac{\partial c(x, t)}{\partial x} + d \frac{\partial^\alpha c(x, t)}{\partial x^\alpha}, \quad 0 < \beta \leq 1, \quad 1 < \alpha \leq 2. \tag{3.4}
  \]

In general, a lot of attention has been given to time fractional partial differential equations, but few consider the space-fractional partial differential equations, especially the space-fractional advection-dispersion equation. Therefore, we will focus on
the space-fractional advection-dispersion equation (3.2). We will recall the derivation of its equation in the next section.

3.2.2 Derivation of the Space-Fractional Advection-Dispersion Equation

From the conservation law for particle mass, we have that the rate of mass change at a specific location is equal to the difference between the mass of the particles entering and leaving. Which lead to the following conservation equation [10]:

\[
\frac{\partial c(x,t)}{\partial t} = - \frac{\partial F(x,t)}{\partial x},
\]  
(3.5)

where \( c \) is the particle concentration in mass per volume, \( F \) is the flux in mass per time. If the flux is by advection and Fickian dispersion, then it will be given by:

\[
F = \nu c - d \frac{\partial c}{\partial x},
\]  
(3.6)

where \( \nu \) is the velocity and \( d \) is the dispersion coefficient. Then, from (3.5) and (3.6) we obtain the following classical advection-dispersion equation:

\[
\frac{\partial c(x,t)}{\partial t} = -\nu \frac{\partial c(x,t)}{\partial x} + d \frac{\partial^2 c(x,t)}{\partial x^2}.
\]  
(3.7)

In a fractal porous medium where velocity of particles varies widely, many authors suggested the use of the following advection fractional Fickian law for the dispersion flux [10]:

\[
F = \nu c - d \frac{\partial^{\alpha-1} c}{\partial x^{\alpha-1}},
\]  
(3.8)
The conservation equation with the fractional dispersive flux leads to the following fractional-in-space ADE:

\[
\frac{\partial c(x, t)}{\partial t} = -\nu \frac{\partial c(x, t)}{\partial x} + d \frac{\partial^\alpha c(x, t)}{\partial x^\alpha}.
\]  (3.9)

In general, the direct problem for the fractional advection-dispersion equation always consists of solving the equation when the parameters and the source term are all given. The inverse problem can have different types according to the unknowns. For example, the unknowns could be the velocity and the dispersion coefficient or the source term. However, for most of the fractional models the differentiation order is unknown and should be identified using available measurements.

### 3.3 Direct Problem

In this section, we construct a closed-form analytic solution for the direct problem, which gives a linear operator that simplifies the mathematical analysis of existence and uniqueness of the solution.

We consider the space-fractional advection-dispersion equation given in (1.1). We assume that \( \nu \) and \( d \) are constant and the source term depends only on \( x \). By assuming that we have both left-to-right and right-to-left flows, we consider the Riesz-Feller fractional derivative of order \( \alpha \), defined as in (2.13). Then, equation (1.1) will have the following form

\[
\frac{\partial c(x, t)}{\partial t} = -\nu \frac{\partial c(x, t)}{\partial x} + d \mathcal{D}^\alpha_{x} c(x, t) + r(x), \quad 0 < x < L, \quad t > 0,
\]  (3.10)
with the following initial and Dirichlet boundary conditions:

\[
\begin{align*}
    c(x, 0) &= g_0(x), & 0 < x < L, \\
    c(0, t) &= 0, & t > 0, \\
    c(L, t) &= 0, & t > 0.
\end{align*}
\]  

(3.11)

### 3.3.1 Analytic Solution

We propose to use the Fourier transform method, which is commonly used to solve fractional differential equations and transfer nonlinear equations to linear equations [26, 17]. Then, we use the integrating factor to obtain the solution of the direct problem. In order to apply the Fourier transform to (3.10), we propose to extend \( c \) and \( r \) to the whole real line by defining: \( \forall x \in \mathbb{R}, \forall t \in \mathbb{R}^* \),

\[
    u(x, t) = c(x, t) \cdot p(x),
\]

(3.12)

\[
    f(x) = r(x) \cdot p(x),
\]

(3.13)

where

\[
    p(x) = \begin{cases} 
    1, & \text{if } x \in [0, L], \\
    0, & \text{else}.
    \end{cases}
\]

(3.14)

Then, we propose to solve the following equation:

\[
\begin{align*}
    \frac{\partial u(x, t)}{\partial t} &= -\nu \frac{\partial u(x, t)}{\partial x} + d \frac{\partial^\alpha u(x, t)}{\partial x^\alpha} + f(x), & x \in \mathbb{R}, \quad t > 0, \\
    u(x, 0) &= g_0(x).
\end{align*}
\]  

(3.15)

**Theorem 3.3.1.** Assuming that \( f, g_0 \in L^2(\mathbb{R}) \), then there exists a unique solution
of the system (3.15), which can be given as follows:

\[
    u(x, t) = \int_{-\infty}^{+\infty} \left\{ \int_{0}^{t} G^\theta_{\alpha}(x - y, t - \tau) \, d\tau \right\} f(y) \, dy + \int_{-\infty}^{+\infty} G^\theta_{\alpha}(x - y, t) g_0(y) \, dy,
\]

where

\[
    G^\theta_{\alpha}(x, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ikx} \hat{G}^\theta_{\alpha}(k, t) \, dk,
\]

with

\[
    \hat{G}^\theta_{\alpha}(k, t) = e^{i\nu k - d\phi^\theta_{\alpha}(k)t}. \tag{3.18}
\]

**Proof.** Applying the superposition principle, the solution of equation (3.15) can be written as \( u = v + w \), where \( w \) and \( v \) are solutions to the following equations, respectively.

\[
    \begin{aligned}
    \frac{\partial w(x, t)}{\partial t} &= -\nu \frac{\partial w(x, t)}{\partial x} + d \frac{\partial^\alpha w(x, t)}{\partial x^\alpha}, & x \in \mathbb{R}, & t > 0, \\
    w(x, 0) &= g_0(x),
    \end{aligned} \tag{3.19}
\]

\[
    \begin{aligned}
    \frac{\partial v(x, t)}{\partial t} &= -\nu \frac{\partial v(x, t)}{\partial x} + d \frac{\partial^\alpha v(x, t)}{\partial x^\alpha} + f(x), & x \in \mathbb{R}, & t > 0, \\
    v(x, 0) &= 0.
    \end{aligned} \tag{3.20}
\]

Applying the Duhamel’s principle [27], the solution \( v \) of (3.20) is given by

\[
    v(x, t) = \int_{0}^{t} V(x, t, \tau) \, d\tau, \tag{3.21}
\]

where \( \tau \) is fixed with \( \tau \in [0, t] \) and \( V(\cdot, \cdot; \tau) \) is the solution of the following equation:

\[
    \begin{aligned}
    \frac{\partial V(x, t; \tau)}{\partial t} &= -\nu \frac{\partial V(x, t; \tau)}{\partial x} + d \frac{\partial^\alpha V(x, t; \tau)}{\partial x^\alpha}, & x \in \mathbb{R}, & t > 0, \\
    V(x; t = \tau) &= f(x). \tag{3.22}
    \end{aligned}
\]
Therefore, we start solving (3.22) by applying the Fourier transform. Then we get:

\[
\mathcal{F}\{\frac{\partial V(x,t)}{\partial t}\} = -\nu\mathcal{F}\{\frac{\partial V(x,t)}{\partial x}\} + d\mathcal{F}\{\frac{\partial^\alpha V(x,t)}{\partial x^\alpha}\},
\]

(3.23)

\[
\frac{\partial \hat{V}(k,t)}{\partial t} = -\nu(-ik)^l \hat{V}(k,t) - d\psi_0^\alpha(k)\hat{V}(k,t),
\]

(3.24)

where the Fourier transform \(\hat{V}\) of \(V\) is obtained using formulas (2.22).

Then, we have:

\[
\frac{\partial \hat{V}(k,t)}{\partial t} = [\nu ik - d\psi_0^\alpha(k)] \hat{V}(k,t).
\]

(3.25)

By multiplying (3.25) by the integrating factor \(e^{\int [\nu ik - d\psi_0^\alpha(k)] dt} = e^{[\nu ik + d\psi_0^\alpha(k)] t}\), we get:

\[
\frac{\partial \hat{V}(k,t)}{\partial t} e^{[\nu ik + d\psi_0^\alpha(k)] t} - e^{[\nu ik + d\psi_0^\alpha(k)] t}[\nu ki - d\psi_0^\alpha(k)]\hat{V}(k,t) = 0,
\]

(3.26)

\[
\frac{d}{dt} \left( \hat{V}(k,t)e^{[\nu ik + d\psi_0^\alpha(k)] t} \right) = 0.
\]

(3.27)

Then, by integrating with respect to \(t\), it yields:

\[
\hat{V}(k,t) = e^{[\nu ik - d\psi_0^\alpha(k)] t} a_1,
\]

(3.28)

where \(a_1 \in \mathbb{R}\) is a constant. Applying the initial condition \(\hat{V}(k,t = \tau) = \hat{f}(k)\) to (3.28) gives us:

\[
\hat{f}(k) = e^{[\nu ik - d\psi_0^\alpha(k)] \tau} a_1,
\]

(3.29)

\[
a_1 = e^{-[\nu ik - d\psi_0^\alpha(k)] \tau} \hat{f}(k).
\]

(3.30)

Substituting (3.30) into (3.28) gives the solution of (7.23):

\[
\hat{V}(k,t) = e^{[\nu ik - d\psi_0^\alpha(k)] (t-\tau)} \hat{f}(k).
\]

(3.31)
Applying the inverse Fourier Transformation to (3.31), we obtain:

\[
V(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i[k - d\psi_{\alpha}^{\theta}(k)](t-\tau)} \hat{f}(k)e^{-ikx}dk. \tag{3.32}
\]

Finally, using (3.21) gives the solution \(v\) of (3.20):

\[
v(x, t) = \frac{1}{2\pi} \int_{0}^{t} \int_{-\infty}^{\infty} e^{i[k - d\psi_{\alpha}^{\theta}(k)](t-\tau)} \hat{f}(k)e^{-ikx}dkd\tau, \tag{3.33}
\]

which can be written as:

\[
v(x, t) = \frac{1}{2\pi} \int_{0}^{t} \int_{-\infty}^{\infty} \hat{G}_{\alpha}^{\theta}(k, t - \tau)\hat{f}(k)e^{-ikx}dkd\tau. \tag{3.34}
\]

Using the same technique the solution \(w\) of (3.19) can be obtained:

\[
w(x, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{G}_{\alpha}^{\theta}(k, t)\hat{g}_{0}(k)e^{-ikx}dk, \tag{3.35}
\]

where \(\hat{g}_{0}\) is the Fourier transform of \(g_{0}\).

Then, by adding (3.34) and (3.35), we can get the solution of (3.15):

\[
u(x, t) = \frac{1}{2\pi} \int_{0}^{t} \int_{-\infty}^{+\infty} \hat{G}_{\alpha}^{\theta}(k, t - \tau)\hat{f}(k)e^{-ikx}dkd\tau + \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{G}_{\alpha}^{\theta}(k, t)\hat{g}_{0}(k)e^{-ikx}dk. \tag{3.36}
\]

By inverting the Fourier transform of \(\hat{f}\) and \(\hat{g}_{0}\) in (3.36), we get:

\[
u(x, t) = \frac{1}{2\pi} \int_{0}^{t} \int_{-\infty}^{+\infty} e^{-ikx}\hat{G}_{\alpha}^{\theta}(k, t - \tau) \int_{-\infty}^{+\infty} f(y)e^{iky}dydkd\tau
\]

\[
+ \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ikx}\hat{G}_{\alpha}^{\theta}(k, t) \int_{-\infty}^{+\infty} g_{0}(y)e^{iky}dydk,
\]

\[
= \int_{-\infty}^{+\infty} \left\{ \int_{0}^{t} \left[ \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ik(x-y)}\hat{G}_{\alpha}^{\theta}(k, t - \tau)dk \right] d\tau \right\} f(y)dy
\]

\[
+ \int_{-\infty}^{+\infty} \left[ \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ik(x-y)}\hat{G}_{\alpha}^{\theta}(k, t)dk \right] g_{0}(y)dy. \tag{3.38}
\]
Then, the fundamental solution of (3.15) is:

\[
    u(x, t) = \int_{-\infty}^{+\infty} \left\{ \int_{0}^{t} G_\alpha^\theta(x - y, t - \tau) d\tau \right\} f(y) dy + \int_{-\infty}^{+\infty} G_\alpha^\theta(x - y, t) g_0(y) dy. \tag{3.39}
\]

The uniqueness of the solution is a direct result from the linearity of the integral operator given in (3.39).

Let \( u_1 \) and \( u_2 \) be two solutions of (3.15) with sources \( f_1 \) and \( f_2 \), respectively and \( f_1 = f_2 \). Then, we have

\[
    u_1(x, t) = \int_{-\infty}^{+\infty} \left\{ \int_{0}^{t} G_\alpha^\theta(x - y, t - \tau) d\tau \right\} f_1(y) dy + \int_{-\infty}^{+\infty} G_\alpha^\theta(x - y, t) g_0(y) dy, \tag{3.40}
\]

\[
    u_2(x, t) = \int_{-\infty}^{+\infty} \left\{ \int_{0}^{t} G_\alpha^\theta(x - y, t - \tau) d\tau \right\} f_2(y) dy + \int_{-\infty}^{+\infty} G_\alpha^\theta(x - y, t) g_0(y) dy. \tag{3.41}
\]

Then the following equality

\[
    u_1(x, t) - u_2(x, t) = \int_{-\infty}^{+\infty} \left\{ \int_{0}^{t} G_\alpha^\theta(x - y, t - \tau) d\tau \right\} [f_1(y) - f_2(y)] dy = 0 \tag{3.42}
\]

completes the proof. \( \square \)

**Remark 3.3.1.** [22] We recall the properties of the Green’s Function \( G_\alpha^\theta(\cdot, \cdot) \):

\[
    \hat{G}_\alpha^\theta(k, t) = e^{i\nu k - d\psi_\alpha^\theta(k)t} = e^{i\nu k t} e^{-d\psi_\alpha^\theta(k)t} = \hat{P}_1^\theta(k; -\nu t) \hat{P}_\alpha^\theta(k; td), \tag{3.43}
\]

and

\[
    \hat{P}_\alpha^\theta(k; c) = e^{-c\psi_\alpha^\theta(k)}, \quad c \in \mathbb{R}. \tag{3.44}
\]

Using the following scale rule for the Fourier transformation,

\[
    f(cx) \longleftrightarrow^F |a|^{-1} \hat{f}(k/c), \tag{3.45}
\]
we get
\[ P_\alpha^\theta(x; c) = |c|^{-\frac{1}{\alpha}} P_\alpha^\theta(x/c^\frac{1}{\alpha}), \] (3.46)

which is non-negative, since \( p_\alpha^\theta \) is a probability density function whose Fourier transformation is \( \hat{p}_\alpha^\theta(k) = e^{-\psi_\alpha^\theta(k)} \).

Therefore, the inverse Fourier transformation of (3.43) is:
\[ G_\alpha^\theta(x, t) = \int_{-\infty}^{+\infty} P_1^1(x - k; \nu t) P_\alpha^\theta(k; td) dk, \] (3.47)

where \( G_\alpha^\theta(x, t) = \int_{-\infty}^{+\infty} P_1^1(x - k; \nu t) P_\alpha^\theta(k; td) dk \) is real and normalized [22].

### 3.3.2 Numerical Simulations

This section deals with numerical solution of the direct problem of the space-fractional advection-dispersion equation (3.10). We propose to discretize (3.10) using a finite difference scheme similar to the one introduced by Meerschaert and Tadjeran [6]. The shifted Grünwald formula is used to discretize the Risze-Feller fractional derivative [26, 28, 29], as follows:

\[ D_\alpha^\theta c(x, t) = -[a_r D_x^\alpha c(x, t) + a_l D_\infty^\alpha c(x, t)], \] (3.48)

where
\[ a_r = \frac{\sin (\alpha-\theta)\pi}{2 \sin (\alpha\pi)}, \quad a_l = \frac{\sin (\alpha+\theta)\pi}{2 \sin (\alpha\pi)}, \] (3.51)
and \( \xi_{\alpha,k} \) is the normalized Grünwald weight defined by:

\[
\xi_{\alpha,k} = \frac{\Gamma(k - \alpha)}{\Gamma(-\alpha)\Gamma(k + 1)}.
\]  

(3.52)

Then, the explicit Euler and the finite difference methods are used to discretize the time and the spatial derivatives, respectively [6]:

\[
\frac{\partial c(x, t)}{\partial t} = \frac{c_i^{j+1} - c_i^j}{\Delta t}, \quad \frac{\partial c(x, t)}{\partial x} = \frac{c_i^{j+1} - c_{i-1}^{j+1}}{\Delta x},
\]

(3.53)

where \( \Delta t \) and \( \Delta x \) are the time step and space step, respectively.

Substituting (3.48) and (7.29) in (3.10), we get the following discretization form:

\[
\frac{c_i^{j+1} - c_i^j}{\Delta t} = -\nu \frac{(c_i^{j+1} - c_{i-1}^{j+1})}{\Delta x} + d \delta_{\alpha,x} c_i^{j+1} + r_i^{j+1},
\]

(3.54)

where

\[
\delta_{\alpha,x} c_i^j = -\frac{1}{(\Delta x)^{\alpha}} \left[ a_r \sum_{k=0}^{i+1} \xi_{\alpha,k} c_{i-k+1}^j + a_l \sum_{k=0}^{N-i+1} \xi_{\alpha,k} c_{i+k-1}^j \right],
\]

(3.55)

with \( i = 1, \ldots, N - 1 \) and \( j = 1, 2, \ldots \) with \( t_j = j\Delta t, \ x_i = i\Delta x, \ c_i^j = c(x_i, t_j), \ r_i = r(x_i), \ c_0^j = 0, \) and \( c_N^j = 0. \)

Then, we get:

\[
(1 - d\Delta t \delta_{\alpha,x}) c_i^{j+1} + \frac{\Delta t}{\Delta x} \nu (c_i^{j+1} - c_{i-1}^{j+1}) = c_i^j + r_i \Delta t.
\]

(3.56)

Thus, the matrix form of the implicit finite difference scheme (7.31) is given by:

\[
[(I - G - L) + V] C^{j+1} = C^j + R,
\]

(3.57)

for \( n = 1, 2, \ldots, N - 1 \) and \( m = 1, 2, \ldots, N - 1, \) where
Example 3.3.1. Let us consider the following space-fractional advection-dispersion equation:

\[
\frac{\partial c(x,t)}{\partial t} = -0.3 \frac{\partial c(x,t)}{\partial x} + 3 \frac{\partial^{1.5} c(x,t)}{\partial x^{1.5}} + 5 \sin \frac{2\pi}{7} x, \quad 0 < x < 7, \quad t > 0, \quad (3.63)
\]

with the following initial and Dirichlet boundary conditions:

\[
\begin{align*}
c(x,0) &= 0, \quad 0 < x < 7, \\
c(0,t) &= 0, \quad t > 0, \\
c(7,t) &= 0, \quad t > 0.
\end{align*}
\]  

(3.64)

Figure 6.1, represents the numerical solution of (3.63) with the conditions (3.64)
at time $T = 1$.

Figure 3.2: Numerical solution of the direct problem.

3.4 Inverse Problems Formulation

We are interested in two types of inverse problems: parameter estimation problem and inverse source problem. First, the measurements of the concentration and the flux will be used to estimate the unknowns. Since in practice it is difficult to measure the concentration and the flux over the whole domain, a non-distributed measurement will also be used. However, for real applications such as groundwater transport, it may be difficult to measure the flux. Therefore, we use the concentration measurements only.

IP1. Parameter Estimation Problem

(a) Identifying the average velocity, dispersion coefficient and differentiation order for the 1D case using the following distributed and non-distributed
concentration and flux measurements at final time $t = T$. In the following
$\xi_1$ and $\xi_2$ are noise contaminating the data

- distributed measurements

$$g_1(x) = c(x, T) + \xi_1, \quad g_2(x) = \frac{\partial c(x, T)}{\partial t} + \xi_2, \quad 0 < x < L, \quad (\text{3.65})$$

- non-distributed measurements

$$g_1(x) = c(x, T) + \xi_1, \quad g_2(x) = \frac{\partial c(x, T)}{\partial t} + \xi_2, \quad 0 < x_i < L, \quad (\text{3.66})$$

for $i = 1, 2, \ldots I$

(b) Identifying the average velocity and the dispersion coefficient for the 2
dimensional space FADE using the measurement of the concentration over
an interval $[0, T]$

$$g_1(x, t) = c(x, t) + \xi_1, 0 < x < L. \quad (\text{3.67})$$

IP2. **Inverse Source Problem** Estimating the source using the

- concentration and the flux measurements given in (3.65),
- concentration measurements given in (3.67).

### 3.5 Chapter Summary

In this chapter, we have recalled the derivation of the fractional advection-dispersion
equation for modeling the solute transport in heterogeneous porous media. In addi-
tion, we have presented an analytic solution for the direct problem of the space-
fractional advection-dispersion equation by applying the Fourier transform method
and the Duhamels principle. Moreover, we have proved the uniqueness of the solution.
Furthermore, we have presented a discretized scheme based on the shifted Grünwald formula and a numerical solution for the direct problem have been presented. Finally, we formulated the inverse problems for the space FADE that we considered in the next chapters. Accurate mathematical modeling for such equations is important to provide information for many applications. However, for fractional models the differentiation order is often unknown and need to be identified by solving an inverse problem. Solving an inverse problem is not trivial especially if the coefficients are also unknown. In the next chapter, we will introduce a novel approach based on the modulating functions method to estimate the coefficients and the differentiation order. The proposed method have several advantages. First, initial values, which are usually unknown in most real life applications, are not required. Second, instead of solving the direct problem and computing the fractional derivative of the solution of the partial differential equation, the fractional derivatives of the modulating functions are computed. Third, a regularization technique is not needed since the proposed estimations involving integral formulae are robust and can help to reduce the effect of noise.
Part I
Chapter 4

Modulating Functions Based Algorithm to Estimate the Coefficients and the Differentiation Order

4.1 Introduction

It has been shown that some physical phenomena can be modeled more accurately using fractional differential equations. As described in the previous chapter, the coefficients and the differentiation order are usually unknown and have to be identified using available measurements. However, this identification problem is not trivial, especially in the presence of varying coefficients. As described in the introduction, several methods exist to identify parameters. Standard methods relying on optimization techniques are computationally expensive, require regularization, and need the initial and boundary conditions. In this chapter, a new method, based on the so-called modulating functions, is proposed to estimate average velocity, dispersion coefficient and differentiation order in a space-fractional advection-dispersion equation, where
the average velocity and the dispersion coefficient are space-varying. First, the average velocity and the dispersion coefficient are estimated by applying the modulating functions method, where the problem is transformed into a linear system of algebraic equations. Then, the modulating functions method combined with a Newton’s iteration algorithm is applied to estimate the coefficients and the differentiation order simultaneously. The local convergence of the proposed method is proved. Numerical results are presented with noisy measurements to show the effectiveness and robustness of the algorithm. It is worth mentioning that this method can be extended to general fractional partial differential equations.

4.2 Definitions and Properties

In 1954, Shinbrot [30] introduced a method called the modulating functions method to identify parameters for linear dynamical systems, then it was used in many applications, such as signal processing and control theory (see, e.g. [31, 32, 33, 34, 35, 36]). For instance, Fedele et al. [34], presented a recursive frequency estimation scheme based on trigonometric and spline-type modulating functions. Janiczek [37] generalized the modulating functions method to fractional differential equations, where he aimed to reduce the fractional order to an integer order in the noise-free case. Recently, Liu et al. [36], applied the modulating functions method to identify unknown coefficients for a class of fractional ordinary differential equations. Furthermore, Sadabadi et al. [33], estimated the parameters for a two-dimensional continuous-time system, based on a two-dimensional modulating functions approach. Recently, the modulating functions method has been extended to the numerical differentiation problem by introducing the so-called generalized modulating functions [38, 39]. However, to the best of our knowledge, there is no study generalizing the modulating functions method to fractional partial differential equations. Moreover, this method has never
been used to estimate the differentiation order.

In this section, we will introduce the definition of the modulating functions and some useful properties.

**Definition 4.2.1.** [40] A function \( \phi \in C^k([0, L]) \), defined over the interval \([0, L]\), is called a modulating function of order \( k \) with \( k \in \mathbb{N}^* \) if:

\[
\phi^{(i)}(0) = \phi^{(i)}(L) = 0, \quad i = 0, 1, \ldots, k - 1.
\] (4.1)

**Proposition 4.2.1.** [1, p. 75-77] If \( f \in C^{k-1}([0, L]) \) and \( f^{(k)} \in \mathcal{L}([0, L]) \) where \( L \in \mathbb{R}_+^* \), then the Riemann-Liouville fractional derivative \( D_x^\alpha f(x) \) exists, where \( k-1 \leq \alpha \leq k \) with \( k \in \mathbb{N}^* \). Moreover, the condition \( \phi^{(i)}(0) = 0 \), for \( i = 0, \ldots, k - 1 \), is equivalent to the condition \( [D_x^\alpha f(x)]_{x=0} = 0 \).

According to Proposition 4.2.1, the modulating function \( \phi \) has also the following properties:

- \( \forall \ 0 \leq \alpha \leq k, \ D_x^\alpha \phi(x) \) exists;

- \( \forall \ 0 \leq \alpha \leq k - 1, \ [D_x^\alpha \phi(x)]_{x=0} = 0 \).

The following lemma describes a useful property of the modulating functions. This lemma was obtained by applying the convolution theorem of the Laplace transform.

**Lemma 4.2.1.** [36] If the \( \alpha \)th order Riemann-Liouville derivative of \( f \in C^n(\mathbb{R}) \) exists where \( n - 1 \leq \alpha < n \), and \( \phi \) is an \( n \)th order modulating function defined on \([0, I]\), then, we have

\[
\int_0^I \phi(I - x) \frac{\partial^n f(x)}{\partial x^n} \, dx = \int_0^I \frac{\partial^n \phi(x)}{\partial x^n} f(I - x) \, dx.
\] (4.2)

*Proof.* Applying the convolution theorem of the Laplace transform to the left side of
(4.2), gives:
\[
\mathcal{L}\left\{ \int_0^L \phi(L - x) D_x^\alpha f(x) \, dx \right\}(s) = \hat{\phi}(s) \mathcal{L}\{D_x^\alpha f(x)\}(s).
\] (4.3)

Since the Laplace transform of (2.8) is [1]:

\[
\mathcal{L}\{D_x^\alpha f(x)\}(s) = s^\alpha \hat{f}(s) - \sum_{i=0}^{n-1} s^i[D_x^{\alpha-i-1} f(x)]_{x=0},
\] (4.4)

then, (4.3) will be:

\[
\hat{\phi}(s) \mathcal{L}\{D_x^\alpha f(x)\}(s) = \hat{\phi}(s)s^\alpha \hat{f}(s) - \sum_{i=0}^{n-1} s^i \hat{\phi}(s)[D_x^{\alpha-i-1} f(x)]_{x=0}.
\] (4.5)

According to Proposition 4.2.1, the fractional derivatives of the modulating function \( \phi \) exists and

\[
[D_x^\alpha \phi(x)]_{x=0} = 0,
\] (4.6)

then the Laplace transform of the fractional derivative of the modulating functions \( \phi \) is:

\[
\mathcal{L}\{D_x^\alpha \phi(x)\}(s) = s^\alpha \hat{\phi}(s),
\] (4.7)

\[
\mathcal{L}\{\phi^{(i)}(x)\}(s) = s^i \hat{\phi}(s),
\] (4.8)

for \( i = 0, 1, \ldots n - 1 \).

Now, by applying Eq. (4.7), Eq. (4.8) and the inverse of the Laplace transform to Eq. (4.5), we obtain:

\[
\mathcal{L}^{-1}\left\{ \hat{\phi}(s) \mathcal{L}\{D_x^\alpha f(x)\}(s) \right\}(L) =
\mathcal{L}^{-1}\left\{ \mathcal{L}\{D_x^\alpha \phi(x)\}(s) \hat{f}(s) \right\}(L) - \sum_{i=0}^{n-1} \phi^{(i)}(L)[D_x^{\alpha-i-1} f(x)]_{x=0}.
\] (4.9)
where the last term will be eliminated by using Eq. (4.1), and the proof can be completed by applying the convolution theorem of the Laplace transform.

4.2.1 Modulating Functions Method for Identification

The procedure of the modulating functions method can be summarized as follows

- **Step 1** Multiply the equation model by the modulating function.

- **Step 2** Integrate over the interval \([0, L]\).

- **Step 3** Apply integration by parts.

The integration will help to reduce the effect of noise. Furthermore, the last step will move the fractional differentiation order from the noisy measurements to the modulating functions. In addition, the initial or boundary conditions will be eliminated, thanks to the boundary conditions of the modulating functions. The problem is then simplified into a system of algebraic equations. These functions are like smooth test functions, which allow writing the system in a discrete form and involves integrations. However, the modulating functions have different constrains.

4.3 Modulating Functions Method for Estimating the Average Velocity and the Dispersion Coefficient

In this chapter, we consider the space FADE given in (1.1) with the conditions (1.2). We define the fractional derivative \( \frac{\partial^\alpha}{\partial x^\alpha} \) using the Riemann-Liouville fractional derivative defined as in (2.8).

In this section, the modulating functions method is applied to estimate the average velocity and the dispersion coefficient by assuming that the differentiation order is
known.

Let \( \{f_k\}_{k=1}^\infty \) and \( \{p_k\}_{k=1}^\infty \) be sets of basis functions where the average velocity \( \nu \) and the dispersion coefficient \( d \) can be written as \( \nu(x) = \sum_{k=1}^\infty \nu_k f_k(x) \), and \( d(x) = \sum_{k=1}^\infty d_k p_k(x) \), where \( \nu_k \) and \( d_k \) are the basis coefficients. In general, \( f_k \) and \( g_k \) can take into account some prior information.

**Proposition 4.3.1.** For \( 0 < L_1 \leq L \), let \( \{\phi_m\}_{m=1}^M \) be a set of \( M \) modulating functions of at least order 2 defined on the interval \([0, L_1]\) where \( M \geq K_1 + K_2 \).

Then, the unknown coefficients \( \nu \) and \( d \) can be estimated by:

\[
\tilde{\nu}(x) = \sum_{k=1}^{K_1} \tilde{\nu}_k f_k(x), \quad \tilde{d}(x) = \sum_{k=1}^{K_2} \tilde{d}_k p_k(x),
\]

where the parameters \( \{\tilde{\nu}_k\}_{k=1}^{K_1} \) and \( \{\tilde{d}_k\}_{k=1}^{K_2} \) are given by the solution to the following linear system:

\[
QX = Y,
\]

with

\[
Q = \begin{bmatrix}
q_{11} & q_{12} & \cdots & q_{1K_1+K_2} \\
q_{21} & q_{22} & \cdots & q_{2K_1+K_2} \\
\vdots & \vdots & \ddots & \vdots \\
q_{M1} & q_{M2} & \cdots & q_{MK_1+K_2}
\end{bmatrix}, \quad X = \begin{bmatrix}
\tilde{\nu}_1 \\
\tilde{\nu}_2 \\
\vdots \\
\tilde{\nu}_{K_1}
\end{bmatrix}, \quad \text{and} \quad Y = \begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_M
\end{bmatrix}.
\]
where
\[ y_m = - \int_0^{L_1} \phi_m(L_1 - x) \left[ r(x, t) - \frac{\partial c(x, t)}{\partial t} \right] \, dx, \quad (4.13) \]

\[ q_{mk} = \begin{cases} 
\int_0^{L_1} \frac{\partial [f_k(x)\phi_m(L_1 - x)]}{\partial x} c(x, t) \, dx, \quad k = 1, 2, \ldots K_1 \\
\int_0^{L_1} \frac{\partial^\alpha \hat{\phi}_{mk}(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx, \quad k = K_1 + 1, K_1 + 2, \ldots K_1 + K_2 
\end{cases} 
\]

\[ \hat{\phi}_{mk}(L_1 - x) = p_k(x)\phi_m(L_1 - x), \quad m = 1, \ldots, M. \quad (4.14) \]

**Proof.** Let \( \{\phi_m(x)\}_{m=1}^M \) be a set of \( M \) modulating functions of at least order 2 and consider the equation given in (1.1). Then by multiplying the modulating functions \( \phi_m(L_1 - \cdot) \) for \( m = 1, \ldots, M \) to (1.1) and by integrating over the interval \([0, L_1]\), we get:

\[ \int_0^{L_1} \phi_m(L_1 - x) \frac{\partial c(x, t)}{\partial t} \, dx = - \int_0^{L_1} \nu(x)\phi_m(L_1 - x) \frac{\partial c(x, t)}{\partial x} \, dx \\
+ \int_0^{L_1} d(x)\phi_m(L_1 - x) \frac{\partial^\alpha c(x, t)}{\partial x^\alpha} \, dx + \int_0^{L_1} \phi_m(L_1 - x) r(x, t) \, dx. \quad (4.15) \]

Substituting (4.10) into (4.15), gives

\[ - \int_0^{L_1} \phi_m(L_1 - x) \left[ r(x, t) - \frac{\partial c(x, t)}{\partial t} \right] \, dx = \\
- \sum_{k=1}^{K_1} \bar{u}_k \int_0^{L_1} f_k(x)\phi_m(L_1 - x) \frac{\partial c(x, t)}{\partial x} \, dx \\
+ \sum_{k=1}^{K_2} \bar{d}_k \int_0^{L_1} \hat{\phi}_{mk}(L_1 - x) \frac{\partial^\alpha c(x, t)}{\partial x^\alpha} \, dx, \quad (4.16) \]

where \( \hat{\phi}_{mk}(L - x) = p_k(x)\phi_m(L_1 - x) \).

Applying integration by parts and Lemma 4.2.1, yields
\[ - \int_0^{L_1} \phi_m(L_1 - x)[r(x, t) - \frac{\partial c(x, t)}{\partial t}] \, dx = \]
\[
+ \sum_{k=1}^{K_1} \bar{\nu}_k \int_0^{L_1} \partial [f_k(x) \phi_m(L_1 - x)] \, c(x, t) \, dx + \sum_{k=1}^{K_2} \bar{d}_k \int_0^{L_1} \partial^{\alpha} \hat{\phi}_{mk}(x) \, c(L_1 - x, t) \, dx, \]

(4.17)

where the boundary conditions are eliminated by the properties of the used modulating functions. Finally, the unknown parameters \( \{\bar{\nu}_k\}_{k=1}^{K_1} \) and \( \{\bar{d}_k\}_{k=1}^{K_2} \) can be estimated by solving the linear system given in (4.11).

**Remark 4.3.1.** In the previous proposition if \( M = K_1 + K_2 \), which means that the number of modulating functions and the number of unknown parameters are equal, then if \( Q \) is nonsingular, the system (4.11) has a unique solution given by \( X = Q^{-1}Y \).

On the other hand, if \( M > K_1 + K_2 \), then system (4.11) is overdetermined and the solution can be obtained using the least square method as: \( X = (Q^TQ)^{-1}Q^TY \).

**Remark 4.3.2.** In proposition 4.3.1, when estimating the velocity and the dispersion coefficients we assume that \( c(x, t) \) is known at a time \( T \).

The next result illustrates the particular case where \( \nu \) and \( d \) are constants.

**Corollary 4.3.1.** For \( 0 < L_1 \leq L \), let \( \{\phi_m(x)\}_{m=1}^M \) be a set of at least a 2\textsuperscript{nd} order modulating functions defined on the interval \([0, L_1]\) where \( 2 \leq M \), then the solution of the following linear system gives the estimations of the parameters \( \nu \) and \( d \):

\[
P \begin{bmatrix} \nu \\ d \end{bmatrix} = Y, \]  

(4.18)
where

\[ P = \begin{bmatrix} A & B \end{bmatrix}, \text{ and } Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix}, \tag{4.19} \]

with

\[ A_m = \int_0^{L_1} -\frac{\partial \phi_m(L_1 - x)}{\partial x} c(x, t) \, dx, \tag{4.20} \]

\[ B_m = \int_0^{L_1} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx, \tag{4.21} \]

\[ y_m = \int_0^{L_1} -\phi_m(L_1 - x) \left[ r(x, t) - \frac{\partial c(x, t)}{\partial t} \right] \, dx, \tag{4.22} \]

for \( m = 1, 2, \cdots M \).

Proof. The proof can be obtained as in Proposition 4.3.1, where the coefficients \( \nu(x) \) and \( d(x) \) are replaced by the constants coefficients \( \nu \) and \( d \).

4.4 Parameters and Differentiation Order Estimation

In this section, the modulating functions method is combined with a Newton’s type method to simultaneously estimate \( \nu, d, \) and \( \alpha \) for the space FADE given in (1.1). The main idea is to split the problem into two stages which allow us to reduce the number of unknowns in the parameter estimation problem into one unknown. Without loss of generality, from now on we will assume that the average velocity and the dispersion coefficient are constant. However, the proposed algorithm can be applied similarly for spatial-varying coefficients.
4.4.1 Combined Newton’s and Modulating Functions Method to Estimate $d$, $\nu$, and $\alpha$

Order of differentiation is usually unknown and often challenging to estimate. However, by using the concept of modulating functions, this difficulty is greatly reduced. Due to the nature of the problem it is demanding that we split the solution algorithm into two stages: the first stage solves the previous problem described in Section 3, and the second stage deals with solving a nonlinear equation. Applying the modulating functions greatly simplifies the second stage of the algorithm, where we avoid solving the direct problem at each iteration and the nonlinear equation problem will depend only on one variable $\alpha$. It also allows us to compute the gradient in an efficient way.

We make the following assumptions on the modulating function $\phi$:

H1. The function $\phi(x) \in C^2([0, L])$.

H2. The function $\frac{\partial}{\partial \alpha} \frac{\partial^\alpha \phi}{\partial x^\alpha} : [0, L] \rightarrow \mathbb{R}$ is continuous.

Now, we introduce the two-stage algorithm to estimate $\nu$, $d$ and $\alpha$.

Stage 1: In this stage, we apply Corollary 4.3.1 to rewrite $\nu$ and $d$ as functions of the unknown $\alpha$: $\nu(\alpha)$ and $d(\alpha)$.

Then, we consider the following equation:

$$\frac{\partial c(x, t)}{\partial t} = -\nu(\alpha) \frac{\partial c(x, t)}{\partial x} + d(\alpha) \frac{\partial^\alpha c(x, t)}{\partial x^\alpha} + r(x, t). \quad (4.23)$$

If $\phi_{M+1}$, which is different than $\phi_m$ used in Proposition 4.3.1, is at least a 2nd order modulating function on $[0, L_1]$, then using a similar way of obtaining (4.17), we get:

$$\nu(\alpha) \int_0^{L_1} \frac{\partial \phi_n(L_1 - x)}{\partial x} c(x, t) \, dx + d(\alpha) \int_0^{L_1} \frac{\partial^\alpha \phi_n(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx = \int_0^{L_1} \phi_n(L_1 - x) \frac{\partial c(x, t)}{\partial t} \, dx - \int_0^{L_1} r(x, t) \phi_n(L_1 - x) \, dx. \quad (4.24)$$
Since \( \alpha \) is the only unknown in equation (4.24), we can write it as follows:

\[
K_t(\alpha) = U_t,
\]

(4.25)

where

\[
K_t(\alpha) := d(\alpha) \int_0^{L_1} \frac{\partial^\alpha \phi_n(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx - \nu(\alpha) \int_0^{L_1} \frac{\partial \phi_n(L_1 - x)}{\partial x} c(x, t) \, dx,
\]

(4.26)

and

\[
U_t := \int_0^{L_1} \phi_n(L_1 - x) \left[ \frac{\partial c(x, t)}{\partial t} - r(x, t) \right] \, dx.
\]

(4.27)

Stage 2: In this stage, the inverse problem is formulated as a solution to a nonlinear equation with respect to the unknown \( \alpha \),

\[
J(\alpha) = K_T(\alpha) - U_T = 0,
\]

(4.28)

where \( K_T(\alpha) \) and \( U_T \) are computed using the measurements given in (3.65) at final time.

**Newton’s Iteration Approach**

We propose to use a first order Newton-type method to solve the nonlinear equation given in (4.28). At each iteration, the order \( \alpha \) is updated using:

\[
K_T(\alpha_k) - U_T = -\Delta \alpha_k K_T'(\alpha_k),
\]

(4.29)

where

\[
\alpha_{k+1} = \alpha_k + \Delta \alpha_k,
\]

(4.30)

and \( K'(\alpha) \) is computed using the following propositions.

In Proposition 4.6.1, the derivatives \( \nu'(\alpha) \) and \( d'(\alpha) \) are obtained using a system of
linear equations, where the modulating functions used to obtain $\nu$ and $d$ in corollary 4.3.1 must be used to obtain the corresponding $\nu'(\alpha)$ and $d'(\alpha)$.

**Proposition 4.4.1.** For $0 < L_1 \leq L$, let $\{\phi_m(x)\}_{m=1}^M$ be a set of $M$ modulating functions of at least order 2 defined on the interval $[0, L_1]$ where $2 \leq M$. Then the parameters $\nu$ and $d$ can be written in terms of $\alpha$ using Corollary 4.3.1, and the following linear system estimates the derivatives of $d$ and $\nu$ with respect to $\alpha$:

\[
\begin{bmatrix}
\nu'(\alpha) \\
\d'(\alpha)
\end{bmatrix} = -d(\alpha) B', \quad \text{where} \quad B' = \begin{bmatrix}
B'_1 \\
B'_2 \\
\vdots \\
B'_M
\end{bmatrix},
\]

(4.31)

with

\[
B'_m = \frac{\partial}{\partial \alpha} B_m = \int_0^{L_1} \frac{\partial}{\partial \alpha} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx,
\]

(4.32)

where $\nu$, $A_m$ and $B_m$ are defined as in (4.19), (4.20), and (4.21), respectively for $m = 1, 2, \ldots M$.

**Proof.** We first write the parameters $\nu$ and $d$ in terms of $\alpha$ using Corollary 4.3.1, then the proof can be obtained by differentiating (4.24) with respect to $\alpha$ where $\phi_n$ is replaced by $\phi_m$, which gives:

\[
\nu'(\alpha) \int_0^{L_1} - \frac{\partial \phi_m(L_1 - x)}{\partial x} c(x, t) \, dx + d'(\alpha) \int_0^{L_1} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx \\
+ d(\alpha) \int_0^{L_1} \frac{\partial}{\partial \alpha} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx = 0,
\]

(4.33)

for $m = 1, 2, \ldots M$.

Similarly as in Corollary 4.3.1, the estimates $\nu'(\alpha)$ and $d'(\alpha)$ can be obtained by
solving the system given in (4.31) using the least square method. The derivative of \( \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} \) with respect to \( \alpha \) can be characterized using Proposition 2.2.3.

Now, using Proposition 4.6.1 we can drive the analytic form of \( K'(\alpha) \).

**Proposition 4.4.2.** Let \( \nu(\alpha) \) and \( d(\alpha) \) be the estimations given by Corollary 4.3.1 and \( K(\alpha) \) is given in (4.26), the gradient \( K'(\alpha) \) exists and is characterized as follows:

\[
K'(\alpha) = d'(\alpha) \int_0^{L_1} \frac{\partial^\alpha \phi_n(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx - \nu'(\alpha) \int_0^{L_1} \frac{\partial \phi_n(L_1 - x)}{\partial x} c(x, t) \, dx
\]

\[
+ d(\alpha) \int_0^{L_1} \frac{\partial}{\partial \alpha} \frac{\partial^\alpha \phi_n(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx,
\]

(4.34)

where \( n = M + 1 \) and \( d'(\alpha), \nu'(\alpha) \) are given by Proposition 4.6.1.

**Proof.** \( K'(\alpha) \) can be obtained directly by differentiating (4.26) with respect to \( \alpha \). The differentiability of \( K(\alpha) \) mainly depends on the differentiability of (2.8) with respect to \( \alpha \), which always exists as the gamma function is differentiable and thanks to H3.

**Remark 4.4.1.** Newton’s iteration is a gradient based method and we know that for any gradient based algorithm, most of the computational effort is spent on computing the gradient at each step. However, here, thanks to the modulating functions method we have analytical closed form of the gradient. This analytical form is more stable and requires less computational power. Furthermore in a similar way, we can efficiently compute higher order derivatives.

**Remark 4.4.2.** In general, when using an iterative method to solve nonlinear equations, it is often difficult to establish theoretically the invertibility of the gradient,
which is the case here. However, from our experiments it seems that $K'$ is nonsingular.

### 4.4.2 Two-Stage Algorithm

The proposed algorithm is described in Figure 4.1.

![Diagram](image)

Figure 4.1: Two-stage algorithm to estimate $\nu$, $d$, and $\alpha$. 
Algorithm 1: Two-stage algorithm to estimate $\nu$, $d$, and $\alpha$.

Step 1: Start with an initial guess $\alpha_0$.

Step 2: Compute the corresponding $d(\alpha_k)$, $\nu(\alpha_k)$.

Step 3: Compute

$$
\frac{K_T(\alpha_k) - U_T}{\|K_T(\alpha_k)\|_2},
$$

if

$$
\frac{\|K_T(\alpha_k) - U_T\|_2}{\|K_T(\alpha_k)\|_2} < \epsilon
$$

then

output: $\nu(\alpha_k)$, $d(\alpha_k)$ and $\alpha_k$.

else

update $\alpha_{k+1} = \alpha_k - \frac{K_T(\alpha_k) - U_T}{K_T(\alpha_k)}$ and go back to step 2.

end

4.4.3 Convergence of the Algorithm

Our goal is to analyze the convergence of the proposed two-stage algorithm when the standard assumptions of the Newton’s iteration algorithm hold. Without loss of generality, the convergence will be proven for $M = 2$.

In order to show the local convergence of the presented algorithm we define the following assumption:

H3. The functions $\frac{\partial^\alpha \phi(x)}{\partial x^\alpha}$ and $\frac{\partial}{\partial \alpha} \frac{\partial^\alpha \phi}{\partial x^\alpha}$ are Lipschitz continuous in $\alpha$, i.e., there exist constants $\gamma_1$ and $\gamma_2$ such that, for all $\alpha_1$ and $\alpha_2$ in $[1, 2]$,

$$
\left| \frac{\partial^\alpha \phi(x)}{\partial x^\alpha_1} - \frac{\partial^\alpha \phi(x)}{\partial x^\alpha_2} \right| \leq \gamma_1 |\alpha_1 - \alpha_2|, \quad (4.35)
$$

and

$$
\left| \frac{\partial}{\partial \alpha_1} \frac{\partial^\alpha \phi(x)}{\partial x^\alpha_1} - \frac{\partial}{\partial \alpha_2} \frac{\partial^\alpha \phi(x)}{\partial x^\alpha_2} \right| \leq \gamma_2 |\alpha_1 - \alpha_2|. \quad (4.36)
$$

Before obtaining the convergence of our proposed two-stage algorithm, we first prove some important results.

Proposition 4.4.3. Under the assumptions H1.-H3. the following hold: for $i = 1, 2, \cdots M + 1$ and $j = 1, 2, \cdots M + 1$
1. \( A_i \) and \( y_i \) defined as in (4.20) and (4.22), respectively, are bounded.

2. The function \( B_i : ]1, 2] \to \mathbb{R} \) defined as in (4.21) is bounded.

3. Then function \( B_i' : ]1, 2] \to \mathbb{R} \) defined as in (4.32) is bounded.

4. The function \( h_{i,j} \) defined as: for \( \alpha \in ]1, 2] \)
   \[
   h_{i,j}(\alpha) = A_i B_j(\alpha) - A_j B_i(\alpha),
   \]
   (4.37)
   is bounded.

5. For \( \alpha \in ]1, 2] \), \( d(\alpha) \) given by (4.18) is bounded.

6. \( B_i(\alpha) \) defined as in (4.21) is Lipschitz continuous in \( \alpha \), that is, there exists a constant \( \eta_1 \) such that, for all \( \alpha_1 \) and \( \alpha_2 \) in \( ]1, 2] \),
   \[
   |B_i(\alpha_1) - B_i(\alpha_2)| \leq \eta_1 |\alpha_1 - \alpha_2|.
   \]
   (4.38)

7. \( B'_i(\alpha) \) defined as in (4.32) is Lipschitz continuous in \( \alpha \), that is, there exists a constant \( \eta_2 \) such that, for all \( \alpha_1 \) and \( \alpha_2 \) in \( ]1, 2] \),
   \[
   |B'_i(\alpha_1) - B'_i(\alpha_2)| \leq \eta_2 |\alpha_1 - \alpha_2|.
   \]
   (4.39)

8. For \( \alpha \in ]1, 2] \) the following functions are Lipschitz continuous
   (a) \( h_{i,j}(\alpha) \) defines as in (4.37).
   (b) \( [h_{i,j}(\alpha)]^2 \).

9. \( g(\alpha) \) defined by: for \( \alpha \in ]1, 2] \)
   \[
   g_{i,j}(\alpha) = \frac{B_i(\alpha) B'_j(\alpha)}{h_{i,j}((\alpha)^2)}.
   \]
   (4.40)
Proof. The proofs of 1-3 can be directly deduced from H1., H2. and the continuity of $\frac{\partial^\alpha \phi}{\partial x^\alpha}$.

4. Can be directly deduced from H1. and the continuity of $\frac{\partial^\alpha \phi}{\partial x^\alpha}$.

5. Can be obtained directly using 1 and 4.

6. Let $\alpha_1, \alpha_2 \in ]1, 2]$, then

$$|B_i(\alpha_1) - B_i(\alpha_2)|$$  \hspace{1cm} (4.41)

$$= \left| \int_0^{L_1} \frac{\partial^{\alpha_1} \phi_i(x)}{\partial x^{\alpha_1}} c(L_1 - x, t) \, dx - \int_0^{L_1} \frac{\partial^{\alpha_2} \phi_i(x)}{\partial x^{\alpha_2}} c(L_1 - x, t) \, dx \right|$$  \hspace{1cm} (4.42)

$$= \left| \int_0^{L_1} \left[ \frac{\partial^{\alpha_1} \phi_i(x)}{\partial x^{\alpha_1}} - \frac{\partial^{\alpha_2} \phi_i(x)}{\partial x^{\alpha_2}} \right] c(L_1 - x, t) \, dx \right|$$  \hspace{1cm} (4.43)

$$\leq \left| \frac{\partial^{\alpha_1} \phi_i(x)}{\partial x^{\alpha_1}} - \frac{\partial^{\alpha_2} \phi_i(x)}{\partial x^{\alpha_2}} \right| |c(L_1 - x, t)| ,$$  \hspace{1cm} (4.44)

by the continuity of $c(\cdot, T)$ and H3. there exist constants $M_c$ and $\gamma_1$ such that:

$$|B_i(\alpha_1) - B_i(\alpha_2)| \leq \gamma_1 M_c |\alpha_1 - \alpha_2| ,$$  \hspace{1cm} (4.45)

setting $\eta_1 = \gamma_1 M_c$, we get inequality (4.38).

7. The proof can be obtained similarly as in 6.

8. (a) The result can be obtained directly by applying 1 and 6.

(b) For $\alpha_1, \alpha_2 \in ]1, 2]$, we get

$$\left| [h_{i,j}(\alpha_1)]^2 - [h_{i,j}(\alpha_2)]^2 \right|$$

$$= \left| [A_i B_j(\alpha_1) - A_j B_i(\alpha_1)]^2 - [A_i B_j(\alpha_2) - A_j B_i(\alpha_2)]^2 \right|. $$  \hspace{1cm} (4.46)
After simplifications, we have

\[
|h_{i,j}(\alpha_1)|^2 - |h_{i,j}(\alpha_2)|^2 = A_i^2[B_j^2(\alpha_1) - B_j^2(\alpha_2)] \\
+ A_j^2[B_i^2(\alpha_1) - B_i^2(\alpha_2)] \\
+ 2A_iA_j[B_j(\alpha_2)B_i(\alpha_2) - B_j(\alpha_1)B_i(\alpha_1)].
\] (4.47)

Now, by adding and subtracting \(B_i(\alpha_2)B_j(\alpha_1)\) from the last term of (4.47) and applying the triangular inequality, we obtain

\[
|h_{i,j}(\alpha_1)|^2 - |h_{i,j}(\alpha_2)|^2 \leq A_i^2|B_j(\alpha_1) + B_j(\alpha_2)||B_j(\alpha_1) - B_j(\alpha_2)| \\
+ |A_j^2[B_i(\alpha_1) + B_i(\alpha_2)]| |B_i(\alpha_1) - B_i(\alpha_2)| \\
+ |2A_iA_jB_i(\alpha_2)||B_j(\alpha_2) - B_j(\alpha_1)| \\
+ |2A_iA_jB_j(\alpha_1)||B_i(\alpha_2) - B_i(\alpha_1)|.
\] (4.48)

Finally, by 1, 2, and 6, there exist constants \(M_a, M_b\) and \(\eta_1\) such that

\[
|h_{i,j}(\alpha_1)|^2 - |h_{i,j}(\alpha_2)|^2 \leq 8M_a^2M_b\eta_1 |\alpha_1 - \alpha_2|,
\] (4.49)

where \(M_b = \max\{M_{b_1}, M_{b_2}\}\) and \(M_a = \max\{M_{a_1}, M_{a_2}\}\) for \(|B_i| \leq M_{b_1} \leq M_{b_2}, |B_j| \leq M_{b_2} \leq M_b\) and \(|A_i| \leq M_{a_1}, |A_i| \leq M_{a_2} \leq M_a\).

9. Let \(\alpha_1, \alpha_2 \in [1, 2]\), then

\[
|g_{i,j}(\alpha_1) - g_{i,j}(\alpha_2)| = \left| \frac{B_i(\alpha_1)B_j'(\alpha_1)}{h_{i,j}(\alpha_1)^2} - \frac{B_i(\alpha_2)B_j'(\alpha_2)}{h_{i,j}(\alpha_2)^2} \right|
\] (4.50)
\begin{align*}
\frac{1}{|h_{i,j}(\alpha_1)h_{i,j}(\alpha_2)|^2} & \left| h_{i,j}(\alpha_2)^2B_i(\alpha_1)B'_j(\alpha_1) - h_{i,j}(\alpha_1)^2B_i(\alpha_2)B'_j(\alpha_2) \right| . \\
(4.51)
\end{align*}

Now, adding and subtracting \( h_{i,j}(\alpha_2)^2B_i(\alpha_2)B'_j(\alpha_1) \) and \( h_{i,j}(\alpha_1)^2B_i(\alpha_1)B'_j(\alpha_2) \) from the last term of (4.51) and by applying the triangular inequality, we have

\begin{align*}
|g_{i,j}(\alpha_1) - g_{i,j}(\alpha_2)| & \leq \frac{1}{|h_{i,j}(\alpha_1)h_{i,j}(\alpha_2)|^2} \\
& \left| \left[ h_{i,j}(\alpha_2)^2B'_j(\alpha_1) + h_{i,j}(\alpha_1)^2B'_j(\alpha_2) \right] \left[ B_i(\alpha_1) - B_i(\alpha_2) \right] \right| \\
& + \left| h_{i,j}(\alpha_2)^2B_i(\alpha_2)B'_j(\alpha_1) - h_{i,j}(\alpha_1)^2B_i(\alpha_1)B'_j(\alpha_2) \right| , \\
(4.52)
\end{align*}

adding and subtracting \( h_{i,j}(\alpha_2)^2B_i(\alpha_2)B'_j(\alpha_2) \) of the last term, we get

\begin{align*}
|g_{i,j}(\alpha_1) - g_{i,j}(\alpha_2)| & \leq \frac{1}{|h_{i,j}(\alpha_1)h_{i,j}(\alpha_2)|^2} \\
& \left| \left[ h_{i,j}(\alpha_2)^2B'_j(\alpha_1) + h_{i,j}(\alpha_1)^2B'_j(\alpha_2) \right] \left[ B_i(\alpha_1) - B_i(\alpha_2) \right] \right| \\
& + \left| h_{i,j}(\alpha_2)^2B_i(\alpha_2)[B'_j(\alpha_1) - B'_j(\alpha_2)] \right| \\
& + B'_j(\alpha_2)|h_{i,j}(\alpha_2)^2B_i(\alpha_2) - h_{i,j}(\alpha_1)^2B_i(\alpha_1)| , \\
(4.53)
\end{align*}

adding and subtracting \( h_{i,j}(\alpha_2)^2B_i(\alpha_1) \) of the last term, we obtain

\begin{align*}
|g_{i,j}(\alpha_1) - g_{i,j}(\alpha_2)| & \leq \frac{1}{|h_{i,j}(\alpha_1)h_{i,j}(\alpha_2)|^2} \\
& \left[ \left| h_{i,j}(\alpha_2)^2B'_j(\alpha_1) + h_{i,j}(\alpha_1)^2B'_j(\alpha_2) \right| \left| B_i(\alpha_1) - B_i(\alpha_2) \right| \right] \\
& + \left| h_{i,j}(\alpha_2)^2B_i(\alpha_2) \right| \left| B'_j(\alpha_1) - B'_j(\alpha_2) \right| \\
& + \left| B'_j(\alpha_2)h_{i,j}(\alpha_2)^2 \right| \left| B_i(\alpha_2) - B_i(\alpha_1) \right| \\
& + \left| B_i(\alpha_1) \right| \left| h_{i,j}(\alpha_2)^2 - h_{i,j}(\alpha_1)^2 \right| . \\
(4.54)
\end{align*}
Finally, by 2, 3, 4 and by applying 6, 7 and 8b, there exist constants $M_b$, $M'_b$, $M_\alpha$, $\eta_1$, $\eta_2$ and $\eta_3$, respectively, such that

$$|g_{i,j}(\alpha_1) - g_{i,j}(\alpha_2)| \leq M_g |\alpha_1 - \alpha_2|,$$  \hfill (4.55)

where $M_g = [3M^2_b M'_b \eta_1 + M^2_\alpha M_b \eta_2 + M_b \eta_3]$.

To prove the convergence, we recall the following theorem referred to in [41].

**Theorem 4.4.1.** [41, p. 30] If the following assumptions hold

\begin{itemize}
  \item \textbf{S1.} The equation $J(\alpha) = 0$ has a solution $\alpha^*$,
  \item \textbf{S2.} $J':]1,2] \to \mathbb{R}$ is Lipschitz continuous with constant $\gamma$,
  \item \textbf{S3.} $J'(\alpha^*)$ is nonsingular,
\end{itemize}

then there exists $\delta$ such that if $\alpha_0 \in B(\delta)$ the Newton iteration

$$\alpha_{k+1} = \alpha_k - \frac{J(\alpha_k)}{J'(\alpha_k)},$$  \hfill (4.56)

converges $q$-quadratically to $\alpha^*$.

Now, we are ready to prove the main result in this section.

**Theorem 4.4.2.** Assume that the solution of $J(\alpha) = 0$, where $J(\alpha)$ is defined as in (4.28), exists and $J'$ is nonsingular. Then, under the assumptions H1.-H3. and for $M = 2$, the proposed two-stage algorithm given in Algorithm 1 converges locally.
Proof. Since we assume that $J(\alpha)$ has a solution and $J'(\alpha^*)$ is nonsingular, then if $J'$ defined in (4.4.1) is Lipschitz continuous, the convergence result of the Newton method holds [41].

Recall that

$$J'(\alpha) = K'(\alpha) = A_n v'(\alpha) + B_n(\alpha) d'(\alpha) + B'_n(\alpha) d(\alpha), \quad (4.57)$$

where $A_n, B_n(\alpha)$, and $B'_n(\alpha)$ are defined as in (4.20), (4.21) and (4.32), respectively, and $n = M + 1$, and using Corollary 4.3.1, we have

$$d(\alpha) = \frac{1}{h_{m_1,m_2}(\alpha)}[-A_{m_2} y_{m_1} + A_{m_1} y_{m_2}], \quad (4.58)$$

and from Proposition 4.6.1, we have

$$\begin{bmatrix} v'(\alpha) \\ d'(\alpha) \end{bmatrix} = \frac{d(\alpha)}{h_{m_1,m_2}(\alpha)} \begin{bmatrix} B_{m_2}(\alpha) B'_{m_1}(\alpha) - B_{m_1}(\alpha) B'_{m_2}(\alpha) \\ -A_{m_2} B'_{m_1}(\alpha) + A_{m_1} B'_{m_2}(\alpha) \end{bmatrix}, \quad (4.59)$$

where $h(\alpha)$ is defined in (4.37).

Now, we can show that $J'$ is Lipschitz continuous. Let $\alpha_1, \alpha_2 \in [1, 2]$, then

$$|J'(\alpha_1) - J'(\alpha_2)| =$$

$$|A_n v'(\alpha_1) + B_n(\alpha_1) d'(\alpha_1) + B'_n(\alpha_1) d(\alpha_1) - A_n v'(\alpha_2) - B_n(\alpha_2) d'(\alpha_2) - B'_n(\alpha_2) d(\alpha_2)|. \quad (4.60)$$

Substituting the values of $v'(\alpha)$ and $d'(\alpha)$ given in (4.59) into (4.60), we get
\[ |J'(\alpha_1) - J'(\alpha_2)| = \left| A_n d(\alpha_1) \frac{B_{m_2}(\alpha_1)B'_{m_1}(\alpha_1) - B_{m_1}(\alpha_1)B'_{m_2}(\alpha_1)}{h_{m_1,m_2}(\alpha_1)} \right. \]
\[ + B_n(\alpha_1)d(\alpha_1) - A_{m_2}B'_{m_1}(\alpha_1) + A_{m_1}B'_{m_2}(\alpha_1) + B'_n(\alpha_1)d(\alpha_1) \]
\[ - A_n d(\alpha_2) \frac{B_{m_2}(\alpha_2)B'_{m_1}(\alpha_2) - B_{m_1}(\alpha_2)B'_{m_2}(\alpha_2)}{h_{m_1,m_2}(\alpha_2)} \]
\[ - B_n(\alpha_2)d(\alpha_2) - A_{m_2}B'_{m_1}(\alpha_2) + A_{m_1}B'_{m_2}(\alpha_2) - B'_n(\alpha_2)d(\alpha_2) \mid \]
\[ (4.61) \]
\[ = \left| A_n \left[ d(\alpha_1) \frac{B_{m_2}(\alpha_1)B'_{m_1}(\alpha_1)}{h_{m_1,m_2}(\alpha_1)} - d(\alpha_2) \frac{B_{m_2}(\alpha_2)B'_{m_1}(\alpha_2)}{h_{m_1,m_2}(\alpha_2)} \right] \right. \]
\[ - A_n \left[ d(\alpha_1) \frac{B_{m_1}(\alpha_1)B'_{m_2}(\alpha_1)}{h_{m_1,m_2}(\alpha_1)} - d(\alpha_2) \frac{B_{m_1}(\alpha_2)B'_{m_2}(\alpha_2)}{h_{m_1,m_2}(\alpha_2)} \right] \]
\[ + A_{m_2} \left[ -d(\alpha_1)B_n(\alpha_1)B'_{m_1}(\alpha_1) + d(\alpha_2) \frac{B_n(\alpha_2)B'_{m_1}(\alpha_2)}{h_{m_1,m_2}(\alpha_2)} \right] \]
\[ + A_{m_1} \left[ d(\alpha_1) \frac{B_n(\alpha_1)B'_{m_2}(\alpha_1)}{h_{m_1,m_2}(\alpha_1)} - d(\alpha_2) \frac{B_n(\alpha_2)B'_{m_2}(\alpha_2)}{h_{m_1,m_2}(\alpha_2)} \right] \]
\[ + B'_n(\alpha_1)d(\alpha_1) - B'_n(\alpha_2)d(\alpha_2) \mid . \]
\[ (4.62) \]

Next, substitute \( d(\alpha_i) \) for \( i = 1, 2 \) by (4.58), then (4.62) becomes

\[ |J'(\alpha_1) - J'(\alpha_2)| = \mid -A_{m_2}C_{m_1} + A_{m_1}C_{m_2} \mid \]
\[ \left| A_n \left[ g_{m_2,m_1}(\alpha_1) - g_{m_2,m_1}(\alpha_2) \right] - A_n \left[ g_{m_1,m_2}(\alpha_1) - g_{m_1,m_2}(\alpha_2) \right] \right. \]
\[ - A_{m_2} \left[ g_{m_1,m_2}(\alpha_1) - g_{m_1,m_2}(\alpha_2) \right] + A_{m_1} \left[ g_{m_2,m_1}(\alpha_1) - g_{m_2,m_1}(\alpha_2) \right] \]
\[ + \frac{1}{h_{m_1,m_2}(\alpha_1)h_{m_1,m_2}(\alpha_2)} \left[ h_{m_1,m_2}(\alpha_2)B'_n(\alpha_1) - h_{m_1,m_2}(\alpha_1)B'_n(\alpha_2) \right] \mid , \]
\[ (4.63) \]

where \( g_{i,j}(\alpha) \) is defined as in (4.40).
Adding and subtracting $h_{m_1,m_2}(\alpha_2)B'_n(\alpha_2)$ of the last term of (4.63) and applying the triangular inequality, we have

$$|J'(\alpha_1) - J'(\alpha_2)| \leq | - A_{m_2}C_{m_1} + A_{m_1}C_{m_2} |$$

$$+ |A_m| |g_{m_2,m_1}(\alpha_1) - g_{m_2,m_1}(\alpha_2)| + |A_m| |g_{m_1,m_2}(\alpha_1) - g_{m_1,m_2}(\alpha_2)|$$

$$+ \frac{1}{h_{m_1,m_2}(\alpha_1)} |B'_n(\alpha_1) - B'_n(\alpha_2)|$$

$$+ \frac{B'_n(\alpha_2)}{h_{m_1,m_2}(\alpha_1)h_{m_1,m_2}(\alpha_2)} |h_{m_1,m_2}(\alpha_2) - h_{m_1,m_2}(\alpha_1)| .$$

(4.64)

Finally, using 1, 3 and 4 and by applying 8a, 7 and 9 of Proposition 4.4.3, we have

$$|J'(\alpha_1) - J'(\alpha_2)| \leq 2M_a M_g \| 4M_a M_y \eta_g + M_h \eta_y + M_h^2 M_y \eta_h \| |\alpha_1 - \alpha_2|$$

where $|A_{m_i}| \leq M_{a_i} \leq M_a = \max \{ M_a, M_y \}$, $|B'_{m_i}| \leq M_{b'_i} \leq M_{b'_i} = \max \{ M_{b'_i}, M_{b'_i} \}$, $|y_{m_i}| \leq M_{y_i} \leq M_y = \max \{ M_{y_i}, M_{y_i} \}$, and $\eta_g, \eta_y, \eta_h$ are the Lipschitz constant for the functions $g, B'$ and $h$, respectively.

\[ \square \]

**Remark 4.4.3.** Note that in the previous theorem, the local convergence was proved for $M = 2$ and assuming that the functions are smooth. However, using Proposition 4.4.3 the local convergence can easily be proved for $M > 2$, where $d(\alpha), d'(\alpha)$ and $\nu(\alpha)$ can be obtained using the least square method and $h(\alpha) = \sum_{i=1}^{M} A_i^2 \sum_{i=1}^{M} B_i^2(\alpha) - (\sum_{i=1}^{M} A_i B_i(\alpha))^2$. 
4.5 Numerical Simulations

In this section, an extensive numerical analysis of the performance of the proposed algorithm is presented. The effect of the following are tested numerically:

- the number and type of modulating functions,
- the length of the integration interval,
- number of basis,
- the noise level,
- type of measurements (distributed and non-distributed).

We propose to use polynomial modulating functions whose fractional derivative is easy to compute analytically. Other types of modulating functions can be used; however they will require the numerical computation of the fractional derivatives which we want to avoid. The polynomial modulating functions used satisfy H1.-H3. and have the following form [36]: for \( b \in \mathbb{N}^*, m = 1, 2, \ldots M \) and \( L_1 \in \mathbb{R} \),

\[
\phi(x) = x^{M+b+1-m}(L_1 - x)^{b+m} = \sum_{k=0}^{b+m} c_k x^{M+b+1-m+k}, \tag{4.65}
\]

the fractional derivative of (4.65) can be easily computed and is given by:

\[
\frac{\partial^\alpha \phi(x)}{\partial x^\alpha} = \sum_{k=0}^{b+m} c_k \frac{\Gamma(M + b - m + k + 2)}{\Gamma(M + b - m + k + 2 - \alpha)} x^{M+b+1-m+k-\alpha}, \tag{4.66}
\]

where \( c_k = \binom{b+m}{k} (-1)^k L_1^{b+m-k} \) and the derivative of (4.66) with respect to \( \alpha \), needed to compute the gradient, can be computed using Proposition 2.2.3 as follows:

\[
\frac{\partial}{\partial \alpha} \frac{\partial^\alpha \phi(x)}{\partial x^\alpha} = -\frac{\partial^\alpha \phi(x)}{\partial x^\alpha} \left[ \ln(x) - \psi_0(n - \alpha) \right], \quad n - 1 \leq \alpha < n, \tag{4.67}
\]
where $\psi_0(n-\alpha) = \frac{\Gamma(n-\alpha)}{\Gamma(n-\alpha)}$.

First, the coefficients $\nu$ and $d$ are estimated by solving the system given in (4.11). Then, we use the algorithm given in Section 4 to estimate the parameters $\nu$, $d$, and $\alpha$ on a finite interval from noisy measurements. The value of $t$ is taken at the time $T$ where we have the measurements of the concentration and the flux given in 3.65. Moreover, we apply the trapezoidal rule to numerically approximate the integrals with grid spacing $\Delta x$.

Example 4.5.1. We consider equation (1.1) with initial and Dirichlet boundary conditions (1.2), where $g_0(x) = x(L-x)$, and

$$ r(x,t) = \begin{cases} 
\cos(-t)[\nu(x)(L-2x) - d(x)(\frac{L\Gamma(2)}{\Gamma(2-\alpha)}x^{1-\alpha} - \frac{\Gamma(3)}{\Gamma(3-\alpha)}x^{2-\alpha})] + \\
\sin(-t)x(L-x), & 0 < x < L, \\
0, & x = 0, L, 
\end{cases} \tag{4.68} $$

for which the analytic solution is $c(x,t) = \cos(-t)x(L-x)$ and the flux is $\frac{\partial c(x,t)}{\partial t} = \sin(-t)x(L-x)$.

1. **Estimating the coefficients $\nu(x)$, $d(x)$ when $\alpha$ is known**

In this part, we assume that the differentiation order $\alpha$ is known and we estimate the variable coefficients $\nu(x)$ and $d(x)$ simultaneously, using the measurements given in (3.67). We set the differentiation order $\alpha = 1.8$, the final time $T = 1$, $b = 1$ and the set of polynomial basis functions $\{1, x, x^2, x^3, \cdots\}$ is selected.

(a) **Noise-free case**

In Figures 4.2 and 4.3, we have the estimated $\nu(x) = 2(\sin(\pi x) + 1)$ and $d(x) = 0.7x$ when using noise-free measurements, where the length of the integration interval $L = 2$. The results are reasonable for different number of modulating functions. This is confirmed in Table 4.1, where the errors of...
the estimated \( \nu \) and \( d \) are less than 1%. However, it is noted that the errors increases as we increase the number of modulating functions which means that the accuracy of the method is affected by the number of modulating functions.

Figure 4.2: Exact and estimated \( \nu \) with different numbers of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1) \), \( d(x) = 0.7x \) and \( \Delta x = \frac{1}{2100} \).

Figure 4.3: Exact and estimated \( d \) with different numbers of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1) \), \( d(x) = 0.7x \) and \( \Delta x = \frac{1}{2100} \).

Table 4.1: Relative errors of \( \nu \) and \( d \), where \( \nu(x) = 2(\sin(\pi x) + 1) \), \( d(x) = 0.7x \), \( \alpha = 1.8 \) and \( \Delta x = \frac{1}{2100} \) in noise-free case.

<table>
<thead>
<tr>
<th>Number of modulating functions</th>
<th>( |\nu - \tilde{\nu}|_2 )</th>
<th>( |d - \tilde{d}|_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0.58E-2</td>
<td>0.25E-2</td>
</tr>
<tr>
<td>9</td>
<td>0.60E-2</td>
<td>0.25E-2</td>
</tr>
<tr>
<td>10</td>
<td>0.61E-2</td>
<td>0.30E-2</td>
</tr>
<tr>
<td>11</td>
<td>0.62E-2</td>
<td>0.41E-2</td>
</tr>
</tbody>
</table>

(b) Noisy case

Figures 4.4 and 4.5 show the estimated \( \nu(x) \) and \( d(x) \) when \( \nu(x) = 2(\sin(\pi x) + 1) \) and \( d(x) = 0.7x \), where 2% white Gaussian noise has been added to the measurements. The results are satisfactory even with different numbers of modulating functions. This is confirmed in Tables 4.2 and 4.3 where the
Table 4.2: Relative errors of $\nu = \frac{\|\nu - \tilde{\nu}\|_2}{\|\nu\|_2}$, where $\nu(x) = 2(\sin(\pi x) + 1)$, $d(x) = 0.7x$, $\alpha = 1.8$ and $\Delta x = \frac{1}{2100}$ with different noise levels.

<table>
<thead>
<tr>
<th>Number of modulating functions</th>
<th>Noise Level</th>
<th>1%</th>
<th>3%</th>
<th>5%</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1%</td>
<td>1.82E-2</td>
<td>5.56E-2</td>
<td>8.88E-2</td>
</tr>
<tr>
<td>9</td>
<td>1%</td>
<td>1.62E-2</td>
<td>4.89E-2</td>
<td>7.66E-2</td>
</tr>
<tr>
<td>10</td>
<td>1%</td>
<td>1.89E-2</td>
<td>5.34E-2</td>
<td>8.13E-2</td>
</tr>
<tr>
<td>11</td>
<td>1%</td>
<td>2.43E-2</td>
<td>6.65E-2</td>
<td>9.79E-2</td>
</tr>
</tbody>
</table>

relative errors of the estimated $\nu$ and $d$ are reasonable even when adding 5% noise to both measurements.

Figure 4.4: Exact and estimated $\nu$ with different number of modulating functions when $\nu(x) = 2(\sin(\pi x) + 1)$, $d(x) = 0.7x$ with 2% noise where $L_1 = 2$ and $\Delta x = \frac{1}{2100}$.

Figure 4.5: Exact and estimated $d$ with different number of modulating functions when $\nu(x) = 2(\sin(\pi x) + 1)$, $d(x) = 0.7x$ with 2% noise where $L_1 = 2$, $\Delta x = \frac{1}{2100}$.

In Figures 4.6 and 4.7, we can see the estimated $\nu(x)$ and $d(x)$ when $\nu(x) = 2(\sin(\pi x) + 1)$ and $d(x) = 5\exp(-4x)$, where we add a 2% white Gaussian noise to the measurements. As shown in Table 4.4, the corresponding relative errors for $\nu(x)$ are around 15% and around 20% for $d(x)$. It is noted that the choice of the basis functions is important and affects the results; however other types of basis functions have not been investigated since this requires the numerical computation of the fractional derivatives of the functions. This will be investigated in our future work.
Table 4.3: Relative errors of \( d(x) = \frac{\|d - \tilde{d}\|_2}{\|d\|_2} \), where \( \nu(x) = 2(\sin(\pi x) + 1) \), \( d(x) = 0.7x \), \( \alpha = 1.8 \) and \( \Delta x = \frac{1}{2100} \) with different noise levels.

<table>
<thead>
<tr>
<th>Number of modulating functions</th>
<th>Noise Level</th>
<th>1%</th>
<th>3%</th>
<th>5%</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>2.99E-2</td>
<td>7.69E-2</td>
<td>10.94E-2</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>3.39E-2</td>
<td>8.47E-2</td>
<td>11.66E-2</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>4.44E-2</td>
<td>10.97E-2</td>
<td>14.70E-2</td>
<td></td>
</tr>
</tbody>
</table>

Figure 4.6: Exact and estimated \( \nu \) with different number of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1) \) and \( d(x) = 5 \exp(-4x) \) with 2% noise where \( L_1 = 2 \) and \( \Delta x = \frac{1}{2100} \).

Figure 4.7: Exact and estimated \( d \) with different number of modulating functions when \( \nu(x) = 2(\sin(\pi x) + 1) \) and \( d(x) = 5 \exp(-4x) \) with 2% noise where \( L_1 = 2 \), \( \Delta x = \frac{1}{2100} \).

Table 4.4: Relative errors of \( \nu \) and \( d \), where \( \nu(x) = 2(\sin(\pi x) + 1) \), \( d(x) = 5 \exp(-4x) \), \( \alpha = 1.8 \) and \( \Delta x = \frac{1}{2100} \) with 2% noise.

<table>
<thead>
<tr>
<th>Number of modulating functions</th>
<th>Relative errors</th>
<th>( \frac{|\nu - \tilde{\nu}|_2}{|\nu|_2} )</th>
<th>( \frac{|d - \tilde{d}|_2}{|d|_2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>0.127</td>
<td>0.213</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>0.159</td>
<td>0.236</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.157</td>
<td>0.235</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>0.150</td>
<td>0.230</td>
<td></td>
</tr>
</tbody>
</table>
2. Estimating constant coefficients $\nu$, $d$ when $\alpha$ is known

In this part, we estimate constant coefficients $\nu$ and $d$ when the differentiation order $\alpha$ is known. We set the average velocity $\nu = 0.4$, the dispersion coefficient $d = 1.1$, the differentiation order $\alpha = 1.8$, and $\Delta x = \frac{1}{2100}$. Three modulating functions are used and the length of the integration interval $[0, L_1]$ has been increased.

(a) **Noise-free case**

Figure 4.8 represents the estimated $\nu$ and $d$ and the corresponding relative errors are given in Figure 4.9. As expected, the results are satisfactory even if we integrate over half the interval.

![Figure 4.8: The estimated $d$ and $\nu$ in noise-free case with different values of $L_1$ when $d = 1.1$, $\nu = 0.4$, $\alpha = 1.8$, $\Delta x = \frac{1}{2100}$.](image1)

![Figure 4.9: The relative errors of $\nu$ and $d$ in noise-free case with different values of $L_1$ when $d = 1.1$, $\nu = 0.4$, $\alpha = 1.8$, $\Delta x = \frac{1}{2100}$.](image2)

(b) **Noisy Case:**

In Figure 4.10, we can see the estimated values of $\nu$ and $d$ when adding a 3% white Gaussian noise to the measurements. From Figure 4.11, we observe that the numerical results are quite satisfactory, where the relative error is less than 5% when integrating over the interval $[0, 4.5]$ and drops to less than 1% as we increase the length of the integration interval. Although
not presented, we would like to note that the results obtained using up to 20 modulating functions are quite similar to those presented in Figure 4.10, which will be discussed later.

Figure 4.10: The estimated $d$ and $\nu$ with 3% noise with different values of $L_1$ when $d = 1.1$, $\nu = 0.4$, $\alpha = 1.8$, $\Delta x = \frac{1}{2100}$.

Figure 4.11: The relative errors of $\nu$ and $d$ with 3% noise with different values of $L_1$ when $d = 1.1$, $\nu = 0.4$, $\alpha = 1.8$, $\Delta x = \frac{1}{2100}$.

3. Estimating $\nu$, $d$ and $\alpha$

Now, we use the combined Newton’s and modulating functions method to estimate all three parameters simultaneously. We set the exact values of the average velocity $\nu = 0.4$, the dispersion coefficient $d = 1.1$, the differentiation order $\alpha = 1.8$, the length of the integration interval $L = 9$ and the initial guess $\alpha_0 = 1.5$.

(a) Noise-free case

In Figure 4.12, we have the relative errors for the estimated parameters with different numbers of modulating functions. As we can see the results are almost accurate as the errors are less than 0.12% for all three parameters.

(b) Noisy case
Figure 4.12: The relative errors of the estimated parameters with different numbers of modulating functions

In Figure 4.13, a comparison under different noise levels 1%, 3%, 5%, 10%, between the exact values of the parameters and the estimated values is given. From this figure, it can be seen that the results are stable and remain reasonable even if adding 10% noise to the measurements. In Table 4.5 the estimated parameters with different numbers of modulating functions when adding a 3% white Gaussian noise to the measurements. Even with different numbers of modulating functions the errors are less than 2% for all parameters and the results are quite satisfactory. However, it is noted that the number of the modulating functions has an effect on the stability and the accuracy of the presented algorithm. This problem will be discussed in the next section.

4. Estimating \( \nu, d \) and \( \alpha \) using non-distributed measurements

In practice, it is difficult to measure the data over the whole domain. Therefore, in this part we use the measurements of the concentration and the flux at few locations, \( x_i = \frac{L}{7} i \):

\[
c(x_i, T) = g_1(x_i), \quad \frac{\partial c(x_i, T)}{\partial t} = g_2(x_i), \quad 0 < x_i < L, \quad i = 1, 2, \ldots, 7.
\] (4.69)
Figure 4.13: The estimated parameters obtained with 5 modulating functions and different noise levels.

Table 4.5: \( d = 1.1, \alpha = 1.8, \nu = 0.4, \) and \( \Delta x = \frac{1}{2100}, \) 3% noise.

<table>
<thead>
<tr>
<th>number of modulating functions</th>
<th>( \hat{\alpha} = (\hat{\nu}, \hat{d}, \hat{\alpha}) )</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>((0.403, 1.098, 1.799))</td>
<td>((0.74E-2, 0.19E-2, 0.07E-2))</td>
</tr>
<tr>
<td>4</td>
<td>((0.406, 1.098, 1.799))</td>
<td>((0.44E-2, 0.15E-2, 0.001E-2))</td>
</tr>
<tr>
<td>5</td>
<td>((0.401, 1.098, 1.800))</td>
<td>((0.33E-2, 0.15E-2, 0.01E-2))</td>
</tr>
<tr>
<td>6</td>
<td>((0.402, 1.098, 1.800))</td>
<td>((0.40E-2, 0.18E-2, 0.03E-2))</td>
</tr>
<tr>
<td>7</td>
<td>((0.402, 1.098, 1.799))</td>
<td>((0.57E-2, 0.22E-2, 0.09E-2))</td>
</tr>
<tr>
<td>8</td>
<td>((0.403, 1.097, 1.797))</td>
<td>((0.83E-2, 0.27E-2, 0.17E-2))</td>
</tr>
<tr>
<td>9</td>
<td>((0.405, 1.097, 1.795))</td>
<td>((1.13E-2, 0.31E-2, 0.26E-2))</td>
</tr>
<tr>
<td>10</td>
<td>((0.406, 1.096, 1.794))</td>
<td>((1.43E-2, 0.33E-2, 0.24E-2))</td>
</tr>
</tbody>
</table>
then use Legendre interpolation to approximate the measurements over the whole domain. We set the exact values of the average velocity $\nu = 0.5$, the dispersion coefficient $d = 1$, the differentiation order $\alpha = 1.6$, the final time $T = 1$, the length of the integration interval $L = 40$, $b = 3$ and the initial guess $\alpha_0 = 1.4$.

(a) Noise-free case

In Figure 4.14, we can see the estimated $\nu$ and $d$ with three modulating functions and different integration intervals. As we can see in Figure 4.15 the corresponding relative errors are less than $7E^{-6}\%$. In Figure 4.16, the relative errors for the estimated $\nu$, $d$ and $\alpha$ with different number of modulating functions. As expected the number of modulating functions has an effect on the accuracy of the algorithm. However, the effect was not significant and the relative errors are less than $0.07\%$ since the measurements are noise-free.

![Figure 4.14: The estimated $\nu$ and $d$ with different values of $L_1$ and $\Delta x = \frac{1}{2000}$](image1)

![Figure 4.15: The relative errors of $\nu$ and $d$ with different values of $L_1$ and $\Delta x = \frac{1}{2000}$](image2)

(b) Noisy Case

In Figure 4.17, the estimated $\nu$ and $d$ when adding a 3% white Gaussian noise to the measurements. Three modulating functions are used and the
length of the integration interval \([0, L_1]\) has been increased. The corresponding relative errors are given in Figure 4.18. From these figures, we note that the results are satisfactory and the relative errors are less than 6\% when \(L_1 = 40\) and less than 10\% when \(L_1\) is between 30 and 40. However, when we estimate all three unknowns \(\nu, d\) and \(\alpha\) the relative errors were slightly greater. In Figure 4.19, the estimated parameters with different noise levels and the corresponding relative errors are given in Figure 4.20. As we can see the relative errors for all three parameters are less than 4\% when adding 1\% noise and less than 6\% for 3\% noisy measurements. Moreover, in Tables 4.6 and 4.7 are the estimated parameters with 1\% and 2\% noise with different number of modulating functions. It is noted that when using 4 and 5 modulating functions the results are more accurate then when increasing the number of modulating functions. As mentioned before the number of modulating functions has an effect on the accuracy of the algorithm and further investigation is needed.

**Remark 4.5.1.** *It is important to point out that in the noisy case the accuracy and*
Figure 4.17: The exact and the estimated $\nu$ with 3% noise with different values and $\Delta x = \frac{1}{2000}$.

Figure 4.18: The exact and the estimated $d$ with 3% noise with different values and $\Delta x = \frac{1}{2000}$.

Table 4.6: $d = 1$, $\alpha = 1.6$, $\nu = 0.5$, and $\Delta x = \frac{1}{2000}$, 1% noise.

<table>
<thead>
<tr>
<th>number of modulating functions</th>
<th>Estimated Value $\hat{\alpha} = (\hat{\nu}, \hat{d}, \hat{\alpha})$</th>
<th>Relative Error $\left( \frac{|\nu - \hat{\nu}|_2}{|\nu|_2}, \frac{|d - \hat{d}|_2}{|d|_2}, \frac{|\alpha - \hat{\alpha}|_2}{|\alpha|_2} \right)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$(0.478, 1.020, 1.620)$</td>
<td>$(4.40E-2, 2.04E-2, 1.26E-2)$</td>
</tr>
<tr>
<td>4</td>
<td>$(0.489, 0.990, 1.597)$</td>
<td>$(2.12E-2, 0.97E-2, 0.19E-2)$</td>
</tr>
<tr>
<td>5</td>
<td>$(0.501, 0.966, 1.575)$</td>
<td>$(0.22E-2, 3.44E-2, 1.55E-2)$</td>
</tr>
<tr>
<td>6</td>
<td>$(0.513, 0.946, 1.555)$</td>
<td>$(2.61E-2, 5.43E-2, 2.81E-2)$</td>
</tr>
<tr>
<td>7</td>
<td>$(0.525, 0.930, 1.536)$</td>
<td>$(5.05E-2, 6.97E-2, 3.98E-2)$</td>
</tr>
</tbody>
</table>

Table 4.7: $d = 1.1$, $\alpha = 1.8$, $\nu = 0.4$, and $\Delta x = \frac{1}{2000}$, 2% noise.

<table>
<thead>
<tr>
<th>number of modulating functions</th>
<th>Estimated Value $\hat{\alpha} = (\hat{\nu}, \hat{d}, \hat{\alpha})$</th>
<th>Relative Error $\left( \frac{|\nu - \hat{\nu}|_2}{|\nu|_2}, \frac{|d - \hat{d}|_2}{|d|_2}, \frac{|\alpha - \hat{\alpha}|_2}{|\alpha|_2} \right)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$(0.446, 1.079, 1.664)$</td>
<td>$(10.9E-2, 7.94E-2, 3.99E-2)$</td>
</tr>
<tr>
<td>4</td>
<td>$(0.471, 1.004, 1.611)$</td>
<td>$(5.89E-2, 0.36E-2, 0.07E-2)$</td>
</tr>
<tr>
<td>5</td>
<td>$(0.498, 0.946, 1.561)$</td>
<td>$(0.417E-2, 5.45E-2, 2.42E-2)$</td>
</tr>
<tr>
<td>6</td>
<td>$(0.528, 0.904, 1.514)$</td>
<td>$(5.51E-2, 9.58E-2, 5.38E-2)$</td>
</tr>
<tr>
<td>7</td>
<td>$(0.559, 0.878, 1.470)$</td>
<td>$(11.9E-2, 12.2E-2, 8.10E-2)$</td>
</tr>
</tbody>
</table>
Figure 4.19: The estimated parameters obtained with five modulating functions and different noise levels.

<table>
<thead>
<tr>
<th>noise level</th>
<th>v</th>
<th>estimated v</th>
<th>d</th>
<th>estimated d</th>
<th>α</th>
<th>estimated α</th>
</tr>
</thead>
<tbody>
<tr>
<td>1%</td>
<td>0.5</td>
<td>0.9911</td>
<td>1</td>
<td>0.96557</td>
<td>1.6</td>
<td>1.59688</td>
</tr>
<tr>
<td>2%</td>
<td>0.5</td>
<td>0.99791</td>
<td>1</td>
<td>1.00356</td>
<td>1.6</td>
<td>1.56116</td>
</tr>
<tr>
<td>3%</td>
<td>0.5</td>
<td>0.986321</td>
<td>1</td>
<td>0.943707316</td>
<td>1.6</td>
<td>1.56381</td>
</tr>
</tbody>
</table>

Figure 4.20: The relative errors for the estimated parameters with five modulating functions with different noise levels.
the stability of the system given in (4.18) do not depend only on the noise, but also depends on the sensitivity of the system, which is the condition number of the matrix. Since the condition number depends on both the input and the output of our system the choice of the modulating functions is critical and should be chosen to give a small condition number.

**Example 4.5.2.** We consider the equation given in (1.1) with initial and Dirichlet boundary conditions given in (1.2), where \( g_0(x) = 10x^2 - x^3 \) and

\[
r(x, t) = \begin{cases} 
  t^2[\nu(x)(20x - 3x^2) - d(x)(\frac{10\Gamma(3)}{\Gamma(3-\alpha)}x^{1-\alpha} - \frac{\Gamma(4)}{\Gamma(4-\alpha)}x^{2-\alpha})] + \\
  2t(10x^2 - x^3), & 0 < x < 10, \\
  0, & x = 0, 10,
\end{cases}
\]

for which its exact solution is \( c(x, t) = t^2(10x^2 - x^3) \) and the flux is \( \frac{\partial c(x, t)}{\partial t} = 2t(10x^2 - x^3) \).

In this example, we set the average velocity \( \nu = 0.3 \), the dispersion coefficient \( d = 1.1 \), the differentiation order \( \alpha = 1.3 \), and the final time \( T = 2 \). In Figures 4.21, we estimated \( \nu \) and \( d \) using 3 modulating functions when adding a 2% noise to the measurements and the corresponding relative errors are given in Figure 4.22. Figure 4.23, represents the relative errors of the estimated \( \nu \), \( d \) and \( \alpha \) when using 4 modulating functions with different noise levels. As we can see the results are satisfactory even with different numbers of modulating functions which is conformed by the errors given in Table 4.8. In Table 4.9, we estimated the parameters with different initial guess \( \alpha_0 = 1.2, 1.35, 1.37, 1.4, 1.5 \) and 1.6, as expected, the algorithm converges to the exact solution when the initial guess is around the true value of \( \alpha \). However, when we chose \( \alpha_0 = 1.5 \) or 1.6 which is more then 15% far from the exact value the algorithm dose not converge to the exact solution.
Figure 4.21: The estimated $d$ and $\nu$ with 2% noise with different values of $L_1$ when $d = 1.1$, $\nu = 0.3$, $\alpha = 1.3$, $\Delta x = \frac{1}{3000}$.

Table 4.8: $d = 1.1$, $\alpha = 1.3$, $\nu = 0.3$, and $\Delta x = \frac{1}{3000}$, 2% noise.

<table>
<thead>
<tr>
<th>number of modulating functions</th>
<th>Estimated Value $\hat{a} = (\hat{\nu}, \hat{d}, \hat{\alpha})$</th>
<th>Relative Error $(|\nu - \hat{\nu}|_2, |d - \hat{d}|_2, |\alpha - \hat{\alpha}|_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>(0.311, 1.110, 1.296)</td>
<td>(3.64E-2, 0.899E-2, 0.308E-2)</td>
</tr>
<tr>
<td>4</td>
<td>(0.300, 1.100, 1.299)</td>
<td>(0.07E-2, 0.003E-2, 0.01E-2)</td>
</tr>
<tr>
<td>5</td>
<td>(0.285, 1.087, 1.305)</td>
<td>(5.01E-2, 1.18E-2, 0.4E-2)</td>
</tr>
<tr>
<td>6</td>
<td>(0.272, 1.076, 1.310)</td>
<td>(9.34E-2, 2.22E-2, 0.77E-2)</td>
</tr>
<tr>
<td>7</td>
<td>(0.264, 1.068, 1.313)</td>
<td>(12.1E-2, 2.89E-2, 10.2E-2)</td>
</tr>
</tbody>
</table>

Table 4.9: $d = 1.1$, $\alpha = 1.3$, $\nu = 0.3$, and $\Delta x = \frac{1}{3000}$, 2% noise.

<table>
<thead>
<tr>
<th>Initial guess $\alpha_0$</th>
<th>Estimated Value $\hat{a} = (\hat{\nu}, \hat{d}, \hat{\alpha})$</th>
<th>Relative Error $(|\nu - \hat{\nu}|_2, |d - \hat{d}|_2, |\alpha - \hat{\alpha}|_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.2</td>
<td>(0.299, 1.1, 1.3)</td>
<td>(0.002E-2, 0.03E-2, 0.002E-2)</td>
</tr>
<tr>
<td>1.35</td>
<td>(0.265, 1.07, 1.313)</td>
<td>(11.6E-2, 2.75E-2, 0.97E-2)</td>
</tr>
<tr>
<td>1.37</td>
<td>(0.265, 1.07, 1.297)</td>
<td>(11.6E-2, 2.75E-2, 0.97E-2)</td>
</tr>
<tr>
<td>1.4</td>
<td>(0.266, 1.07, 1.312)</td>
<td>(11.4E-2, 2.72E-2, 0.95E-2)</td>
</tr>
<tr>
<td>1.5</td>
<td>(0.163, 0.766, 1.62)</td>
<td>(45.7E-2, 30.3E-2, 24.6E-2)</td>
</tr>
<tr>
<td>1.6</td>
<td>(0.163, 0.766, 1.62)</td>
<td>(45.7E-2, 30.3E-2, 24.6E-2)</td>
</tr>
</tbody>
</table>

Figure 4.22: The relative errors of $\nu$ and $d$ with 2% noise with different values of $L_1$ when $d = 1.1$, $\nu = 0.3$, $\alpha = 1.3$, $\Delta x = \frac{1}{3000}$. 
Figure 4.23: The relative errors of the estimated parameters obtained with 4 modulating functions and different noise levels.

4.6 Estimating the Coefficients $\nu$ and $d$ in Case Flux Measurements are Not Available

In case flux measurements are not available, but only the concentration can be measured, the previous algorithm can not be used in its current form. The solution we propose for this case is to use two sets of modulating functions: space-dependent modulating functions and time-dependent modulating functions.

In the next proposition, the coefficients $\nu$ and $d$ for the space FADE give in (1.1) are estimated.

**Proposition 4.6.1.** For $0 < L_1 \leq L$, let \( \{\phi_m(x)\}_{m=1}^M \) and \( \{\psi_m(t)\}_{m=1}^M \) be sets of $M$ modulating functions of at least order 2 defined on the intervals [0, $L_1$] and [0, $T_1$] respectively, where $2 \leq M$. Then the solution of the following linear system
gives the estimations of the parameters $d$ and $\nu$:

$$
P \begin{bmatrix} \nu \\ d \end{bmatrix} = Y,
$$

(4.71)

where

$$
P = \begin{bmatrix} A & B \end{bmatrix}, \text{ and } Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix},
$$

(4.72)

with

$$
A_n = - \int_0^T \int_0^{L_1} \psi_n(t) \frac{\partial \phi_n(L_1 - x)}{\partial x} c(x, t) \, dx \, dt,
$$

(4.73)

$$
B_n = \int_0^T \int_0^{L_1} \psi_n(t) \frac{\partial^n \phi_n(x)}{\partial x^n} c(L_1 - x, t) \, dx \, dt,
$$

(4.74)

$$
y_n = - \int_0^T \int_0^{L_1} \frac{\partial \psi_n(t)}{\partial t} \phi_n(L_1 - x) c(x, t) \, dx \, dt - \int_0^T \int_0^{L_1} r(x, t) \psi_n(t) \phi_n(L_1 - x) \, dx \, dt.
$$

(4.75)

for $m = 1, 2, \ldots M$.

Proof. The proof can be obtained similarly as in proposition 4.3.1, where instead of multiplying by the modulating functions $\phi_m(x)$ we will also multiply by $\psi_m(t)$ and integrate with respect to $t$.

\qed

4.6.1 Numerical Simulations

The same polynomial modulating functions that have been used in Section 5 are used here and we apply the trapezoidal rule to numerically approximate the integrals. We
Example 4.6.1. Let us consider the following space fractional advection-dispersion equation:

\[
\frac{\partial c(x,t)}{\partial t} = -\nu \frac{\partial c(x,t)}{\partial x} + d \frac{\partial^{\alpha} c(x,t)}{\partial x^{\alpha}} + r(x,t), \quad 0 < x < L, \quad t > 0,
\]

(4.76)

with the following initial and Dirichlet boundary conditions:

\[
\begin{align*}
    c(x,0) &= x(L - x), \\
    c(0,t) &= 0, \\
    c(L,t) &= 0,
\end{align*}
\]

(4.77)

where

\[
r(x,t) = \begin{cases} 
\cos(-t)[\nu(L - 2x) - d(\frac{L(2-\alpha)}{\Gamma(2-\alpha)}x^{1-\alpha} - \frac{\Gamma(3-\alpha)}{\Gamma(3-\alpha)}x^{2-\alpha})] + \\
\sin(-t)x(L - x), & 0 < x < L, \\
0, & x = 0, L,
\end{cases}
\]

(4.78)

for which its exact solution is \( c(x,t) = \cos(-t)x(10 - x) \) and the flux is \( \frac{\partial c(x,t)}{\partial t} = \sin(-t)x(10 - x) \).

In Figure 4.24, we can see the estimated values of \( \nu \) and \( d \) when adding 3% white Gaussian noise to the measurement. As expected the results are satisfactory and the relative errors are less than 8% even if we integrate over half the interval.

### 4.7 Discussion

A two-stage algorithm has been used to estimate the coefficients and the differentiation order for a fractional differential equation. In the proposed approach, we take advantage of the properties of the modulating functions to overcome the difficulties
in estimating the differentiation order. The main advantage is that we simplify the
Newton’s algorithm by reducing the number of variables in the nonlinear equation
problem and the efficient computation of the gradient. Moreover, the presented algo-


rithm is fast compared to other standard optimization methods. The efficiency and
the robustness against corrupting noise with different numbers of modulating func-
tions have been confirmed by numerical examples. It is noted that the choice and the
number of modulating functions can affect the accuracy of the proposed algorithm.
As we can see in Figures 4.26 and 4.27, for 3 up to 20 modulating functions the relative
errors vary, but still less than 10%. It is also noted that the numerical accuracy can
become worse if the number of modulating functions increases. This is because the
stability of the algebraic system given in (4.11) depends on the modulating functions.
Indeed, as we increase the number of modulating functions the number of equations
increases. In all cases, the results are stable and remain reasonable even for up to 20
modulating functions and the presented algorithm works well with reasonable number
of modulating functions, which is further confirmed by the errors in Table 4.5. The
type of modulating functions is also important as in the noisy case the stability of the
system (4.11) (i.e. the condition number) depends on the noise and the used mod-
Figure 4.26: The relative errors of $\nu$.

Figure 4.27: The relative errors of $d$.

Therefore, we should choose a modulating functions that give a small condition number. Finally, we briefly comment on the length of the integration interval. In Tables 4.10 and 4.11, we present the relative errors when estimating the average velocity and the dispersion coefficient with different integration intervals. We observe that the length of the integration interval also has an effect on the accuracy of the performed algorithm. However, the relative errors are still reasonable and less than 1% for $L_1 = 5$. In fact, there is an optimal value for the length of the integration interval and further investigation is needed. Further, in Table 4.12, we present the relative errors when estimating all three parameters.

Table 4.10: Estimating $d$ when the exact values are $d = 1.1$, $\alpha = 1.8$, $\nu = 0.4$, and $\Delta x = \frac{1}{2100}$, 3% noise on both measurements.

<table>
<thead>
<tr>
<th>Number of modulating functions</th>
<th>$L_1 = 5$</th>
<th>$L_1 = 6$</th>
<th>$L_1 = 7$</th>
<th>$L_1 = 8$</th>
<th>$L_1 = 9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.81E-2</td>
<td>0.40E-2</td>
<td>0.20E-2</td>
<td>0.20E-2</td>
<td>0.17E-2</td>
</tr>
<tr>
<td>4</td>
<td>0.76E-2</td>
<td>0.40E-2</td>
<td>0.18E-2</td>
<td>0.18E-2</td>
<td>0.16E-2</td>
</tr>
<tr>
<td>5</td>
<td>0.67E-2</td>
<td>0.38E-2</td>
<td>0.14E-2</td>
<td>0.14E-2</td>
<td>0.14E-2</td>
</tr>
<tr>
<td>6</td>
<td>0.56E-2</td>
<td>0.35E-2</td>
<td>0.08E-2</td>
<td>0.08E-2</td>
<td>0.11E-2</td>
</tr>
<tr>
<td>7</td>
<td>0.43E-2</td>
<td>0.31E-2</td>
<td>0.03E-2</td>
<td>0.03E-2</td>
<td>0.08E-2</td>
</tr>
</tbody>
</table>

Remark 4.7.1. The presented two-stage algorithm has two sources of errors: numerical errors and noise error contributions. The numerical errors come from the iterative method and the numerical integration method. As mentioned in the discussion the nu-
Table 4.11: Estimating $v$ when the exact values are $d = 1$, $\alpha = 1.8$, $\nu = 0.5$, and $\Delta x = \frac{1}{2100}$, 2% noise on both measurements.

<table>
<thead>
<tr>
<th>Number of modulating functions</th>
<th>Relative Errors</th>
<th>$L_1 = 5$</th>
<th>$L_1 = 6$</th>
<th>$L_1 = 7$</th>
<th>$L_1 = 8$</th>
<th>$L_1 = 9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1.13E-2</td>
<td>0.60E-2</td>
<td>0.05E-2</td>
<td>0.05E-2</td>
<td>0.07E-2</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1.07E-2</td>
<td>0.56E-2</td>
<td>0.02E-2</td>
<td>0.02E-2</td>
<td>0.08E-2</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.97E-2</td>
<td>0.49E-2</td>
<td>0.02E-2</td>
<td>0.02E-2</td>
<td>0.08E-2</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.83E-2</td>
<td>0.39E-2</td>
<td>0.07E-2</td>
<td>0.07E-2</td>
<td>0.08E-2</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.67E-2</td>
<td>0.28E-2</td>
<td>0.12E-2</td>
<td>0.12E-2</td>
<td>0.07E-2</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.12: When estimating all parameters $d = 1.1$, $\alpha = 1.8$, $\nu = 0.4$, and $\Delta x = \frac{1}{2100}$, 2% noise on both measurements.

<table>
<thead>
<tr>
<th>M</th>
<th>$L_1 = 7.5$</th>
<th>Relative Error</th>
<th>$L_1 = 8$</th>
<th>$L_1 = 8.5$</th>
<th>$L_1 = 9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>(26.8E-2, 4.1E-2, 4.9E-2)</td>
<td>(13.5E-2, 2.3E-2, 2.3E-2)</td>
<td>(7.0E-2, 1.6E-2, 1.0E-2)</td>
<td>(1.1E-2, 1.1E-2, 0.3E-2)</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>(23.6E-2, 3.9E-2, 4.3E-2)</td>
<td>(10.1E-2, 2.3E-2, 1.6E-2)</td>
<td>(4.8E-2, 1.3E-2, 0.5E-2)</td>
<td>(2.3E-2, 0.9E-2, 0.1E-2)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>(20.4E-2, 3.6E-2, 3.8E-2)</td>
<td>(7.2E-2, 1.9E-2, 0.8E-2)</td>
<td>(3.6E-2, 1.3E-2, 0.3E-2)</td>
<td>(1.8E-2, 0.9E-2, 0.0E-2)</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>(17.0E-2, 3.3E-2, 3.2E-2)</td>
<td>(4.8E-2, 1.7E-2, 0.8E-2)</td>
<td>(3.4E-2, 1.4E-2, 0.4E-2)</td>
<td>(2.2E-2, 1.1E-2, 0.1E-2)</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>(13.5E-2, 3.1E-2, 2.7E-2)</td>
<td>(0.3E-2, 1.7E-2, 0.6E-2)</td>
<td>(4.2E-2, 1.6E-2, 0.8E-2)</td>
<td>(3.4E-2, 1.4E-2, 0.5E-2)</td>
<td></td>
</tr>
</tbody>
</table>

Numerical errors are also affected by the type and number of modulating functions. The noise error contributions are affected by the step size and as we increase the step size the errors tend to zero. [36].

4.8 Chapter Summary

In this chapter, we have presented a new approach to estimate the coefficients and the differentiation order in a space-fractional advection-dispersion equation. First, we have estimated the dispersion coefficient and the average velocity by applying the modulating functions method which transformed the coefficients identification problem into solving a linear system of algebraic equations. Second, the modulating functions method has been combined with Newton’s iterative algorithm to estimate the average velocity, the dispersion coefficient and the differentiation order simultaneously, where the first order derivatives with respect to $\alpha$ of the dispersion
Coefficient and the average velocity have also been estimated using a modulating functions approach, which simplifies the calculation of the gradient. Moreover, the local convergence of the presented method has been proved. Furthermore, the modulating functions method have been applied using two sets of modulating functions to estimate the velocity and the dispersion coefficients using the concentration measurement only. Numerical simulations have been performed using polynomial modulating functions, for which the fractional derivative is known analytically. The results have shown the effectiveness of the proposed algorithm for the 1D space FADE. However, for real world applications it is more practical to use a 2D model. The generalization to the 2D case is not straightforward and some adjustments need be done. Therefore, in the next chapter we generalize the two-stage algorithm to estimate the coefficients and the differentiation orders for the 2D space FADE.
Chapter 5

Parameters and Differentiation
Order Estimation for a 2D Space
FADE

5.1 Introduction

When modeling real physical phenomena such as groundwater flow and transport, it is more realistic to use a 2D model. Thus, we aim to generalize the combined modulating functions method and Newton-type algorithm presented in Chapter 4, to identifying the coefficients and the differentiation orders for a two-dimensional space-fractional advection-dispersion equation. Despite the importance of such models very little progress has been made on the inverse problem for 2D fractional partial differential equations. Xiong et al. [42], investigated an inverse problem for a two-dimensional time-fractional diffusion equation. They established the stability of determining heat flux from a measured temperature history at a fixed point using Fourier regularizing method. Kirane et al. [43], showed the existence and the uniqueness of an inverse source problem for a two-dimensional fractional diffusion equation using the properties of the biorthogonal system of functions. Qian et al. [44], presented a numerical
solution for the two-dimensional inverse heat conduct problem based on Kernel approximation in the frequency domain.

In this chapter, we consider the two-dimensional space FADE, and show that the combined modulating functions method and Newton’s type algorithm can be generalized to estimate all the parameters. However, there are some obstacles that we need to overcome before applying the method. First, we need to use more sets of modulating functions and integrate with respect to more than one variable. Second, instead of computing the derivative of the coefficients with respect to one variable, we compute it with respect to both differentiation orders and compute the corresponding Jacobian matrix. Third, the cost function has to be minimized with respect to more than one unknown.

5.2 Problem Statement

We consider the following 2D space FADE [45]: for any $0 < x < L_1$, $0 < y < L_2$, $t > 0$ and $1 < \beta, \alpha \leq 2$,

$$
\frac{\partial c(x, y, t)}{\partial t} = -\nu_1 \frac{\partial c(x, y, t)}{\partial x} - \nu_2 \frac{\partial c(x, y, t)}{\partial y} + d_1 \frac{\partial^\alpha c(x, y, t)}{\partial x^\alpha} + d_2 \frac{\partial^\beta c(x, y, t)}{\partial y^\beta} + f(x, y, t)
$$

(5.1)

with the following initial and Dirichlet boundary conditions:

$$
\begin{aligned}
&c(x, 0) = g_0(x, y), \quad 0 < x < L_1, \quad 0 < y < L_2, \\
&c(0, y, t) = 0, \quad 0 < y < L_2, \quad t > 0 \\
&c(x, 0, t) = 0, \quad 0 < x < L_1, \quad t > 0, \\
&c(L_x, y, t) = h_1(y, t), \quad 0 < y < L_2, \quad t > 0 \\
&c(x, L_y, t) = h_2(x, t), \quad 0 < x < L_1, \quad t > 0.
\end{aligned}
$$

(5.2)

We assume that the velocities $\nu_1, \nu_2$ and the dispersion coefficients $d_1, d_2$ are con-
stants and \( \nu_1, \nu_2, d_1, d_2 > 0 \).

We are interested in identifying the coefficients and the differentiation orders for the two-dimensional space FADE defined by (5.1) - (5.2) using the measurement of the concentration

\[
c(x, y, t) + \zeta, \quad 0 < x < L_1, \quad 0 < y < L_2, \quad 0 < t < T_1
\]

where \( \zeta \) is a noise contaminating the data.

### 5.3 Modulating Functions Method for Estimating the Coefficients

Similar to the approach developed in the previous chapter, we will first apply the modulating functions method to estimate the coefficients by assuming that the differentiation orders are known.

**Proposition 5.3.1.** Let \( \{\phi_m(x)\}_{m=1}^{M} \), \( \{\psi_n(y)\}_{n=1}^{N} \) and \( \{\eta_\kappa(t)\}_{\kappa=1}^{K} \) be sets of 2nd order modulating functions defined on the intervals \([0, L_1]\), \([0, L_2]\) and \([0, T_1]\) respectively, where \(M+N+K \leq 4\), \(L_x \leq L_1\), \(L_y \leq L_2\) and \(T \leq T_1\), then the solution of the following linear system gives the estimations of the parameters \( \nu_1, \nu_2, d_1 \) and \( d_2 \) :

\[
\begin{pmatrix}
A & B & C & D
\end{pmatrix}_{(M \times N \times K) \times 4}
\begin{pmatrix}
\nu_1 \\
\nu_2 \\
d_1 \\
d_2
\end{pmatrix}_{4 \times 1} = E, \quad (5.4)
\]
\[
\begin{bmatrix}
A_{1,1,1} \\
A_{2,1,1} \\
\vdots \\
A_{M,1,1} \\
A_{1,2,1} \\
\vdots \\
A_{2,2,1} \\
A_{M,2,1} \\
\vdots \\
\vdots \\
A_{M,N,K}
\end{bmatrix} (M \times N \times K) \times 1 \quad \begin{bmatrix}
E_{1,1,1} \\
E_{2,1,1} \\
\vdots \\
E_{M,1,1} \\
E_{1,2,1} \\
\vdots \\
E_{2,2,1} \\
E_{M,2,1} \\
\vdots \\
\vdots \\
E_{M,N,K}
\end{bmatrix} (M \times N \times K) \times 1
\]

and \( \mathbf{B}, \mathbf{C}, \mathbf{D} \) have the same structure as \( \mathbf{A} \) with

\[
A_{m,n,k} = \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial \phi_m(L_x - x)}{\partial x} \psi_n(L_y - y) \eta(T - t)c(x, y, t) \, dx \, dy \, dt
\]

\[
B_{m,n,k} = \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \psi_n(L_y - y)}{\partial y} \eta(T - t)c(x, y, t) \, dx \, dy \, dt
\]

\[
C_{m,n,k} = \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial^2 \psi_n(x)}{\partial x^2} \psi_n(L_y - y) \eta(T - t)c(L_x - x, y, t) \, dx \, dy \, dt
\]

\[
D_{m,n,k} = \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial^2 \psi_n(y)}{\partial y^2} \psi_n(L_y - y) \eta(T - t)c(x, L_y - y, t) \, dx \, dy \, dt
\]

\[
E_{m,n,k} = \int_0^T \int_0^{L_y} \int_0^{L_x} \left[ \phi_m(L_x - x) \psi_n(L_y - y) \right] \frac{\partial \eta(T - t)}{\partial t} c(x, y, t) - \eta(T - t) f(x, y, t) \, dx \, dy \, dt
\]

**Proof.** Step 1: Multiply (5.1) by the modulating functions \( \phi_m(L_x - x), \psi_n(L_y - y) \)
\[ \eta_\kappa(T - t) \text{ for } m = 1, \ldots, M, n = 1, \ldots, N \text{ and } \kappa = 1, \ldots, K \text{ then we get:} \]

\[ \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial c(x, y, t)}{\partial t} = -\nu_1 \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial c(x, y, t)}{\partial x} \]

\[ - \nu_2 \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial c(x, y, t)}{\partial y} + d_1 \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial^\alpha c(x, y, t)}{\partial x^\alpha} \]

\[ + d_2 \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial^\beta c(x, y, t)}{\partial y^\beta} + \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) f(x, y, t). \]

**Step 2:** Integrating over the intervals \([0, L_x], [0, L_y]\) and \([0, T]\) gives us:

\[
\int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial c(x, y, t)}{\partial t} \, dx \, dy \, dt =
\]

\[ - \nu_1 \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial c(x, y, t)}{\partial x} \, dx \, dy \, dt \]

\[ - \nu_2 \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial c(x, y, t)}{\partial y} \, dx \, dy \, dt + d_1 \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial^\alpha c(x, y, t)}{\partial x^\alpha} \, dx \, dy \, dt \]

\[ + d_2 \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) \frac{\partial^\beta c(x, y, t)}{\partial y^\beta} \, dx \, dy \, dt + \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) f(x, y, t) \, dx \, dy \, dt. \]

**Step 3:** By applying integration by parts and Lemma 4.2.1 to equation (5.7), we obtain:
\[
\int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \frac{\partial \eta_\kappa(T - t)}{\partial t} c(x, y, t) \, dx \, dy \, dt =
\]

\[
- \nu_1 \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \phi_m(L_x - x)}{\partial x} \psi_n(L_y - y) \eta_\kappa(T - t) c(x, y, t) \, dx \, dy \, dt
\]

\[
- \nu_2 \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \psi_n(L_y - y)}{\partial y} \eta_\kappa(T - t) c(x, y, t) \, dx \, dy \, dt
\]

\[
+ d_1 \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} \psi_n(L_y - y) \eta_\kappa(T - t) c(L_x - x, y, t) \, dx \, dy \, dt
\]

\[
+ d_2 \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial^\beta \psi_n(y)}{\partial y^\beta} \eta_\kappa(T - t) c(x, L_y - y, t) \, dx \, dy \, dt
\]

\[
+ \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_\kappa(T - t) f(x, y, t) \, dx \, dy \, dt.
\]

(5.8)

where the boundary conditions are eliminated by the properties of the used modulating functions.

Finally, the unknown coefficients can be estimated by solving the linear system given in (5.4).

\[\square\]

5.4 Parameters and Differentiation Order Estimation

In this section, we combine the modulating functions method with a Newton’s type algorithm to simultaneously, estimate the coefficients and the differentiation orders for the 2D space FADE given in (5.1).
5.4.1 Combined Newton’s and Modulating Functions Method to Estimate the Coefficients and the Differentiation Orders

An important problem for fractional models is the estimation of the parameters that best fit the model. However, the problem becomes more difficult for the 2D models as the number of unknown parameters increases and using the standard optimization techniques may lead to an ill-conditioning problem. This difficulty and complexity can be reduced by applying the algorithm presented in the previous chapter. However, to extend the combined algorithm to the 2D case we need to use more sets of modulating functions, represents the unknown coefficients in terms of two variables, compute the Jacobian matrix and minimize a cost function with respect to both differentiation orders.

Now, we introduce the two-stage algorithm to estimate coefficients and the differentiation orders and provide an exact characterization of the Jacobian matrix which is the main challenge for most optimization methods.

Stage 1: In this stage, we apply Proposition 5.3.1 to re-write the coefficients as functions of the unknown differentiation orders $\alpha$ and $\beta$:

Then, we consider the following equation:

$$
\frac{\partial c(x, y, t)}{\partial t} = -\nu_1(z) \frac{\partial c(x, y, t)}{\partial x} - \nu_2(z) \frac{\partial c(x, y, t)}{\partial y} + d_1(z) \frac{\partial^\alpha c(x, y, t)}{\partial x^\alpha} + d_2(z) \frac{\partial^\beta c(x, y, t)}{\partial y^\beta} + f(x, y, t)
$$  

(5.9)

where $z = (\alpha, \beta)$.

If \{\phi_m(x)\}_{m=1}^{M}, \{\psi_n(y)\}_{n=1}^{N}$ and $\eta_{K+1}(t)$ are 2nd order modulating functions, then using a similar way of obtaining (5.8), we get:
\[
\int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \frac{\partial \eta_k(T - t)}{\partial t} c(x, y, t) \, dx \, dy \, dt = \\
- \nu_1(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial \phi_m(L_x - x)}{\partial x} \psi_n(L_y - y) \eta_k(T - t) c(x, y, t) \, dx \, dy \, dt \\
- \nu_2(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \psi_n(L_y - y)}{\partial y} \eta_k(T - t) c(x, y, t) \, dx \, dy \, dt \\
+ d_1(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} \psi_n(L_y - y) \eta_k(T - t) c(L_x - x, y, t) \, dx \, dy \, dt \\
+ d_2(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial^\beta \psi_n(y)}{\partial y^\beta} \eta_k(T - t) c(x, L_y - y, t) \, dx \, dy \, dt \\
+ \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_k(T - t) f(x, y, t) \, dx \, dy \, dt.
\]

(5.10)

Since \( z \) is the unknown in equation (5.10), we can write it as follows:

\[
K_{m,n,K+1}(z) = U_{m,n,K+1} \quad \text{for} \quad m = 1, 2, \ldots, M \quad \text{and} \quad n = 1, 2, \ldots, N \quad (5.11)
\]

\[
K_{m,n,K+1}(z) = \\
- \nu_1(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial \phi_m(L_x - x)}{\partial x} \psi_n(L_y - y) \eta_k(T - t) c(x, y, t) \, dx \, dy \, dt \\
- \nu_2(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \psi_n(L_y - y)}{\partial y} \eta_k(T - t) c(x, y, t) \, dx \, dy \, dt \\
+ d_1(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} \psi_n(L_y - y) \eta_k(T - t) c(L_x - x, y, t) \, dx \, dy \, dt \\
+ d_2(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial^\beta \psi_n(y)}{\partial y^\beta} \eta_k(T - t) c(x, L_y - y, t) \, dx \, dy \, dt \\
+ \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \eta_k(T - t) f(x, y, t) \, dx \, dy \, dt.
\]

(5.12)

and

\[
U_{m,n,K+1} := \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \psi_n(L_y - y) \\
\cdot \left[ \frac{\partial \eta_k(T - t)}{\partial t} c(x, y, t) - \eta_k(T - t) f(x, y, t) \right] \, dx \, dy \, dt.
\]

(5.13)
Stage 2: In this stage, the inverse problem is formulated as a solution to the following nonlinear system of equations with respect to the unknown $z$:

$$ F_{m,n,K+1}(z) = K_{m,n,K+1}(z) - U_{m,n,K+1} = 0, \quad (5.14) $$

where $m = 1,2,\cdots M+1$ and $n = 1,2,\cdots N+1$. Which can be written in the following matrix form:

$$ F = K - U = 0, \quad (5.15) $$

where

$$ F = \begin{pmatrix}
K_{1,1,K+1} - U_{1,1,K+1} \\
K_{1,2,K+1} - U_{1,2,K+1} \\
\vdots \\
K_{1,N+1,K+1} - U_{1,N+1,K+1} \\
K_{2,1,K+1} - U_{2,1,K+1} \\
K_{2,2,K+1} - U_{2,2,K+1} \\
\vdots \\
K_{2,N+1,K+1} - U_{2,N+1,K+1} \\
\vdots \\
K_{M+1,1,K+1} - U_{M+1,1,K+1} \\
K_{M+1,2,K+1} - U_{M+1,2,K+1} \\
\vdots \\
K_{M+1,N+1,K+1} - U_{M+1,N+1,K+1}
\end{pmatrix}_{(M+1\times N+1)\times 1}, \quad (5.16) $$

with $K_{m,n,K+1}$ and $U_{m,n,K+1}$ defined as in (4.26) and (4.27), respectively.
Newton’s Approach

We use a first order Newton’s type method to solve the nonlinear system given in (5.15). At each iteration, $z$ is updated using:

$$z_{k+1} = z_k + \Delta z_k,$$  \hfill (5.17)

where $\Delta z_k$ is the solution of the following equation

$$F(z_k) = -J[F(z_k)] \Delta z_k,$$  \hfill (5.18)

and the Jacobian matrix $J[F(z)]$ is exactly characterized using the following proposition.

**Proposition 5.4.1.** Let $\{\phi_m(x)\}_{m=1}^M$, $\{\psi_n(y)\}_{n=1}^N$ and $\{\eta_\kappa(t)\}_{\kappa=1}^K$ be sets of 2nd order modulating functions defined on the intervals $[0,L_1]$, $[0,L_2]$ and $[0,T_1]$ respectively, where $M+N+K \leq 4$, $L_x \leq L_1$, $L_y \leq L_2$ and $T \leq T_1$, then the solution of the following linear system gives the estimations of the derivatives of the parameters $\nu_1, \nu_2, d_1$ and $d_2$ with respect to the differentiation order $\alpha$:

$$\begin{pmatrix} A & B & C & D \end{pmatrix}_{(M \times N \times K) \times 4} \frac{\partial}{\partial \alpha} \begin{pmatrix} -\nu_1 \\
-\nu_2 \\
1 \\
2 \end{pmatrix}_{4 \times 1} = -d_1(z)C'_{(M \times N \times K) \times 1},$$  \hfill (5.19)

where $A, B, C$ and $D$ are defined as in Proposition 5.3.1 with

$$\frac{\partial}{\partial \alpha} C_{m,n,\kappa} = \int_0^T \int_0^{L_x} \int_0^{L_y} \frac{\partial^{\alpha} \phi_m(x)}{\partial x^\alpha} \frac{\partial^{\alpha} \psi_n(y)}{\partial x^\alpha} \psi_n(L_y-y) \eta_\kappa(T-t)c(L_x-x,y,t),$$  \hfill (5.20)
where
\[ C' = \frac{\partial}{\partial \alpha} C \quad (5.21) \]

**Proof.** This proof can be obtained by differentiating (5.8) with respect to \( \alpha \).

**Remark 5.4.1.** In the previous proposition, we will determine the derivative of the coefficients \( \nu_1, \nu_2, d_1 \) and \( d_2 \) with respect to the differentiation order \( \alpha \). However, the derivatives of the coefficients with respect to the differentiation order \( \beta \) can be obtained similarly.

**Proposition 5.4.2.** Using the coefficients \( \nu_1(z), \nu_2(z), d_1(z) \) and \( d_2(z) \) which are the estimations given in proposition (5.3.1) and \( F \) is given in (4.28), the Jacobian \( J[F(z)] \) exists and is given as follows:

\[
J[F(z)] = \left( \frac{\partial F}{\partial \alpha}, \frac{\partial F}{\partial \beta} \right)^T \quad \text{where} \quad \frac{\partial F}{\partial \beta} = \left( \begin{array}{c}
\frac{\partial K_{1,1,K+1}}{\partial} \\
\frac{\partial K_{1,2,K+1}}{\partial} \\
\vdots \\
\frac{\partial K_{1,N+1,K+1}}{\partial} \\
\frac{\partial K_{2,1,K+1}}{\partial} \\
\vdots \\
\frac{\partial K_{2,N+1,K+1}}{\partial} \\
\vdots \\
\frac{\partial K_{M+1,1,K+1}}{\partial} \\
\frac{\partial K_{M+1,2,K+1}}{\partial} \\
\vdots \\
\frac{\partial K_{M+1,N+1,K+1}}{\partial}
\end{array} \right)_{(M+1 \times N+1) \times 1} \quad (5.22)
\]
with

\[
\frac{\partial K_{m,n,K+1}}{\partial \alpha} = \\
- \frac{\partial \nu_1(z)}{\partial \alpha} \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial \phi_m(L_x - x)}{\partial x} \psi_n(L_y - y) \eta_c(T - t) c(x, y, t) \, dx \, dy \, dt \\
- \frac{\partial \nu_2(z)}{\partial \alpha} \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \psi_n(L_y - y)}{\partial y} \eta_c(T - t) c(x, y, t) \, dx \, dy \, dt \\
+ d_1(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial \phi_m(x)}{\partial x} \psi_n(L_y - y) \eta_c(T - t) c(L_x - x, y, t) \, dx \, dy \, dt \\
+ \frac{\partial d_1(z)}{\partial \alpha} \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial^2 \psi_n(y)}{\partial y^2} \eta_c(T - t) c(x, L_y - y, t) \, dx \, dy \, dt, \\
\]

(5.23)

and

\[
\frac{\partial K_{m,n,K+1}}{\partial \beta} = \\
- \frac{\partial \nu_1(z)}{\partial \beta} \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial \phi_m(L_x - x)}{\partial x} \psi_n(L_y - y) \eta_c(T - t) c(x, y, t) \, dx \, dy \, dt \\
- \frac{\partial \nu_2(z)}{\partial \beta} \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \psi_n(L_y - y)}{\partial y} \eta_c(T - t) c(x, y, t) \, dx \, dy \, dt \\
+ \frac{\partial d_1(z)}{\partial \beta} \int_0^T \int_0^{L_y} \int_0^{L_x} \frac{\partial \phi_m(x)}{\partial x} \psi_n(L_y - y) \eta_c(T - t) c(L_x - x, y, t) \, dx \, dy \, dt \\
+ \frac{\partial d_2(z)}{\partial \beta} \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial^2 \psi_n(y)}{\partial y^2} \eta_c(T - t) c(x, L_y - y, t) \, dx \, dy \, dt \\
+ d_2(z) \int_0^T \int_0^{L_y} \int_0^{L_x} \phi_m(L_x - x) \frac{\partial \psi_n(y)}{\partial y} \eta_c(T - t) c(x, L_y - y, t) \, dx \, dy \, dt. \\
\]

(5.24)

**Proof.** The elements of \( J[F(z)] \) can be obtained directly by differentiating (5.12) with respect to the fractional orders \( \alpha \) and \( \beta \). The existence of the Jacobian \( J[F(z)] \) depends on the existence of the derivative of (2.8) with respect to the fractional orders \( \alpha \) and \( \beta \), which always exists as shown in Proposition 2.2.3.\]

□
5.4.2 Two-Stage Algorithm

For the convenience, we present a description of the proposed algorithm in Figure 5.1

<table>
<thead>
<tr>
<th>Algorithm 2: Two-stage algorithm to estimate the parameters and the fractional order.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 1: Start with an initial guess $z_0 = (\alpha^o, \beta^o)$.</td>
</tr>
<tr>
<td>Step 2: Compute the corresponding $\nu_1(z_k), \nu_2(z_k), d_1(z_k)$ and $d_2(z_k)$.</td>
</tr>
<tr>
<td>Step 3: Compute $|F(z_k)|^2_2$,</td>
</tr>
<tr>
<td>if $|F(z_k)|^2_2 &lt; \epsilon$ then</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>else</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>end</td>
</tr>
</tbody>
</table>

5.5 Numerical Results

In this section, we present some numerical results to show the performance and the robustness of the presented method.

First, we estimate $\nu_1, \nu_2, d_1$ and $d_2$ by solving the system given in (5.4). Then, we use the algorithm given in Section 4 to estimate the parameters $\nu_1, \nu_2, d_1$ and $d_2$ and $z$ on a finite interval from noisy measurements. We consider the following polynomial modulating functions whose fractional derivatives are simple to calculate. Other modulating functions can be used, but this will require the numerical computation of the fractional derivatives of the modulating functions if it cannot not be easily determined analytically: $\phi_m(x) = x^{M+b+1-m}(L_x - x)^{b+m}, \psi_n(y) = y^{N+b+1-n}(L_y - y)^{b+n}$ and $\eta_n(y) = t^{K+b+1-\kappa}(T_1 - t)^{b+\kappa}$ where $L_x \leq L_1, L_y \leq L_2, T \leq T_1, b = 3$, and $m = 1, 2, \cdots M$, $n = 1, 2, \ldots, N$ and $\kappa = 1, 2, \cdots K$, where $M, N$ and $K$ are the number of modulating functions. The fractional derivatives and the derivative with respect to the fractional derivatives of the modulating functions can be computed as given in
Figure 5.1: Two-stage algorithm to estimate $\nu_1, \nu_2, d_1, d_2, \alpha$ and $\beta$. 
and (4.67), respectively. Moreover, we apply the trapezoidal rule to numerically approximate the integrals.

**Example 5.5.1.** We consider the space fractional advection-dispersion equation given in 5.1 with the following initial and Dirichlet boundary conditions:

\[
\begin{align*}
  c(x, y, 0) &= x^{4.8} y^3, \\
  c(0, y, t) &= 0, \\
  c(x, 0, t) &= 0, \\
  c(x, 10, t) &= -e^{-t} 10^{4.8} y^3, \\
  c(10, y, t) &= e^{t} 10^{4.8} y^3, \\
  c(x, 10, t) &= -e^{-t} 10^{4.8} y^3,
\end{align*}
\]

(5.25)

where

\[
f(x, y, t) = \exp(-t)[-x^{4.8} y^3 + 4.8 \nu_1 x^{3.8} y^3 + 3 \nu_2 x^{4.8} y^2 - d_1 \frac{\Gamma(5.8)}{\Gamma(5.8 - \alpha)} x^{4.8 - \alpha} y^3
\]

\[-d_2 \frac{\Gamma(4)}{\Gamma(4 - \beta)} x^{4.8} y^{3 - \beta}]

The exact solution of the forward problem is \( c(x, y, t) = e^{-t} x^{4.8} y^3 \) and the flux is \( \frac{\partial c(x, y, t)}{\partial t} = -e^{-t} x^{4.8} y^3 \).

1. **Estimating \( \nu_1, \nu_2, d_1 \) and \( d_2 \) when \( \alpha \) and \( \beta \) are known**

   In this part, we assume that the differentiation orders \( \alpha \) and \( \beta \) are known and we estimate \( \nu_1, \nu_2, d_1 \) and \( d_2 \). We set the exact values of the average velocities as \( \nu_1 = 0.2 \) and \( \nu_2 = 0.5 \), the dispersion coefficients \( d_1 = 1 \) and \( d_2 = 0.8 \), the differentiation orders \( \alpha = 1.5 \) and \( \beta = 1.6 \). In Figure 5.2, the estimated values of \( \nu_1, \nu_2, d_1 \), and \( d_2 \) when adding a white Gaussian noise with \( \sigma = 2\% \) to the measurements.

2. **Estimating \( \nu_1, \nu_2, d_1, d_2, \alpha \) and \( \beta \)**
Figure 5.2: The estimated parameters with 2% stationary noise case with $\Delta x = \frac{1}{50}$

Figure 5.3: Relative errors for different integration interval

Table 5.1: $\nu_1 = 0.5$, $\nu_2 = 0.3$ $d_1 = 1$, $d_2 = 0.8$, $\alpha = 1.5$, $\beta = 1.6$, and $\Delta x = \frac{1}{50}$, $\sigma = 0.05$

<table>
<thead>
<tr>
<th>Number of modulating functions</th>
<th>Relative errors</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$(|\nu_1 - \hat{\nu}_1|_2, |\nu_2 - \hat{\nu}_2|_2, |\hat{d}_1 - \hat{d}_1|_2, |\hat{d}_2 - \hat{d}_2|_2, |\alpha - \hat{\alpha}|_2, |\beta - \hat{\beta}|_2)$</td>
</tr>
<tr>
<td>5</td>
<td>(0.025, 0.034, 0.012, 0.011, 0.004, 0.004)</td>
</tr>
<tr>
<td>6</td>
<td>(0.032, 0.043, 0.015, 0.014, 0.005, 0.006)</td>
</tr>
<tr>
<td>7</td>
<td>(0.041, 0.054, 0.019, 0.017, 0.006, 0.007)</td>
</tr>
<tr>
<td>8</td>
<td>(0.051, 0.067, 0.023, 0.022, 0.008, 0.009)</td>
</tr>
<tr>
<td>9</td>
<td>(0.063, 0.082, 0.023, 0.026, 0.009, 0.010)</td>
</tr>
<tr>
<td>10</td>
<td>(0.077, 0.099, 0.035, 0.032, 0.011, 0.012)</td>
</tr>
</tbody>
</table>

In this part, we will use the combined Newton’s and modulating functions method to estimate all parameters simultaneously. We set the exact values of the average velocities $\nu_1 = 0.5$, $\nu_2 = 0.3$, and the dispersion coefficients $d_1 = 1$ and $d_2 = 0.8$, the differentiation orders $\alpha = 1.5$ $\beta = 1.6$, the final time $T = 1$, the initial guess $z_0 = (\alpha_o, \beta_o) = (1.2, 1.2)$. As we see in Table 5.1, the results are satisfactory even with different number of modulating functions.
5.6 Chapter Summary

We successfully generalized the combined modeling functions method to estimate the coefficients and the differentiation orders for a 2D space FADE. To overcome the difficulties when moving to the 2D model some adjustments have been made to the 1D algorithm. First, more sets of modulating functions have been used. Second, the unknown coefficients have been represented in terms of two variables and their derivatives were computed with respect to two variables. As a result, the parameter estimation problem has been solved with respect to two unknowns. Finally, instead of computing the gradient of the cost function, the Jacobian matrix has been analytically computed. Numerical simulations have been performed and the results have shown the effectiveness of the proposed algorithm.
Part II
Chapter 6

Inverse Source Problem for the
Space FADE

6.1 Introduction

We will theoretically and numerically study an inverse source problem for a space FADE on a bounded domain, where we aim to recover the unknown source from the concentration measurement at a final time.

Progress has been made on the direct problem for different types of fractional advection-dispersion equations [46, 47, 48, 49, 22]. While, few studies have considered the inverse problem.

The inverse source problem of the space FADE has been considered by Chi et al. [18] where they solved the problem numerically in the presence and in the absence of noise using an optimal perturbation regularization algorithm. However, the stability of the proposed method depends on the initial guess and the choice of some base functions.

In this chapter, we will study the uniqueness and the stability of the inverse source problem. In addition, a numerical method based on the Tikhonov regularization will be presented. Finally, we illustrate the results with a numerical example.
6.2 Inverse Source Problem

Our inverse problem consists of estimating the source for the space FADE given in (3.10) using the measurement of the concentration given in (3.67). We consider the Riesz-Feller fractional derivative of order $\alpha$, defined as in (2.13). We start from the solution given in Theorem 3.3.1 of the direct problem of the space FADE given in (3.15), which shows that the operator relating the unknown source to the final observation is linear which simplifies the analysis of the properties of the inverse problem and its numerical solution.

In this section, we study the uniqueness and the stability of the Inverse Source Problem (ISP) consisting in the estimation of the source from the knowledge of the concentration at time $t = T$:

$$f = K(g_T).$$  \hspace{2cm} (ISP)

**Proposition 6.2.1.** Consider the system given in (3.15) and assume that $f,g_0 \in L^2(\mathbb{R})$, then $f$ is the solution of the following equation:

$$\int_{-\infty}^{+\infty} \left\{ \int_0^T G_\alpha^{\alpha}(x - y, T - \tau) d\tau \right\} f(y) dy = h(x),$$  \hspace{2cm} (6.1)

where

$$h(x) := g_T(x) - \int_{-\infty}^{+\infty} G_\alpha^{\alpha}(x - y, T) g_0(y) dy.$$  \hspace{2cm} (6.2)

**Proof.** The proof can be obtained by substituting (3.67) into (3.39). \hfill \Box

Now, we will study the uniqueness and the stability of the inverse problem.
6.2.1 Uniqueness

In the next Theorem, we prove the unique determination of the source term from given measurements at a specific or a final time.

**Theorem 6.2.1.** Let \( u_1(\cdot, T) \) and \( u_2(\cdot, T) \) be solutions of (3.15) with sources \( f_1 \) and \( f_2 \), respectively. Then, the condition \( u_1(\cdot, T) = u_2(\cdot, T) \) implies that \( f_1 = f_2 \) almost everywhere.

**Proof.** Let \( u_1(x, T) = u_2(x, T) \). Since \( u_1 \) and \( u_2 \) are solutions of (3.15), then using (3.36) we get:

\[
u_1(x, T) - u_2(x, T) = \frac{1}{2\pi} \int_0^T \int_{-\infty}^{+\infty} \hat{G}_\alpha^d(k, T - \tau)[\hat{f}_1(k) - \hat{f}_2(k)]e^{-ikx} dk d\tau, \quad (6.3)
\]

which is equivalent to:

\[
0 = \frac{1}{2\pi} \int_0^T \int_{-\infty}^{+\infty} \hat{G}_\alpha^d(k, T - \tau)[\hat{f}_1(k) - \hat{f}_2(k)]e^{-ikx} dk d\tau. \quad (6.4)
\]

By applying the Fourier transform, we get:

\[
\int_0^T \hat{G}_\alpha^d(k, T - \tau)d\tau [\hat{f}_1(k) - \hat{f}_2(k)] = 0. \quad (6.5)
\]

Computing the following integration gives us:

\[
\int_0^T \hat{G}_\alpha^d(k, T - \tau)d\tau = \frac{1}{(i\nu k - d\psi_\theta^\alpha(k))} \left[e^{(i\nu k - d\psi_\theta^\alpha(k))T} - 1\right]. \quad (6.6)
\]

Therefore, equation (6.5) holds if and only if

\[
\frac{1}{(i\nu k - d\psi_\theta^\alpha(k))} \left[e^{(i\nu k - d\psi_\theta^\alpha(k))T} - 1\right] = 0 \iff (i\nu k - d\psi_\theta^\alpha(k))T = 0, \quad (6.7)
\]
which implies that:

\[ Re(\imath \nu k - d \psi^\alpha(\kappa)) = 0, \quad \text{and} \quad Im(\imath \nu k - d \psi^\alpha(\kappa)) = 0. \]  

(6.8)

The real part

\[ Re(\imath \nu k - d \psi^\alpha(\kappa)) = 0, \]  

(6.9)

if

\[ \nu k \pm d|k|^\alpha \sin \theta \pi /2 = 0. \]  

(6.10)

Then either \( k = 0 \), or \( \theta = 1 \), but \( \theta \neq 1 \), since \( \theta \leq 2 - \alpha \) and \( \alpha > 1 \).

The imaginary part

\[ Im(\imath \nu k - d \psi^\alpha(\kappa)) = 0, \]  

(6.11)

if

\[ \nu k \pm d|k|^\alpha \sin \theta \pi /2 = 0, \]  

(6.12)

\[ \Rightarrow \begin{cases} k = 0 \\ \eta(k) := \frac{|k|^\alpha}{k} = \mp \frac{\nu}{d \sin(\theta \pi /2)} \end{cases}. \]  

(6.13)

This implies that:

\[ \int_0^T \hat{G}^\theta_\alpha(k, T - \tau) d\tau \neq 0, \quad \forall k \in \mathbb{R}. \]  

(6.14)

Therefore

\[ \hat{f}_1(k) - \hat{f}_2(k) = 0, \]  

(6.15)

which completes the proof.
6.2.2 Stability

In this subsection, we show that the third Hadamard condition [23], is not satisfied, i.e. an arbitrarily small error in the measurement data leads to a large error in the solution [23]. To prove this instability, we show that a bounded perturbation in the source will not affect the final observation of the concentration [23].

**Theorem 6.2.2.** The inverse problem ISP is not stable in the sense of Hadamard.

*Proof.* If we perturb $f$ in the $L^2$ norm $\| \cdot \|_2$ by a bounded perturbation (we can, for example, perturb $f$ by $\delta_n(x) = A \sin(\frac{n\pi x}{L})$), then the error of the solution (with respect to the $\| \cdot \|_2$) is

$$
\| f^{\delta_n}(x) - f(x) \|_2^2 = \| f(x) + A \sin(\frac{n\pi x}{L}) - f(x) \|_2^2
= \| A \sin(\frac{n\pi x}{L}) \|_2^2 = \int_0^L A^2 \sin^2(\frac{n\pi x}{L}) dx = \frac{1}{2} A^2 L \neq 0.
$$

(6.16)

Thus

$$
\| f^{\delta_n}(x) - f(x) \|_2^2 \to \frac{1}{2} A^2 L \quad \text{as} \quad n \to \infty
$$

(6.17)

Now, if we assume that $u$ and $u^{\delta_n}$ are solutions of (3.15) with sources $f$ and $f^{\delta_n}$ respectively, then the error of the data is

$$
\| u^{\delta_n}(x, T) - u(x, T) \|_2^2 = \left\| \int_{-\infty}^{+\infty} \left\{ \int_0^T G_\alpha^a(x - y, T - \tau) d\tau \right\} [f^{\delta_n}(y) - f(y)] dy \right\|_2^2
$$

$$
= \left\| \int_{-\infty}^{+\infty} \left\{ \int_0^T G_\alpha^a(x - y, T - \tau) d\tau \right\} [A \sin(\frac{n\pi y}{L})] dy \right\|_2^2.
$$

(6.18)

Applying the Riemann-Lebesgue lemma we get [50]:

$$
\lim_{n \to \infty} \| u^{\delta_n}(x, T) - u(x, T) \|_2^2 = 0,
$$

(6.19)
which means that the error in the solution is a constant when the error in the data tends to zero. Thus the solution does not depend continuously on the data. Therefore, the problem is not stable.

\[ \square \]

### 6.3 Numerical Analysis

In this section, we present a numerical solution to reconstruct the source term for the space-fractional advection-dispersion equation (3.10) from the measurement \( c(\cdot, T) \). Due to the instability of the inverse problem the Tikhonov regularization will be used.

Recall from chapter 3 that the matrix form of the finite difference scheme for the solution of the direct problem is given by:

\[
[(I - G - L) + V]C^{j+1} = C^j + R
\]  

(6.21)

where \( G, L, V, R \) and \( C^{j+1} \) are defined in (3.58), (3.59), (3.60), (3.61) and (3.62) respectively.

Let \( A = [(I - G - L) + V]^{-1} \), then equation (6.21) can be written as:

\[
C^{j+1} = A(C^j + R).
\]  

(6.22)

By induction, we get the following equation:

\[
C^N - A^N C^0 = (I - A)^{-1}(I - A^N)AR,
\]  

(6.23)

which can be written in the following form:

\[
Y = KR,
\]  

(6.24)
where

\[ K = (I - A)^{-1}(I - A)^N A, \]  

(6.25)

and

\[ Y = C^N - A^N C^0. \]  

(6.26)

In order to estimate the unknown source, we propose to minimize the following cost function with the Tikhonov regularization:

\[ J_\lambda(R) = \|Y - KR\|^2 + \lambda \Omega(R), \]  

(6.27)

where \( Y \) is the observation and \( \Omega(R) = \left\| \frac{d^m R}{dx^m} \right\|^2 \) with \( m = 0, 1 \) is a stabilization functional of \( R \) which usually includes a priori information on the problem. The regularization parameter \( \lambda \) can be determined using the L-curve [23].

### 6.3.1 Numerical Simulations

Let us consider the following space-fractional advection-dispersion equation:

\[ \frac{\partial c(x,t)}{\partial t} = -0.3 \frac{\partial c(x,t)}{\partial x} + 3 \frac{\partial^{1.5} c(x,t)}{\partial x^{1.5}} + r(x), \quad 0 < x < 7, \quad t > 0, \]  

(6.28)

with the following initial and Dirichlet boundary conditions:

\[
\begin{aligned}
&c(x, 0) = 0, \\
&c(0, t) = 0, \\
&c(7, t) = 0.
\end{aligned}
\]  

(6.29)

In this example, we assume that the source term \( r(x) = 5 \sin \frac{2\pi}{7} x \) is unknown.

Figure 6.1, represents the numerical solution of (6.28) with the conditions (6.29)
at time $T = 1$, which will be used as the exact solution when recovering the source term numerically.

Figure 6.1: Numerical solution of the direct problem.

Figure 6.2: Solution of the inverse problem without noise.

Figure 6.2, represents the approximated solution $r^0$ of the inverse problem without regularization in noise free case. As we can see, if we have the exact measurement (i.e. without noise) then, the numerical solution matches the approximated solution. While, recovering the source term from noisy measurements is severely ill-posed (see Figure 6.3).

In Figure 6.3, a comparison of the approximated solutions with and without regularization, between the exact source term and the approximated $r^\lambda$ is given, where
Figure 6.3: Solution of the inverse problem with and without regularization with 5% noisy measurements.

Figure 6.4: The exact and the regularized solution with different noise levels.
the stabilization functional is \( \Omega(R) = \|R\|^2 \). Clearly from the figure, the presence of noise in the data affects greatly the reconstruction and with the use of the Tikhonov regularization the numerical results are quite satisfactory.

In Figure 6.4, comparisons under different noise levels 1\%, 2\% and 5\%, between the exact source term and the approximated \( r^\lambda \) are given. In all three cases, the results are stable and reasonable, which are further confirmed by the errors in Table 6.1.

As shown in Figure 6.4, the Tikhonov regularization with \( \Omega(R) = \|R\|^2 \) produces a stable solution, but the solution is not smooth enough. Therefore, we minimized the cost function given in (6.27) with

\[
\Omega(R) = \left\| \frac{dR}{dx} \right\|_2^2,
\]

which produces a smooth solution (see Figures 6.5 and 6.6). Better results obtained using (6.30) is due to regularity of the source term considered. Thus, minimizing (6.27) with the stabilization functional given in (6.30) will force the solution to be smooth.

In Tables 6.1, the relative errors of the approximated source term \( r^\delta \) to the exact source \( r \) are given. It can be seen that the smaller the noise level, the better the approximative effect.

Table 6.1: The relative errors with different stabilizing functional \( \Omega(R) \) when: \( N = 100, \theta = 0.5 \).

<table>
<thead>
<tr>
<th>Noise level</th>
<th>( \Omega(R) = |R|^2 )</th>
<th>( \Omega(R) = |R^\prime|^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1%</td>
<td>16.66%</td>
<td>3.96%</td>
</tr>
<tr>
<td>2%</td>
<td>21.69%</td>
<td>5.23%</td>
</tr>
<tr>
<td>3%</td>
<td>21.67%</td>
<td>6.14%</td>
</tr>
</tbody>
</table>
Figure 6.5: Exact solution and the regularization solution with 5% noisy measurement.

Figure 6.6: The exact and the regularized solution with different noise levels.
6.4 Chapter Summary

In this chapter, we have analyzed the mathematical properties of recovering the source term for a space-fractional advection-dispersion equation. We have proved the unique determination of the source term from a final observation. Moreover, we have analytically showed that the inverse source problem is ill-posed due to the lack of stability requirements. Furthermore, we have presented a numerical solution using the Tikhonov-based optimization technique. However, to overcome some of the optimization limitations other approaches should be considered. Therefore, in the next chapter we propose to use the modulating functions method to estimate the source term and compare the method to the standard Tikhonov-based optimization technique.
Chapter 7

Inverse Source Problem Using Modulating Functions

7.1 Introduction

In this chapter, we aim to adopt the modulating functions method for estimating the source term for the space FADE using different measurements. We propose to compare the proposed modulating functions method to a standard optimization technique, based on Tikhonov regularization. We illustrate the results by numerical simulations and discuss the performance of both methods and focus on the choice of the design parameters.

7.2 Problem Statement

We consider the space-fractional advection-dispersion equation given in (1.1) with initial and Dirichlet boundary conditions in (1.2). We assume that $\nu$ and $d$ are constants and the source term depends only on $x$. The fractional derivative $\frac{\partial^\alpha}{\partial x^\alpha}$ is a Riemann-Liouville derivative of order $\alpha$ defined as in (2.8). Then, equation (1.1) will
have the following form: for any \(0 < x < L\) and \(t > 0\),

\[
\begin{cases}
\frac{\partial c(x, t)}{\partial t} = -\nu \frac{\partial c(x, t)}{\partial x} + d \frac{\partial^\alpha c(x, t)}{\partial x^\alpha} + r(x), \\
c(x, 0) = g_0(x), \quad 0 < x < L \\
c(0, t) = 0, \quad t \geq 0 \\
c(L, t) = 0, \quad t \geq 0
\end{cases}
\] (7.1)

We would like to estimate the unknown source \(r(x)\) using two different types of measurements. First, the measurements of the concentration \(c\) and the flux \(\frac{\partial c}{\partial t}\) given in (3.65). Then, we will use the measurements of the concentration \(c\) given in (3.67).

### 7.2.1 Modulating Function Method to Estimate \(r(x)\)

In this section, we apply the modulating functions method to estimate the source for the considered space-fractional advection-dispersion equation.

Assuming that \(\{f_k(x)\}_{k=1}^\infty\) is a set of basis functions where source term \(r(x)\) can be written as:

\[
\hat{r}(x) = \sum_{k=1}^{\infty} a_k f_k(x),
\] (7.2)

which can be approximated by:

\[
\hat{r}(x) \approx \sum_{k=1}^{K} a_k f_k(x).
\] (7.3)

Then, the source estimation problem is transferred into determining the coefficients \(\{a_k\}_{k=1}^{K}\). There are a number of commonly used basis functions, for example, Polynomial basis, Spline basis, and Fourier basis [18, 51, 52]. In the numerical simulations, we will use the shifted Jacobi orthogonal polynomial basis define in Definition (2.1.2).

In the next proposition, the modulating functions method is applied to determine the unknown coefficients \(\{a_k\}_{k=1}^{K}\) using the measurements given in (3.65).
Proposition 7.2.1. Let \( \{\phi_m\}_{m=1}^M \) be a set of modulating functions of at least order 2 defined on the interval \([0, L_1]\) where \( L_1 \leq L \) and \( M \geq K \). Then, the unknown source \( r \) can be estimated, using the measurements given in (3.65) as follows:

\[
\tilde{r}(x) = \sum_{k=1}^K a_k f_k(x). \tag{7.4}
\]

The estimations of the parameters \( \{a_k\}_{k=1}^K \) are the solution of the following linear system:

\[
\begin{pmatrix}
A_{11} & A_{12} & \cdots & A_{1K} \\
A_{21} & B_{22} & \cdots & A_{2K} \\
\vdots & \vdots & \ddots & \vdots \\
A_{M1} & B_{M2} & \cdots & A_{MK}
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_K
\end{pmatrix}
= \begin{pmatrix}
B_1 \\
B_2 \\
\vdots \\
B_M
\end{pmatrix}, \tag{7.5}
\]

where for \( m = 1, \ldots, M, \ k = 1, \ldots, K, \)

\[
A_{mk} = \int_0^{L_1} \phi_m(L_1 - x) f_k(x) \, dx, \tag{7.6}
\]

\[
B_m = -d \int_0^{L_1} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} c(L_1 - x, t) \, dx \nonumber \\
+ \nu \int_0^{L_1} \frac{\partial \phi_m(L_1 - x)}{\partial x} c(x, t) \, dx \\
+ \int_0^{L_1} \phi_m(L_1 - x) \frac{\partial c(x, t)}{\partial t} \, dx. \tag{7.7}
\]

**Proof.** Let \( \{\phi_m(x)\}_{m=1}^M \) be a set of \( M \) modulating functions of at least order 2 and consider the equation given in (7.1). Then by multiplying the modulating functions \( \phi_m(L_1 - \cdot) \) for \( m = 1, \ldots, M \) to (7.1) and by integrating over the interval \([0, L_1]\), we get:
\[ \int_0^{L_1} r(x)\phi_m(L_1-x) \, dx = \int_0^{L_1} \phi_m(L_1-x) \frac{\partial c(x,t)}{\partial t} \, dx + \nu \int_0^{L_1} \frac{\partial c(x,t)}{\partial x} \phi_m(L_1-x) \, dx \]

\[ -d \int_0^{L_1} \frac{\partial^\alpha c(x,t)}{\partial x^\alpha} \phi_m(L_1-x) \, dx. \]

(7.8)

Applying integration by parts and Lemma 4.2.1 gives:

\[ \int_0^{L_1} r(x)\phi_m(L_1-x) \, dx = \]

\[ \int_0^{L_1} \phi_m(L_1-x) \frac{\partial c(x,t)}{\partial t} \, dx + \nu \int_0^{L_1} \frac{\partial \phi_m(L_1-x)}{\partial x} c(x,t) \, dx \]

\[ -d \int_0^{L_1} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} c(L_1-x,t) \, dx, \]

(7.9)

where the boundary conditions are eliminated by the property of the used modulating functions. Finally, substituting (7.3) into (7.9) gives:

\[ \sum_{k=1}^{K} a_k \int_0^{L_1} \phi_m(L_1-x)f_k(x) \, dx = \]

\[ \int_0^{L_1} \phi_m(L_1-x) \frac{\partial c(x,t)}{\partial t} \, dx + \nu \int_0^{L_1} \frac{\partial \phi_m(L_1-x)}{\partial x} c(x,t) \, dx \]

\[ -d \int_0^{L_1} \frac{\partial^\alpha \phi_m(x)}{\partial x^\alpha} c(L_1-x,t) \, dx. \]

(7.10)

Consequently, the unknown coefficients \( \{a_k\}_{k=1}^{K} \) can be estimated by solving the linear system given in (7.5).

Remark 7.2.1. In the next proposition the source term will be estimated using the concentration measurement only, given in (3.67). In this case we need to apply the modulating functions method using a space and time dependent sets of modulating functions.
Proposition 7.2.2. Let $\{\phi_m\}$ and $\{\psi_m\}_{m=1}^M$ be two sets of modulating functions of at least order 2 defined on the intervals $[0, L_1]$ and $[0, T_1]$ respectively, where $L_1 \leq L$, $T_1 \leq T$ and $M \geq K$. Then, the unknown source $r$ can be estimated, using the measurement given in (3.67) as follows:

$$
\tilde{r}(x) = \sum_{k=1}^{K} a_k f_k(x).
$$

(7.11)

The estimations of the parameters $\{a_k\}_{k=1}^K$ are the solution of the following linear system:

$$
\begin{pmatrix}
A_{11} & A_{12} & \cdots & A_{1K} \\
A_{21} & A_{22} & \cdots & A_{2K} \\
\vdots & \vdots & \ddots & \vdots \\
A_{M1} & B_{M2} & \cdots & A_{MK}
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_K
\end{pmatrix}
= 
\begin{pmatrix}
B_1 \\
B_2 \\
\vdots \\
B_M
\end{pmatrix},
$$

(7.12)

where for $m = 1, \ldots, M$, $k = 1, \ldots, K$,

$$
A_{mk} = -\int_0^T \int_0^{L_1} f_k(x) \psi_m(t) \phi_m(L_1 - x) dx dt,
$$

(7.13)

$$
B_m = -\nu \int_0^{T_1} \int_0^{L_1} \psi_m(t) \frac{\partial \phi_m(L_1 - x)}{\partial x} c(x, t) dx dt \\
+ d \int_0^{T_1} \int_0^{L_1} \psi_m(t) \frac{\partial^a \phi_m(x)}{\partial x^a} c(L_1 - x, t) dx dt \\
+ \int_0^{T_1} \int_0^{L_1} \psi_m(t) \frac{\partial \psi_m(t)}{\partial t} \phi_m(L_1 - x) c(x, t) dx dt,
$$

(7.14)

Proof. The proof can be obtained similarly as explained in proposition 4.6.1. □
7.2.2 Optimization Methods: Tikhonov Regularization

We aim to compare the modulating functions method to standard optimization techniques. Since the process of computing inverse solutions are often extremely unstable and a regularization technique is needed to stabilize the solution, we propose to use the standard Tikhonov regularization and minimize the following cost function:

\[ J_\lambda(A) = \| Y - KA \|^2 + \lambda \| A \|^2, \tag{7.15} \]

where the regularization parameter \( \lambda \) can be determined using the L-curve or the GCV [53, 23].

In order to define \( Y, A \) and the operator \( K \) we discretize equation (7.1) using a finite difference scheme, where the fractional derivative is discretized using the shifted Grunwald formula defined in (2.5). Then the discrete form of (7.1) is:

\[ \frac{\partial c_i^j}{\partial t} = -\nu \frac{c_i^j - c_{i-1}^j}{\Delta x} + d \delta_{\alpha,x} c_i^j + \sum_{k=1}^{K} a_k P_k(x_i), \tag{7.16} \]

where the source term \( r(x) \) is approximated by (7.4).

Which can be written as:

\[ \frac{\partial c_i^j}{\partial t} - d \delta_{\alpha,x} c_i^j + \frac{1}{\Delta x} \nu (c_i^j - c_{i-1}^j) = \sum_{k=1}^{K} a_k P_k(x_i), \tag{7.17} \]

where

\[ \delta_{\alpha,x} c_i^j = \frac{1}{(\Delta x)^{\alpha}} \sum_{k=0}^{i+1} \xi_{\alpha,k} c_{i-k+1}^j, \tag{7.18} \]

for \( i = 1, \ldots, N - 1 \) and \( j = 0, 1, 2, \ldots, N - 1 \) with \( t_j = j \Delta t, x_i = i \Delta x, c_i^j = c(x_i, t_j) \), \( c_0^j = 0, c_N^j = 0 \) and \( \xi_{\alpha,k} \) is the normalized Grunwald weight defined by:

\[ \xi_{\alpha,k} = \frac{\Gamma(k - \alpha)}{\Gamma(-\alpha) \Gamma(k + 1)}. \tag{7.19} \]
Thus, the matrix form of the implicit finite difference scheme (7.17) is given by:

\[ D^j + [F + V]C^j = PA \]  \hspace{1cm} (7.20)

where

\[
PA = \begin{pmatrix}
\begin{array}{cccc}
P_1(x_1) & P_2(x_1) & \cdots & P_K(x_1) \\
P_1(x_2) & P_2(x_2) & \cdots & P_K(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
P_1(x_N) & P_2(x_N) & \cdots & P_K(x_N)
\end{array}
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_K
\end{pmatrix},
\]  \hspace{1cm} (7.21)

\[
F(l, n) = -\frac{d}{(\Delta x)^\alpha} \begin{cases}
\xi_{\alpha,n+1} & \text{if } n \geq l + 1, \\
\xi_{\alpha,1} & \text{if } n = l, \\
\xi_{\alpha,0} & \text{if } n = l - 1, \\
0 & \text{else},
\end{cases}
\]  \hspace{1cm} (7.22)

\[
V(l, n) = \frac{v}{\Delta x} \begin{cases}
1 & \text{if } n = l, \\
-1 & \text{if } l = n - 1, \\
0 & \text{else},
\end{cases}
\]  \hspace{1cm} (7.23)

\[
C^j = [c_1^j, c_2^j, \ldots, c_{N-1}^j]^T, \hspace{1cm} (7.24)
\]

\[
D^j = \frac{\partial}{\partial t} [c_1^j, c_2^j, \ldots, c_{N-1}^j]^T. \hspace{1cm} (7.25)
\]

Then at a final time T, we get

\[ D^N + [F + V]C^N = PA \]  \hspace{1cm} (7.26)

Using the measurements given in (3.67), Equation (7.26) can be written in the
following form:

\[ C^N = K[PA - D^N] \]  \hfill (7.27)

where \( C^N \) and \( D^N \) are the measurements at the final time and \( K = [F + V]^{-1} \).

In order to estimate the source term, we minimize the following cost function with Tikhonov regularization [23].

\[ J_\lambda(A) = \|KP[A] - KD^N - C^N\|_2^2 + \lambda \|A\|^2. \]  \hfill (7.28)

The above equation will be used to estimate the source when using the measurements of the concentration and the flux given in (3.65). However, when using the measurement of the concentration only the backward Euler method, which is defined as follow will be used to discretize the time derivative:

\[ \frac{\partial c(x,t)}{\partial t} = \frac{c^{j+1} - c^j}{\Delta t} \]  \hfill (7.29)

where \( \Delta t \) is the time step.

Therefore, the discrete form of (7.1) will be

\[ \frac{c^{j+1}_i - c^j_i}{\Delta t} = -\nu \frac{(c^{j+1}_i - c^{j+1}_{i-1})}{\Delta x} + d_i \delta_{\alpha,x}c^j_i + \sum_{k=1}^{K} a_k P_k(x_i), \]  \hfill (7.30)

with \( t_j = j\Delta t \), \( x_i = i\Delta x \), \( c^j_i = c(x_i, t_j) \), \( c^j_0 = 0 \), and \( c^j_N = 0 \).

Which can be written as:

\[ (1 - d\Delta t\delta_{\alpha,x})c^{j+1}_i + \frac{\Delta t}{\Delta x} \nu (c^{j+1}_i - c^{j+1}_{i-1}) = c^j_i + \sum_{k=1}^{K} a_k P_k(x_i)\Delta t; \]  \hfill (7.31)

\[ i = 1, \ldots, N - 1 \) and \( j = 1, 2, \ldots \)

where \( \delta_{\alpha,x}c^j_i \) is defined in (7.18).
Thus, the matrix form of the implicit finite difference scheme (7.31) is given by:

\[
[(I + \Delta t(F + V))]C^{j+1} = C^j + PA,\]  

(7.32)

for \(n = 1, 2, \ldots, N - 1\) and \(m = 1, 2, \ldots, N - 1\), where \(F, V\) and \(PA\) are defined as in (7.22), (7.23) and (7.21), respectively and \(C^{j+1} = [c_1^{j+1}, c_2^{j+1}, \ldots, c_{N-1}^{j+1}]^T\).

Now, to solve the inverse source problem, we propose to write the problem in the form (2.25). Therefore, we will start by defining the operator \(K\).

Let \(G = [(I + \Delta t(F + V))]^{-1}\), then equation (7.32) can be written as:

\[
C^{j+1} = A(C^j + PA),\]  

(7.33)

by induction we can get the following:

\[
C^{N+1} - (A)^{N+1}C^0 = (I - A)^{-1}(I - (A)^{N+1})APX,\]  

(7.34)

which can be written in the following form:

\[
Y = KA\]  

(7.35)

where

\[
K_{(N-1) \times (N-1)} = (I - A)^{-1}(I - (A)^{N+1})AP\]  

(7.36)

and

\[
Y = C^{N+1} - (A)^{N+1}C^0.\]  

(7.37)

In order to solve the inverse problem and estimate the unknown source, we propose to use the Tikhonov regularization. Then according to (2.35) we need to minimize the following cost function:
\[ J_\lambda(A) = \| Y - KA \|_2^2 + \lambda \| A \|_2^2, \]  
where \( Y \) is the observation.

Now, we will find \( \text{argmin}_F J \) which is the value of \( A \) when, \( \frac{dJ_\lambda(F)}{dA} = 0 \).

\[
\frac{dJ_\lambda(A)}{dA} = -2K^*(Y - KA) + 2\lambda A
\]  
\[
= -2K^*Y + 2K^*KA + 2\lambda A
\]  
\[
= -2K^*Y + 2(K^*K + \lambda I)A. \]  
\[
\frac{dJ_\lambda(A)}{dA} = 0 \iff -2K^*Y + 2(K^*K + \lambda I)A = 0. \]

\[
\iff A = (K^*K + \lambda I)^{-1}K^*Y. \]

Therefore, the solution of \( \text{argmin}_F J \) is given by [23]:

\[ \hat{A} = (K^*K + \lambda I)^{-1}KY. \]

The regularization parameter \( \lambda \) is determined using the L-curve.

### 7.2.3 Numerical Simulations

In this subsection, some numerical results, showing the efficiency and the robustness of the modulating functions method, are presented. We consider the space-fractional advection-dispersion equation given in equation (7.1) and we assume that the unknown source term is \( r(\cdot) = \sin(\frac{\pi}{L} \cdot) \). The value of \( t \) for the measurements given in
(3.65) and (3.67), are taken at the time where the source is estimated. Since it is difficult to find the exact analytical solution of (7.1), we use finite difference scheme based on the shifted Grünwald formula given in (2.7) combined with a finite difference scheme in time, to obtain the measurements given in (3.65) and (3.67). We consider the following polynomial modulating functions whose fractional derivatives are simple to calculate: \( \phi_m(\cdot) = (\cdot)^{M+b+1-m}(L_1 - \cdot)^b+m \), where \( b = 3, \ m = 1, 2, \ldots, M \), and \( M \) is the number of modulating functions [36]. Moreover, we apply the trapezoidal rule to numerically approximate the integrals obtained in Proposition 7.2.1.

For the series expansion of the source given in (7.3), we consider the shifted Jacobi orthogonal polynomial \( P_n^{(\mu, \kappa)}(\cdot) \) as the basis function, that is defined on \([0,1]\) as follows [19]:

\[
P_n^{(\mu, \kappa)}(x) := \sum_{j=0}^{n} \left( \frac{n + \mu}{j} \right) \left( \frac{n + \kappa}{n - j} \right) (x - 1)^{n-j} x^j,
\]

with \( \mu, \kappa \in ]-1, \infty[ \).

**Example 7.2.1.** In this example, we use the measurements of the concentration and the flux at final time \( T \). We set the average velocity \( \nu = 0.5 \), the dispersion coefficient \( d = 1 \), the differentiation order \( \alpha = 1.6 \), \( L_1 = L = 9 \), \( \Delta x = \frac{1}{100} \), and \( K = 6 \). Moreover, we take \( \mu = \kappa = 0.5 \) in the Jacobi polynomial basis. Figure 7.1 represents the estimated source when using 6 modulating functions \( (M = 6) \). A 1% and a 3% white gaussian noise were added to the measurements, respectively, where the standard deviation is adjusted such that the relative error of the concentration and the flux measurements: \( \frac{\|g_1 - g_1^\dagger\|}{\|g_1\|} \times 100\% \) and \( \frac{\|g_2 - g_2^\dagger\|}{\|g_2\|} \times 100\% \) are equal to the noise level.

The relative errors obtained by different numbers of modulating functions are given in Figure 7.2, where a 3% white gaussian noise is added to the measurements. The results are satisfactory even with different numbers of modulating functions. Moreover, according to Table II, the modulating functions method is robust against noises.
Figure 7.1: The exact and the estimated sources using the modulating functions method with different noise levels.

Figure 7.2: The relative errors with different numbers of modulating functions.

Table 7.1: The relative errors using the modulating functions method.

<table>
<thead>
<tr>
<th>Noise level</th>
<th>Relative Error: $\frac{|r - r^\parallel}{|r|}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1%</td>
<td>0.027245929322316</td>
</tr>
<tr>
<td>3%</td>
<td>0.036223635806968</td>
</tr>
<tr>
<td>5%</td>
<td>0.068071934193359</td>
</tr>
<tr>
<td>10%</td>
<td>0.157435207543781</td>
</tr>
</tbody>
</table>
Table 7.2: The relative errors $\|r-r^d\|_2/\|r\|_2$ with different noise levels.

<table>
<thead>
<tr>
<th>Noise level</th>
<th>Modulating Functions=15</th>
<th>Tikhonov Regularization</th>
</tr>
</thead>
<tbody>
<tr>
<td>1%</td>
<td>0.028259347437407</td>
<td>0.046557583351492</td>
</tr>
<tr>
<td>3%</td>
<td>0.035887236848630</td>
<td>0.052646581046958</td>
</tr>
<tr>
<td>5%</td>
<td>0.061714020509659</td>
<td>0.060190460392725</td>
</tr>
</tbody>
</table>

Example 7.2.2. In this example, the measurements of the concentration and the flux at final time $T$ were used to estimate the source $r(x)$. We set $\nu = 0.7$, $d = 2$, $\alpha = 1.2$, $L_1 = L = 9$, $\Delta x = \frac{1}{100}$, $\mu = \kappa = 0.5$, $\Delta x = \frac{1}{100}$ and $K = 6$. A comparison between the estimated sources obtained using the modulating functions method and the Tikhonov regularization is given in Figure 7.3, where the noise level is 3%. The regularization parameter $\lambda$ is obtained using the GCV and we set the number of modulating functions as $M = 12$. Table 7.2 represents the relative errors with different noise levels. Hence, we can see that the results are satisfactory with both methods. However, it is noted that the accuracy of both methods depends on the design parameter: the regularization parameters $\lambda$ for the Tikhonov regularization, the number of modulating functions $M$ for the modulating functions method.

Figure 7.3: The exact source and the estimated source using 15 polynomial modulating functions and the Tikhonov regularization with 3% noise levels.
Example 7.2.3. In this example, we use the measurement of the concentration only to estimate the source term. We set \( r(x) = \sin\left(\frac{\pi x}{L}\right) \), \( \nu = 0.3 \), \( d = 0.5 \), \( \alpha = 1.2 \), \( L_1 = L = 10 \), \( \Delta x = \frac{1}{15} \), \( \mu = \kappa = 0.5 \) and \( K = 5 \). In figure 7.4, the exact and the estimated source when applying the modulating functions method with different number of modulating functions. A comparison between the estimated sources obtained using the modulating functions method and the Tikhonov regularization is given in Figure 7.5, where the noise level is 3%. The regularization parameter \( \lambda \) is obtained using the GCV and we set the number of modulating functions as \( M = 6 \).

![Figure 7.4](image-url)

Figure 7.4: The exact and the approximated source different number of modulating functions with 3% noise.

Example 7.2.4. In this example, we use the measurement of the concentration only. We set \( r(x) = \sin\left(\frac{2\pi x}{L}\right) \), \( \nu = 0.3 \), \( d = 0.5 \), \( \alpha = 1.2 \), \( L_1 = L = 10 \), \( \Delta x = \frac{1}{15} \), \( \mu = \kappa = 0.5 \), \( T = 1 \) and \( K = 5 \). In figure 7.7, the exact and the estimated source when applying the modulating functions method with different number of modulating functions in noise free case and in Figure 7.7 is the estimated source from a 3% noisy measurement.

Remark 7.2.2. In the considered inverse source problem we assumed that the source is time independent. However, the method can easily be applied to estimate time-dependent source using the concentration measurement over the time domain.
Figure 7.5: Comparison between the Tik and the modulating functions method when M=6 with 3% noise.

Figure 7.6: The exact and the approximated source with 5 basis in noise free case with $\Delta x = \frac{1}{15}$.
7.3 Chapter Summary

In this chapter, we have presented the modulating functions method to estimate the source for a space-fractional advection-dispersion equation on a finite domain using two different types of measurements. Then, a comparison between the presented method and the standard optimization technique based on the Tikhonov regularization has been given throughout some numerical examples. Like Tikhonov based regularization which is affected by the value of the regularization parameter $\lambda$, the choice and number of modulating functions affects the accuracy of the proposed method, further investigation is needed.
Chapter 8

Concluding Remarks

8.1 Conclusion

In this work we analyzed, both from theoretical and numerical perspective, some inverse problems for space-fractional advection-dispersion equation (FADE). A novel algorithm is presented to estimate the coefficients and the differentiation order for a space-FADE. Further, we extended and generalized the algorithm to estimate parameters for two-dimensional domains. Estimation of the source term for the 1D space-FADE is also provided.

Our numerical results show the efficiency of the developed two-stage algorithm. It is found that the number of modulating functions can affect the accuracy of the proposed algorithm and may require deeper investigation. However, this was not a major problem in the particular scenario under investigation, and the errors were not significant while using a reasonable number of modulating functions. Also, the type of the modulating functions is important as the stability of the algebraic system when estimating the coefficients depends on the condition number. A set of modulating functions that gives a small condition number is found to be more appropriate. To give a guide on how to choose modulating functions some error analysis need to be done, which was out of the scope of this work.

It is important to point out that accuracy of the algorithm also depends on the
number of measurements. However, in the noise free case, the number of points can be reduced, and the results are satisfactory even with various numbers of modulating functions. It is also noted that when estimating scalar parameters from noisy data the results are reasonably satisfactory. However, in order to use a small amount of data when estimating variable coefficients, an interpolation method can be used to approximate the data over the whole domain. In comparison with Tikhonov based optimization technique the modulating functions method give comparable results. As the accuracy of the Tikhonov regularization is affected by the value of the regularization parameter, choice and number of modulating functions can affect the accuracy of proposed method.

In a nutshell, we proposed and validated a new algorithm to solve inverse problems that can be generalized to various integer and fractional or PDE systems.

8.2 Future Research Work

Work presented in this thesis report can be extended in following directions:

- Study the effect of using different types of modulating functions while applying combined modulating functions approach and Newton’s algorithm in cascade. In order to have a clue on how to choose modulating functions some error analysis needs to be done.

- Optimal number of modulating functions is found to be application specific and it can be further studied to improve the results.

- Method presented in this work can be applied using any of the definitions of the fractional derivatives, however; some theoretical studies in this particular direction are highly encouraged to be done.

- Proposed method is simple to implement and potentially it will be very useful
to extend it to general fractional partial differential equations.
REFERENCES


156


A Papers Submitted and Under Preparation

A.1 Journal Papers

- A. Aldoghaither, T.M. Laleg-Kirati and D.Y. Liu, Modulating Functions Based Algorithm for the Estimation of the Coefficients and Differentiation Order for a Space Fractional Advection Dispersion Equation. (accepted to SIAM Journal on Scientific Computing)

- A. Aldoghaither, T.M. Laleg-Kirati, and D.Y. Liu, Direct and Inverse Source Problem for a Space Fractional Advection Dispersion Equation. (Submitted to the Journal of Inverse and Ill Posed Problems)

- A. Aldoghaither and T.M. Laleg-Kirati, Parameter and Differentiation Order Estimation for a Two Dimensional Space Fractional Differential Equation. (under preparation)

A.2 Conference Papers

A. Aldoghaither and T.M. Laleg-Kirati, Inverse Source Problem for a Space Fractional Advection Dispersion Equation, the 11th International Conference on Mathematical and Numerical Aspects of Waves (WAVES 2013), Gammarth, Tunisia.


A.3 Presentations


A.4 Posters

