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par

**S**oumeya **D**jellali [1]

Sous la direction de

**Dr. S**oumia **I**drissi

**Thème:**

# Anomalous diffusion modeling based on stochastic fractional calculus: theory and application.

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| | | |
|---|---|---|
| **Dr. I. M**ekkaoui | Université de Saïda Dr. Moulay Tahar | Président |
| **Dr. S. I**drissi | Université de Saïda Dr. Moulay Tahar | Encadreur |
| **Dr. F. B**enziadi | Université de Saïda Dr. Moulay Tahar | Examinatrice |

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[1]e-mail: bouchradhouha@gmail.com

***Dedication***

*To you*

*Bouchra,*

*Doha,*

*Azzedine.*

*I dedicate this work.*

You have made me stronger, better and more fulfilled than I could have ever imagined.

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# Contents

# Abstract

Numerous processes, both natural and man-made, entail the dispersion of small particles that move in chaotic or random ways. The so-called anomalous-diffusion regimes are possible in addition to normal diffusion, which is defined by a Gaussian probability density function whose variance increases linearly with time. A variance rising slower (subdiffusive) or faster (superdiffusive) than typical characterizes them.

In order to replace normal diffusion by anomalous diffusion, -path properties- must be present. Brownian motion is intimately associated with normal diffusion. Likewise, many different underlying processes can lead to anomalous diffusion, such as Fractional Brownian motion, continuous random walks and fractional Itô motion.

In this work we recapitulate the state of art in the study of properties for some popular anomalous diffusion processes. Whith regard to their significance in real life we discuss an example of application using basis from fractional calculus theory.

# List Of Notations And Symbols & Acronyms

Throughout this master thesis we will use the following terminology and notation:

| | | |
|---|---|---|
| $\mathbb{N}$ | = | The set of natural numbers. |
| $\mathbb{R}$ | = | The set of all real numbers. |
| $[a, b]$ | = | The set of all real numbers between $a$ and $b$. |
| $\beta > 0$ | = | All positive real values of $\beta$. |
| $\beta \in [a, b]$ | = | All real values of $\beta$ between $a$ and $b$ . |
| $\overset{d}{=}$ | = | Equality in distribution (equality of all finite-dimensional distributions). |

| | | |
|---|---|---|
| a.s. | = | Almost surely |
| iff | = | If, and only if |
| m.s. | = | Mean-square |
| psd | = | Power spectral density |
| r.m.s | = | Root mean-square |
| r.v. | = | Random variable |
| w.r.t. | = | With respect to |
| MSD | = | mean squared displacement |
| H-ss | = | Self-similar with index $H \geq 0$ |
| H-sssi | = | **H-ss** with stationary increments |
| MSD | = | Mean squred displacement |
| CTRW | = | Continuous Time Random Walk |
| iid | = | Identically distributed and independent |
| pdf | = | probability density function |
| FIM | = | Fractional Itô motion |
| gBm | = | Grey Brownian motion |
| ggBm | = | Generalized grey Brownian motion |
| MR | = | Magnetic Resonance |

# Introduction

The world in our surrounding moves. No matter its scale, objects move in exceptionally specific ways, driven by their properties and their interaction with the envirodynamics of particles in atomic experiments, their speed: how fast or slowing down they'renment. From the motion of black holes in the middle of our galaxy to the going, direction and acceleration, among others, are widely used to understand their nature. Indeed, numerous hypotheses and theories have been created to study such systems just by looking at their motion.

Since Albert Einstein provided a theoretical foundation for Robert Brown's observation of the movement of microscopic granules contained in pollen grains, significant deviations from the laws of Brownian motion have been uncovered in an impressively wide variety of animate and inanimate systems, from biology to the stock market [13]. Anomalous diffusion, as it has come to be called, extends the concept of Brownian motion and is connected to disordered systems, non-equilibrium phenomena, flows of energy and information, and transport in living systems. In theoretical terms, anomalous diffusion has a well-developed framework, able to explain most of the current experimental observations. However, it has been usually focused in describing the systems in terms of its macroscopic behaviour. This means that the processes are described by means of general models, able to predict the average or collective features; such as ergodicity, Gaussianity, or ageing are now crucial for in the understanding of diffusion processes, well beyond Brownian motion. Anomalous diffusion took off in 1973 when Scher and Lax discussed [23] transport processes in disordered systems and in particular carrier diffusion in amorphous semiconductor films. Using recent estimates from 1973 by Montroll and Scher [23] and 1974 by Shlesinger [6], Scher and Montroll proposed a success model based on continuous-time random walk (CTRW) in 1975. The extraordinary spread proved too much during the years 1973-1975. Subsequently, new applications of diffusion theory began to require new modeling methods and through several other applications like physics [6], living systems [23] and finance [8].

Simultaneously, the field of fractional calculus that generalizes the concept of a derivative operator of integer order to a derivative operator of arbitrary order (real or complex), has found its great application in modeling anomalous diffusion thanks to the fractional time generalization of the diffusion equation. This connection between anomalous diffusion and fractional differential calculus is demonstrated by the so-called memory effect that governs diffusion and is encoded in the power-law kernel of the differential operators. The history of fractional models for anomalous diffusion began in 1986 with Nigmatullin[13], who modeled diffusion in porous media using comb-shaped fractal structures and derived the diffusion equation fractional dispersion over time, see the reference [6, 16, 23] for other pioneering applications of the fraction calculus. The work presented in this master thesis has the goal of explore models to understand anomalous diffusion. It is organized as follows.

In Chapter 1, various results and techniques from the theory of stochastic processes are presented, we will first give some preliminary definitions, results and notion of stochastic processes such as self-similarity, Mean squared displacement, then some of their properties, second we will discuss some useful mathematical definitions that are inextricably linked to fractional calculus.

In Chapter 2, we will survey the topic of stochastic anomalous diffusion processes, defined as stochastic processes that deviate from Brownian motion, with mean squared displacement not linearly related to time. First we will present different behaviors those follow a power law and manifest in sub-diffusion, super-diffusion, ballistic motion, and hyper-ballistic motion. Second some important stochastic processes lead to anomalous diffusion are discussed like the fractional Brownian motion (fBm), grey Brownian motion (gBm), continuous random walks and the fractional Itô motion (FIM). A visual comparisons that examine profound differences between fBm and FIM is considered at the end of this chapter.

In Chapter 3, the subject of fractional anomalous diffusion is discussed, we will first introduce the basic notions of fractional calculus. The area of mathematics that allows non-integer order integrals and derivatives. Then due to the importance of fractional calculus in real life, an example of application using basis from fractional calculus theory is presented. Where a novel model to analyzing anomalous diffusion in human brain tissues in vivo at high b-values up to $4700 sec/mm^2$ have been applied. This model is based on solutions of fractionalized Bloch-Torrey differential equation.

Chapter 1

# Concepts in Diffusion and Stochastic Processes

This chapter presents various results and techniques from the theory of stochastic processes that are useful in the study of stochastic problems in the natural sciences. [22, 15, 5]

## 1.1 Preliminary Background

For the sake of clarity, in this section we introduce notations, definitions, and preliminary facts that will be used.

### 1.1.1 Stochastic Processes

The stochastic processes serve as useful concepts for modeling random changes in time with stochastic differential equations, similar to the use of ordinary differential equations to model deterministic (non-stochastic) problems.

**Definition 1.1.1.** ***Stochastic Processes.***
A real-valued stochastic process, defined on a probabilistic space $(\Omega, \mathcal{F}, \mathbb{P})$, is a family of random variables denoted $X := (X(t), t \in I), (or (X_t)_{t\in I}$ or $(X(t))_{t\in I})$, where $I$ is a part of $\mathbb{R}^+$.
$X$ is therefore a function of two variables which associates to $(t, \omega) \in I \times \Omega$, the image $X_t(\omega) \in \mathbb{R}$.

- If I is a part of $\mathbb{N}$, we speak of a discrete-time stochastic process.
- If I is an interval of $\mathbb{R}^+$ we speak of a continuous-time stochastic process.

- At a fixed time $t$, the random function $\omega \to X_t(\omega)$ is a random variables.
- At a fixed individual $\omega$, the deterministic function $t \to X_t(\omega)$ is said to be the trajectory of the process.
- $X$ is said to be continuous when for any $\omega$, the trajectories $t \to X_t(\omega)$ are continuous.

**Definition 1.1.2.** ***Finite-dimensional distributions.***
For any natural number $k \in \mathbb{N}$ and a "time" sequence $\{t_i\}_{i=1,\dots,k} \in I$, the finite-dimensional distributions of the real valued stochastic process $X_t = \{X_t\}_{t\in I}$ are the measures $\mu_{t_1,\dots,t_k}$, defined on $\mathbb{R}^k$, such that

$$\mu_{t_1,\dots,t_k}(A_1 \times \cdots \times A_k) = \mathbb{P}(\{X_{t_1} \in A_1, \cdots, X_{t_k} \in A_k\}),$$

where $\{A_1, \dots, A_k\}$ are Borel sets on $\mathbb{R}$.

**Definition 1.1.3.** We say that two processes $X_t$ and $Y_t$ are equivalent if they have same finite-dimensional distributions.

### 1.1.2 Gaussian Stochastic Processes

A very important class of continuous-time processes is that of Gaussian processes, which arise in many applications.

**Definition 1.1.4.** A one-dimensional continuous-time Gaussian process is a stochastic process for which $\mathbb{E} = \mathbb{R}$ and all the finite-dimensional distributions are Gaussian.

**Remark.** A Gaussian process $x(t)$ is characterized by its mean

$$m(t) := \mathbb{E}(X(t))$$

and the covariance (or auto-correlation) matrix

$$C(t, s) = \mathbb{E}\left((X(t) - m(t)) \times (X(s) - m(s))\right).$$

Thus, the first two moments of a Gaussian process are sufficient for a complete characterization of the process.

### 1.1.3 Stationary Processes

The statistics of a large number of stochastic processes that arise in applications are time-invariant. We refer to such stochastic processes as stationary.

**Definition 1.1.5.** A stochastic process is called stationary if all finite-dimensional distributions are invariant under time translation: for every integer $k$ and for all times $t_i \in T$, the distribution of $(X(t_1), X(t_2), ..., X(t_k))$ is equal to that of $(X(s+t_1), X(s+t_2), ..., X(s+t_k))$ for every $s$ such that $s+t_i \in T$ for all $i \in 1, ..., k$. In other words,

$$\{X_{t_1}, X_{t_2}, ...., X_{t_k}\} \stackrel{d}{=} \{X_{s+t_1}, X_{s+t_2}, ..., X_{s+t_k}\}.$$

**Definition 1.1.6.** A stochastic process $\{X_t\}_{t\geq 0}$ is said a stationary increment process, shortly **si**, if for all $t \geq 0$ and for any $h \geq 0$ :

$$\{X_{t+h} - X_h\}_{t\geq 0} \stackrel{d}{=} \{X_t - X_0\}_{t\geq 0}.$$

### 1.1.4 Self-similarity

Self-similar objects in mathematics resemble a portion of itself precisely or roughly, with the whole having the same shape as one or more parts. Real-world phenomena, like coastlines, exhibit statistical self-similarity, with scale invariance being a precise type. Self-similarity occurs when the numerical value of an observable quantity changes but the corresponding dimensionless quantity remains unchanged.

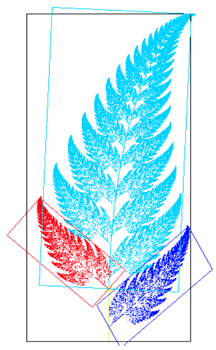

Figure 1.1: An image of the Barnsley fern which exhibits affine self-similarity

#### Self-similar processes

Self-similar processes (shortly **ss**) are stochastic processes that are invariant in distribution under suitable scaling of time and space. These processes also enter naturally in the analysis of random phenomena (in time) exhibiting certain forms of long-range dependence. In the last few years there has been an explosive growth in the study of self-similar processes.

**Definition 1.1.7.** ***Self-similar processes.***
A real valued stochastic process $X = \{X_t\}_{t\geq 0}$ is said self-similar with index $H \geq 0$, shortly **H-ss**, if for all $t \geq 0$ and for any $a > 0$

$$\{X_{at}\}_{t\geq 0} \stackrel{d}{=} \{a^H X_t\}_{t\geq 0}.$$

**Remark.** Observe that, if $X$ is an **H-ss** process, then all the finite-dimensional distributions of $X$ in $[0, \infty[$ are completely determined by the distribution in any finite real interval.

**Corollary 1.1.1.** For $H > 0$, a $H - ss$ process starts at 0 a.s.

**Proof.** We have $\forall a$ that $X_0 = X_{a0} \stackrel{d}{\sim} a^H X_0$. Then, letting $a \to 0$, we obtain the result.

**Proposition 1.1.1.** Let $X = \{X_t\}_{t\geq 0}$ be a non-degenerate[1] stationary process, then X can not be an **H-ss** process.

**Proof.** Indeed, for any $a > 0$:

$$X_t \stackrel{d}{=} X_{at} \stackrel{d}{=} a^H X_t,$$

by stationarity and self-similarity of the process $X$. Let $a \longrightarrow \infty$. Then the family of random variables on the right diverge with positive probability, whereas the random variable on the left is finite with probability one, leading to a contradiction.

Nevertheless, there is an important connection between self-similar and stationary processes.

**Proposition 1.1.2.** Let $\{X_t\}_{t\geq 0}$ be an **H-ss** process; then the process

$$Y(t) = e^{-tH} X(e^t), \quad t \in \mathbb{R} \tag{1.1.1}$$

is stationary. We have the converse, in the sense that if $(Y_t)_{t\in\mathbb{R}}$ is stationary, then

$$X_t = t^H Y(ln(t)), \quad t \geq 0 \tag{1.1.2}$$

is $H-$ss.

[1] A process $\{X_t\}_{t\geq 0}$ is said to be degenerate if for any $t \geq 0$, $X_t = 0$ almost surely.

**Proof.** Let $\theta_1, ....\theta_d$ be real numbers. If $\{X(t), 0 < t < \infty\}$ is H-ss, then for any $t_1, ...., t_d \in \mathbb{R}^1$ and $h > 0$,

$$\begin{aligned}\sum_{j=1}^{d} \theta_j Y(t_j + h) &= \sum_{j=1}^{d} \theta_j e^{-t_j H} e^{-hH} X(e^h e^{t_j}) \\ &\overset{d}{=} \sum_{j=1}^{d} \theta_j e^{-t_j H} X(e^{t_j}) \\ &= \sum_{j=1}^{d} \theta_j Y(t_j)\end{aligned}$$

proving that $\{Y(t), t \in \mathbb{R}\}$ is stationary.

Conversely, if $\{Y(t), t \in \mathbb{R}\}$ is stationary, then for $t_1, ...., t_d > 0$ and $a > 0$

$$\begin{aligned}\sum_{j=1}^{d} \theta_j X(at_j) &= \sum_{j=1}^{d} \theta_j a^H t_j^H Y(ln(a) + ln(t_j)) \\ &\overset{d}{=} \sum_{j=1}^{d} \theta_j a^H t_j^H Y(ln(t_j)) \\ &= \sum_{j=1}^{d} \theta_j a^H X(t_j)\end{aligned}$$

proving that $\{X(t), t > 0\}$ is H-ss. The transformation defined by Eq. (1.1.1) is called the Lamperti transformation

### 1.1.5 H-sssi processes

**Definition 1.1.8.** A stochastic process $X = \{X_t\}_{t\in I}$, $\mathcal{F}$-adapted, which is **H-ss** with stationary increments, is said **H-sssi** process with exponent H.

In the following we always suppose that $\mathbb{E}(X_t^2) < \infty$, $t \in I$. let $X = \{X_t\}_{t\in I}$. $\mathcal{F}$-adapted, be an **H-sssi** process with finite variance [2], the following properties hold:

1. $X_0 = 0$ almost surely.

[2]We always consider finite variance H-sssi process because it have many interesting properties.

2. If $H \neq 1$, then for any $t \geq 0$, $\mathbb{E}(X_t) = 0$.

3. One has:
$$X(-t) \stackrel{d}{=} -X(t),$$
it follows from the first property and the stationarity of the increments:
$$X(-t) \stackrel{a.s.}{=} X(-t) - X(0) \stackrel{d}{=} X(0) - X(t) \stackrel{a.s.}{=} -X(t).$$
The above property allows us to extend the definition of an H-sssi process to the whole real line: $\{X_t\}_{t\in\mathbb{R}}$.

4. Let $\sigma^2 = \mathbb{E}(X_1^2)$. Then,
$$\mathbb{E}(X_t^2) = |t|^{2H}\sigma^2. \tag{1.1.3}$$
Indeed, from the third property and the self-similarity:
$$\mathbb{E}X(t)^2 = \mathbb{E}X^2(|t|sign(t)) = |t|^{2H}\mathbb{E}X^2(sign(t)) = |t|^{2H}\mathbb{E}(X_1^2) = |t|^{2H}\sigma^2.$$

5. The autocovariance function of an **H-sssi** process [3] X, with $\mathbb{E}(X_1^2) = \sigma^2$, turns out to be:
$$\gamma_{s,t}^H = \frac{\sigma^2}{2}(|t|^{2H} + |s|^{2H} - |t-s|^{2H}). \tag{1.1.4}$$
It follows from the fourth property and the stationarity of the increments
$$\mathbb{E}(X_s X_t) = \frac{1}{2}(\mathbb{E}X_s^2 + \mathbb{E}X_t^2 - \mathbb{E}(X_t - X_s)^2).$$

6. If $X = \{X_t\}_{t\in I}$ is an H-sssi process, then one must have $H \leq 1$.
The constraint of the scaling exponent follows directly from the stationarity of the increments:
$$2^H\mathbb{E}|X_1| = \mathbb{E}|X_2| = \mathbb{E}|X_2 - X_1 + X_1| \leq \mathbb{E}|X_2 - X_1| + \mathbb{E}|X_1| = 2\mathbb{E}|X_1|,$$
therefore, $2^H \leq 2 \iff H \leq 1$.

### 1.1.6 Brownian Motion (BM)

Brownian motion and the diffusion processes derived from it play a central role in the theory of stochastic processes. They provide simple models for a wide range of applications. Brownian motion takes its name from the botanist Robert Brown, who in 1827 observed the movement of fine particles (pollen) suspended in a fluid.

[3] Sometimes, we refer to the **H-sssi** process $\{X_t\}_{t\in I}$ with the word standard if $\sigma^2 = 1$

**Definition 1.1.9.** ***Brownian motion.***

A stochastic process $\{B(t), t \geq 0\}$ is said to be a Brownian motion if

(i) $B(0) = 0$.

(ii) (**Independent increments.**) For each $0 \leq t_1 < t_2 < \ldots < t_m$,

$$B(t_1), B(t_2) - B(t_1), \ldots, B(t_m) - B(t_{m-1}),$$

are independent r.v.'s.

(iii) (**Stationary increments.**) For each $0 \leq s < t$, $B(t) - B(s)$ has a normal distribution with mean zero and variance $\sigma^2 = t - s$.

(iv) (**Continuity of paths.**) $\{B(t)\}_{t \geq 0}$ are continuous functions of $t$.

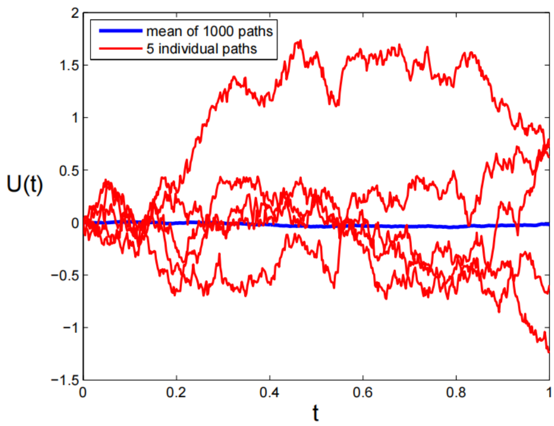


Figure 1.2: Brownian sample paths

**Remark.**

- Notice that the natural filtration of the Brownian motion is $\mathcal{F}_t^B = \sigma(B_s, s \leq t)$.
- If $\sigma^2 = 1$, we said that $\{B(t) : t \geq 0\}$ is a standard Brownian motion.

### 1.7.1.1 Properties of Brownian motion

### 1- Martingale property

A martingale is a very special type of stochastic process.

**Lemma 1.1.1.** An $\mathcal{F}_t$-Wiener process $B_t$ is an $\mathcal{F}_t$-martingale.

**Proof.**

We need to prove that $\mathbb{E}(B_t|\mathcal{F}_s) = B_s$ for any $t > s$. But as $B_s$ is $\mathcal{F}_s$-measurable (by adeptness) this is equivalent to $\mathbb{E}(B_t - B_s|\mathcal{F}_s) = 0$, and this is clearly true by the definition of the Wiener process (as $B_t - B_s$ has zero mean and is independent of $\mathcal{F}_s$) .

**2- Markov property**

The reason why Markov processes are so important comes from the fact that they are fundamental class of stochastic processes, with many applications in real life problems outside mathematics.

**Definition 1.1.10.** An $\mathcal{F}_t$ adapted process $X_t$ is called an $\mathcal{F}_t$-Markov process if we have $\mathbb{E}(f(X_t)|\mathcal{F}_s) = \mathbb{E}(f(X_t)|X_s)$ for all $t \geq s$ and all bounded measurable functions $f$. When the filtration is not specified, the natural filtration $\mathcal{F}_t^X$ is implied.

**Lemma 1.1.2.** [15] An $\mathcal{F}_t$-Wiener process $B_t$ is an $\mathcal{F}_t$-Markov process.

**3- Self-similarity**

**Theorem 1.1.1.** $B$ is a H-ss process with $H = 1/2$.

**Proof.** It is enough to show that for every $a > 0$, $\{a^{1/2}B(t)\}$ is also Brownian motion. Conditions (i), (ii) and (iv) follow from the same conditions for $\{B(t)\}$. As to (iii), Gaussianity and mean-zero property also follow from the properties of $\{B(t)\}$.
As to the variance, $\mathbb{E}\left[\left(a^{1/2}B(t)^2\right)\right] = t$. And for all $t_1, t_2 \in \mathbb{R}$, the autocovariance function

$$\mathbb{E}\left[(B(at_1)B(at_2))\right] = \min(at_1, at_2) = a\min(t_1, t_2) = \mathbb{E}\left[\left(a^{1/2}B(t_1)a^{1/2}B(t_2)\right)\right].$$

Thus $\{a^{1/2}B(t)\}$ is a Brownian motion.

**4- Non-differentiability**

**Theorem 1.1.2.** [15] For any $t$ almost all trajectories of Brownian motion are not differentiable at $t$.

**5- Hölder continuity**

**Proposition 1.1.3.** [15] Brownian motion paths are a.s. locally $\gamma$-Hölder continuous for $\gamma \in [0, 1/2)$.

**6- Quadratic variation**

**Definition 1.1.11.** The quadratic variation of Brownian motion $B(t)$ is defined as

$$[B, B](t) = [B, B]([0, t]) = \lim_{n\to\infty} \sum_{i=1}^{n} \left| B_{t_i^n} - B_{t_{i-1}^n} \right|^2,$$

where for each $n$, $\{t_i^n, 0 \leq i \leq n\}$ is a partition of $[0, t]$, and the limit is taken over all partitions with $\delta_n = \max_i (t_{i+1}^n - t_i^n) \to 0$ as $n \to \infty$, and in the sense of convergence in probability.

**Theorem 1.1.3.** [15] Quadratic variation of a Brownian motion over $[0, t]$ is $t$.

### 1.1.7 Mean squared displacement (MSD)

MSD is a fundamental metric for understanding particle dynamics, especially in Brownian motion and random walk scenarios, providing insights into diffusion coefficients and mechanical properties of the medium in which particles move.

**Definition 1.1.12.** ***Mean squared displacement (MSD)***.
An averaged quantity that is often calculated is called the mean-squared displacement. Its generic formula is given by:

$$MSD(\tau) = \left\langle x^2(\tau) \right\rangle = \left\langle \ [x(t+\tau) - x(t)]^2 \ \right\rangle$$

where $x(\tau)$ is is the position of the particle at time $t$, and $\tau$ is the lag time between the two positions taken by the particle used to calculate the displacement

$$\Delta x(\tau) = x(t+\tau) - x(t).$$

The average $< ., . >$ designates a time-average over $t$ and/or an ensemble-average over several trajectories.

**Remark.** MSDs can be computed from the following expression, known as the Einstein formula:

$$MSD(x_d) = \left\langle \frac{1}{N} \sum_{i=1}^{N} |x_d(t) - x_d(t_0)|^2 \right\rangle$$

### 1.1.8 Special Functions

In this section we will discuss some useful mathematical definitions that are inextricably linked to fractional calculus. These include the Gamma function, the Beta function and the Mittag-Leffler function.

#### 3.1.1.1 The Gamma Function

The most basic interpretation of the Gamma function is simply the generalization of the factorial for all real numbers.

**Definition 1.1.13.**

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt, \qquad x \in \mathbb{R}^+.$$

The Gamma function has some properties.

$$\begin{aligned} \Gamma(x+1) &= x\Gamma(x), \qquad x \in \mathbb{R}^+. \\ \Gamma(x) &= (x-1)!, \qquad x \in \mathbb{R}^+. \end{aligned}$$

**Example 1.1.1.**

$$\begin{aligned} \Gamma(1) &= \Gamma(2) = 1. \\ \Gamma(1/2) &= \sqrt{\pi}. \\ \Gamma(n+1/2) &= \frac{\sqrt{\pi}}{2^n}(2n-1)!, \qquad n \in \mathbb{N}. \end{aligned}$$

### 3.1.1.2 The Beta Function

Like the Gamma function, the Beta function is defined by a definite integral.

**Definition 1.1.14.** It's given by:

$$\mathbf{B}(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1} dt, \qquad x, y \in \mathbb{R}^+$$

The Beta function can also be defined in terms of the Gamma function:

$$\mathbf{B}(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}, \qquad x, y \in \mathbb{R}^+ \tag{1.1.5}$$

### 3.1.1.3 The Mittag-Leffler Function

The Mittag-Leffler function named after a Swedish mathematician who defined and studied it in 1903, is a direct generalization of the exponential function.

**Definition 1.1.15.** The standard definition of the Mittag-Leffler is given by :

$$\mathrm{E}_\alpha(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\alpha k + 1)}, \quad \alpha > 0$$

The Mittag-Leffler function with two parameters $\alpha$ and $\beta$, is defined as:

$$\mathrm{E}_{\alpha,\beta}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\alpha k + \beta)}, \quad \beta > 0 \quad \alpha > 0 \tag{1.1.6}$$

As a result of the definition given in Eq. (1.1.6), the following relations hold:

$$E_{\alpha,\beta}(x) = \frac{1}{\Gamma(\beta)} + xE_{\alpha,\alpha+\beta}(x).$$

and

$$E_{\alpha,\beta}(x) = \beta E_{\alpha,\beta+1}(x) + \alpha x \frac{d}{dx} E_{\alpha,\beta+1}(x).$$

**Example 1.1.2.**

$$\begin{aligned}
E_{\alpha,\beta}(0) &= 1. \\
E_{1,1}(x) &= \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \frac{x^k}{k!} = e^x. \\
E_{1,2}(x) &= \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(k+2)} = \frac{1}{x} \sum_{k=0}^{\infty} \frac{x^{k+1}}{(k+1)!} = \frac{e^x - 1}{x}.
\end{aligned}$$

Chapter 2

# Anomalous diffusion processes.

Anomalous diffusion processes deviate from Brownian motion, with mean squared displacement not linearly related to time. These complex behaviors follow a power law and manifest in sub-diffusion, super-diffusion, ballistic motion, and hyper-ballistic motion. Examples of anomalous diffusion stochastic processes are discussed in this chapter, this include fractional Brownian motion, continuous-time random walks, grey Brownian motion and fractional Itô motion. The main references for this chapter are [1, 3, 4, 13, 20].

## 2.1 Classes of anomalous diffusion

In recent years many processes have been observed that deviated from the normal diffusion. Such processes are described by anomalous diffusion for which MSD scales as a power law

$$\langle x^2(\tau)\rangle = K_\alpha \tau^\alpha$$

where $K_\alpha$ is the so-called generalized diffusion coefficient and $\tau$ is the elapsed time. The main classes of anomalous diffusion's are classified as follows:

- $\alpha < 1$ : Subdiffusion.
- $\alpha = 1$ : Brownian motion.
- $1 < \alpha < 2$ : Superdiffusion.
- $\alpha = 2$ : Ballistic motion.
- $\alpha > 2$ : Hyperballistic.

## 2.2 Models of anomalous diffusion

There are many possible ways to mathematically define a stochastic process which then has the right kind of power law. Currently the most studied types of anomalous diffusion processes are those involving the following: Generalizations of Brownian motion, such as the fractional Brownian motion and Grey Brownian motion, Continuous time random walks.

**Definition 2.2.1.** Embedding Principle for anomalous diffusion. Anomalous diffusion process can be represented as time-changed Brownian motion if and only if it is a semi-martingale.

### 2.2.1 Fractional Brownian Motion (fBm)

The fractional Brownian motion is one of the most widely used anomalous diffusion processes. It was formulated in 1968 by Mandelbrot and van Ness as a family of Gaussian random functions. We note that a similar process was introduced by Kolmogorov in 1940. For instance, it is a standard model for stock market dynamics. Moreover, it is commonly used to model single particle diffusion experiments in living cells.

**Definition 2.2.2.** The fractional B rownian motion (fBm) with Hurst index ($H \in (0,1)$) is a Gaussian process $B^H = \{B_t^H, t \in \mathbb{R}\}$ on $(\Omega, \mathcal{F}, \mathbb{P})$, having the properties:

1. $B_0^H = 0$,
2. $\mathbb{E}[B_t^H] = 0$; $t \in \mathbb{R}$,
3. $\mathbb{E}[B_t^H B_s^H] = \frac{1}{2}\Big(|t|^{2H} + |s|^{2H} - |t-s|^{2H}\Big)$; $s, t \in \mathbb{R}$.

**Remark.** Since $\mathbb{E}[B_t^H - B_s^H]^2 = |t-s|^{2H}$ and $B_H$ is a Gaussian process, it has a continuous modification, according to the Kolmogorov theorem.

**Remark.** For $H = 1$, we set $B_t^H = B_t^1 = t\xi$, where $\xi$ is a standard normal Random variable.
For $H = \frac{1}{2}$, the characteristic function has the form

$$\phi_\lambda(t) = \mathbb{E}\Big[exp(i\sum_{k=1}^{n} \lambda_k B_{t_k}^H)\Big] = exp\Big(-\frac{1}{2}(C_t\lambda, \lambda)\Big),$$

where $C_t = (\mathbb{E}[B_{t_K}^H B_{t_i}^H])_{1 \le i,k \le n}$ and $(.,.)$ is the inner product on $\mathbb{R}^n$.

**Proposition 2.2.1.** (**fBm characterization**). Let $X = \{X_t\}_{t\geq 0}$ be a stochastic process defined on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$, such that:

- $\mathbb{P}(X_0 = 0) = 1$.
- $X$ is a zero-mean Gaussian process such that, for any $t > 0, \mathbb{E}(X_t^2) = \sigma^2 t^\alpha$ for some $\sigma > 0$ and $0 < \alpha < 2$.
- $X$ is a **si**-process.

Then, $\{X_t\}_{t>0}$ is a (one-sided) fractional Brownian motion of order $H = \alpha/2$.

**Proof.** Since $X$ is a zero-mean Gaussian process, its finite-dimensional distributions are completely characterized by its autocovariance function. Given that, for any $t > 0$ :

$$\mathbb{E}(X_t^2) = \sigma^2 |t|^\alpha$$

and $X$ has stationary increments, it follows that the autocovariance function is given by Eq. (2.2.2), which is the autocovariance of a fBm with $H = \alpha/2$.

**Corollary 2.2.1.** [18] Let $X = \{X_t\}_{t\geq 0}$ be a stochastic process defined on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Let $0 < H < 1$ and $\sigma^2 = E(X_1^2)$. The following statements are equivalent:

1. $X$ is an **H-sssi** Gaussian process.
2. $X$ is a (one-sided) fractional Brownian motion with scaling exponent $H$.

## Fractional Brownian motion proprieties

### 1-Selfsimilarity.

There is an other classic definition of the fBm using selfsimilar properties, which we give as a theorem.

**Theorem 2.2.1.** For $H \in (0, 1)$, the fBm $(B_t^H)_{t\in\mathbb{R}_+}$ is a gaussian $H-$sssi process.

**Proof.** First, let us prove the selfsimilarity property. We have that

$$\begin{aligned}
\mathbb{E}\left(B_{at}^{(H)} B_{as}^{(H)}\right) &= \frac{1}{2}\left((at)^{2H} + (as)^{2H} - (a|t-s|)^{2H}\right) \\
&= a^{2H}\mathbb{E}\left(B_t^{(H)} B_s^{(H)}\right) \\
&= \mathbb{E}\left((a^H B_t^{(H)})(a^H B_s^{(H)})\right)
\end{aligned}$$

Thus, since all processes are centered and gaussian, it implies that

$$\left(B_{at}^{(H)}\right) \stackrel{d}{=} \left(a^H B_t^{(H)}\right).$$

Second, we show that it has stationary increments. Note that if, for $h > 0$, we have

$$\mathbb{E}\left((B_{t+h}^{(H)} - B_h^{(H)})(B_{s+h}^{(H)} - B_h^{(H)})\right) = \mathbb{E}\left(B_t^{(H)} B_s^{(H)}\right), \tag{2.2.1}$$

we conclude that $(B_{t+h}^{(H)} - B_h^{(H)}) \stackrel{d}{=} B_t^{(H)}$. We have,

$$\begin{aligned}
\mathbb{E}\left((B_{t+h}^{(H)} - B_h^{(H)})(B_{s+h}^{(H)} - B_h^{(H)})\right) &= \mathbb{E}\left((B_{t+h}^{(H)} B_{s+h}^{(H)})\right) - \mathbb{E}\left((B_{t+h}^{(H)} B_h^{(H)})\right) - \mathbb{E}\left((B_{s+h}^{(H)} B_h^{(H)})\right) \\
&+ \mathbb{E}\left((B_h^{(H)})^2\right) \\
&= \frac{1}{2}\Big(((t+h)^{2H} + (s+h)^{2H} - |t-s|^{2H}) \\
&- ((t+h)^{2H} + h^{2H} - t^{2H}) \\
&- ((s+h)^{2H} + h^{2H} - s^{2H}) + 2h^{2H}\Big) \\
&= \frac{1}{2}(t^{2H} + s^{2H} - |t-s|^{2H}) \\
&= \mathbb{E}\left(B_t^{(H)} B_s^{(H)}\right).
\end{aligned}$$

Therefore the fBm is a H-sssi process.

**2-Markovian property.**

**Proposition 2.2.2.** [1] Fractional Brownian motion is non-Markovian provided that $H \neq 1/2$.

**3- Hölder continuity**

**Theorem 2.2.2.** [1] (**Kolmogorov continuity theorem**). A stochastic process $\{X_t\}_{t\in I}$ has a version with continuous trajectories if there exist: $p \geq 1$ and $\eta > 1$ and a constant $c$, such that, for any $t_1, t_2 \in I$ :

$$\mathbb{E}|X_{t_2} - X_{t_1}|^p \leq c|t_2 - t_1|^\eta. \tag{2.2.2}$$

**Theorem 2.2.3.** Let $H \in (0,1)$. The fBm $B^{(H)}$ admits a version whose sample paths are almost surely Hölder continuous of order strictly less than $H$.

**Proof.** We recall that a function $f : \mathbb{R} \longrightarrow \mathbb{R}$ is Hölder continuous of order $\alpha$, $0 < \alpha \leq 1$ and write $f \in \mathcal{C}^\alpha(\mathbb{R})$, if there exists $M > 0$ such that

$$|f(t) - f(s)| \leq M|t-s|^\alpha,$$

for every $s, t \in \mathbb{R}$. For any $\alpha > 0$ we have

$$\mathbb{E}\big[|B^H(t) - B^H(s)|^\alpha\big] = \mathbb{E}\big[|B^H(1)|^\alpha\big]|t-s|^{\alpha H};$$

hence, by the Kolmogorov criterion we get that the sample paths of $B^H$ are almost everywhere Hölder continuous of order strictly less than $H$. Moreover, by ([1]) we have

$$\limsup_{t\longrightarrow 0_+} \frac{|B^{(H)}(t)|}{t^H\sqrt{log(log(t^{-1}))}} = c_H$$

with probability one, where $c_H$ is a suitable constant. Hence $B^H$ can not have sample paths with Hölder continuity's order greater than $H$.

**4- Differentiability**

By ([14]) we also obtain that the process $B^H$ does not have differentiable sample paths.

**Proposition 2.2.3.** Let $H \in (0,1)$. The fBm sample path $B^H(.)$ is not differentiable. In fact, for every $t_0 \in [0,\infty)$

$$\limsup_{t\to t_0} \left|\frac{B^H(t) - B^H(t_0)}{t-t_0}\right| = \infty$$

with probability one.

**Proof.** Here we recall the proof of ([14]). Note that we assume $B^H(0) = 0$. The result is proved by exploiting the self-similarity of $B^H$. Consider the random variable

$$\mathcal{R}_{t,t_0} := \frac{B^H(t) - B^H(t_0)}{t-t_0}$$

that represents the incremental ratio of $B^H$. Since $B^H$ is self-similar (see[1]), we have that the law of $\mathcal{R}_{t,t_0}$ is the same of $(t-t_0)^{H-1}B^H(1)$. If one considers the event

$$A(t,w) := \left\{\sup_{0\le s\le t}\left|\frac{B^H(s)}{s}\right| > d\right\},$$

then for any sequence $(t_n)_{n\in\mathbb{N}}$ decreasing to 0, we have

$$A(t_n, w) \supseteq A(t_{n+1}, w),$$

and

$$A\left(t_n, w\right) \supseteq \left(|\frac{B^H(t_n)}{t_n}| > d\right) = \left(|B^H(1)| > t_n^{1-H}d\right).$$

But,

$$\lim_{n\longrightarrow\infty}\left(|B^H(1)| > t_n^{1-H}d\right)$$

Since this is true for any $d$, it must be the case that the derivative does not exist at any point along any sample path of $B^H(t)$.

**5- Non semi-martingale property**

The definition of the Itô integral is a direct consequence of the martingale property of Brownian motion. But fBm does not exhibit this property.

**Definition 2.2.3.** The $p$-variation of a stochastic process $(X(t))_{t\in[0,T]}$ is defined as

$$\mathcal{V}_p(X,[0,T]) := sup_\pi \sum_{i=1}^{n} |X(t_i) - X(t_{i-1})|^p, \tag{2.2.3}$$

where $\pi$ is a finite partition of $[0,T]$. The index of $p$-variation of a process is defined to be

$$I(X,[0,T]) := \inf\{p > 0; \mathcal{V}_p(X,[0,T]) < \infty\}. \tag{2.2.4}$$

**Lemma 2.2.1.** $I(B^H,[0,T]) = \dfrac{1}{H}$ Moreover, $V_p(B^H(t),[0,T]) = 0$ when $pH > 1$ and $V_p(B^H(t),[0,T]) = \infty$ when $pH < 1$.

**Proof.** A proof can be found in [1].

**Theorem 2.2.4.** $\{B^H(t) : t \geq 0\}$, for $H \neq 1/2$, is not semimartingale.

**Proof.** A process $\{X(t), \mathcal{F}_t, t \geq 0\}$ is called a semimartingale if it admits the Doob-Meyer decomposition $X(t) = X(0) + M(t) + A(t)$, where $M(t)$ is an $\mathcal{F}_t$ local martingale with $M(0) = 0, A(t)$ is a càdlàg adapted process of locally bounded variation and $X(0)$ is $\mathcal{F}_0$-measurable. Moreover, any semimartingale has locally bounded quadratic variation[1].

Now, let $X(t) = B^H(t)$. If $H \in (0,1/2)$, then $B^H(t)$ cannot even be a martingale since it has infinite quadratic variation, hence, it is not a semimartingale.

If $H \in (1/2,1)$ then the quadratic variation of $B^H(t)$ is zero. So, let's suppose that it is a semimartingale. Then, $M(t) = B^H(t) - A(t)$ has quadratic variation equal to zero. So, from [12], $M(t) = 0$ for all t a.s. Then that would mean that $B^H(t) = A(t)$, but this can't be the case since $B^H(t)$ has unbounded variation. Hence $B^H(t)$ is not a semimartingale for any $H \neq 1/2$.

**6- Long-Range Dependence**

Note also that the fBm is one of the simplest process which exhibits long-range dependency.

Define $X(n) = B^H(n+1) - B^H(n), n \geq 1$. Then clearly $X(n)$ is a Gaussian stationary sequence with unit variance. Moreover the covariance function of $X(t)$ is

$$r^H(n) = \mathbb{E}[X(0)X(n)] = 1/2((n+1)^{2H} - 2n^{2H} + (n-1)^{2H}).$$

If $H = 1/2$ then we get that $r(n) = 0$ implying that the increments of $X(n)$ are uncorrelated.

But, if $H \neq 1/2$, we get that as $n$ tends to infinity $r^H(n) \backsim H(2H-1)n^{2H-2}$. Thus we get

- If $0 < H < 1/2$ then $\sum_{n=0}^{\infty} |r^H(n)| < \infty$.
- If $1/2 < H < 1$ then $\sum_{n=0}^{\infty} |r^H(n)| = \infty$, in this case the process $B^H$ is a long memory process.

Depending on the qualitative behavior of the fBm trajectories, it is common the following fBm partitioning, which can be actually used to characterize any $H-$sssi process:

1. If $0 < H < 1/2$, the fBm is termed anti-persistent.
2. If $H = 1/2$, the fBm is termed purely random, or chaotic.
3. If $1/2 < H < 1$, the fBm is termed persistent.

This division is due to the behavior of the autocovariance function

### 2.2.2 Generalized Grey Brownian Motion (ggBm)

Grey Brownian motion (gBm) was introduced by W. Schneider as a model for slow anomalous diffusions, i.e., the marginal density function of the gBm is the fundamental solution of the time-fractional diffusion equation. This is a class $\{B_\beta(t), t \geq 0, 0 < \beta \leq 1\}$ of processes which are self-similar with stationary increments. More recently, this class was extended to the, so called "generalized" grey Brownian motion (ggBm) to include slow and fast anomalous diffusions which contain either Gaussian or non-Gaussian processes e.g., fBm, gBm and others. In this chapter we will not reproduce the all construction of the ggBm, but we will refer to the mention of the latter and some of its properties and then recall the differential equations driven by it, the interested reader can find it in [17],[16] and references therein.

### Grey Brownian Motion

We begin by introducing some basic concepts and facts

**Definition 2.2.4.** (**Schwartz space**) The space $\mathcal{S}(\mathbb{R}^n)$ is the space of all the functions $f \in \mathcal{C}^\infty(\mathbb{R}^n)$, such that for any multi-indices $j = (j_1, j_2, \ldots, j_n)$ and $k = (k_1, k_2, ..., k_n)$ :

$$\sup_{x\in\mathbb{R}^n} |x^j D^k f(x)| < \infty. \tag{2.2.5}$$

**Definition 2.2.5.** (**Tempred distribution**) The space of all tempered distributions on $\mathbb{R}$, denoted $\mathcal{S}'(\mathbb{R}^n)$, is the dual space of $\mathcal{S}(\mathbb{R}^n)$. That is, it is the set of all functions that are linear and continuous .

**Definition 2.2.6.** (**Completely monotonic function**) A function f with domain $(0, \infty)$ is said to be completely monotonic (c.m.), if it possesses derivatives $f^{(n)}(x)$ for all
$n = 0, 1, 2, \cdot ..$ and if

$$(-1)^n f^{(n)}(x) \geq 0$$

for all $x > 0$
The limit $f^{(n)}(0) = \lim_{x\to 0^+} f^{(n)}(x)$, finite or infinite,exists.

**Definition 2.2.7.** A continuous map $\Phi : X \longrightarrow \mathbb{C}$ is called a characteristic functional on X if it is:

1. Normalized: $\Phi(0) = 1$,
2. Positive defined: $\sum_{i,j=1}^{m} \overline{c_i}\Phi(\xi_i - \xi_j)c_j \geq 0,\ m \in \mathbb{Z},\ \{c_i\}_{i=1,....,m} \in \mathbb{C},\ \{\xi_i\}_{i=1,...,m} \in X$

**Proposition 2.2.4.** [16] Let F be a completely monotonic function defined on the positive real line.Therefore, there exists a unique characteristic functional, defined on a real separable Hilbert space H, such that:

$$\Phi(\xi) = F(\|\xi\|^2), \xi \in H.$$

**Definition 2.2.8.** (**Nuclear space**) A topological vector space X, with the topology defined by a family of Hilbert norms, is said a nuclear space if for any Hilbert norm $\|\cdot\|_p$ there exists a larger norm $\|\cdot\|_q$ such that the inclusion map $X_q \hookrightarrow X_p$ is an Hilbert−Schmidt operator.

**Remark.** Nuclear spaces have many of the good properties of the finite-dimensional Euclidean spaces $\mathbb{R}^d$. For example, a subset of a nuclear space is compact if and only if is bounded and closed. Moreover, spaces whose elements are '**smooth**' in some sense tend to be nuclear spaces.

**Theorem 2.2.5.** (**Bochner's theorem**, [16]) For any characteristic functional $\Phi$ on $\mathbb{R}^n$ there exists a **unique** probability measure $\mu$ on $\mathbb{R}^n$ such that $\Phi$ is its generating functional. Namely,

$$\Phi(\xi) = \int_{\mathbb{R}^n} e^{i\langle x,\xi\rangle} d\mu(x), \quad \xi \in \mathbb{R}^n.$$

**Theorem 2.2.6.** (**Minlos theorem**, [16]) Let X be a nuclear space. For any characteristic functional $\Phi$ defined on X there exists a unique probability measure $\mu$ defined on the measurable space $(X', \mathcal{B})$, where $\mathcal{B}$ is regarded as the Borel $\sigma$-algebra generated by the weak topology on $X'$, such that:

$$\int_{X'} e^{i\langle w,\xi\rangle} d\mu(w) = \Phi(\xi), \quad \xi \in X. \tag{2.2.6}$$

**Proposition 2.2.5.** Let F be a completely monotonic function defined on the positive real line.Therefore, there exists a unique characteristic functional, defined on a real separable Hilbert space H, such that:

$$\Phi(\xi) = F(\|\xi\|^2), \xi \in H.$$

**Proof.** A proof can be found in [16]. Using this proposition and Minlos theorem [16], the following definition makes sense.

**Definition 2.2.9.** For any $\beta \in (0, 1]$ the Mittag-Leffler measure is defined as the unique probability measure $\mu_\beta$ on $\mathcal{S}'(\mathbb{R})$ by fixing its characteristic functional

$$\int_{\mathcal{S}'} e^{i\langle w,\varphi\rangle} d\mu_\beta(w) = E_\beta(-\frac{1}{2}\langle \varphi, \varphi\rangle), \quad \varphi \in \mathcal{S}(\mathbb{R}) \tag{2.2.7}$$

**Remark.**

1. The measure $\mu_\beta$ is also called grey noise (reference) measure [17, 16].

2. In the approach of (Mura, [16]) the grey noise measure is defined via the characteristic function $E_\beta(-(.,.)_\alpha)$ and denoted by $\mu_{\alpha,\beta}$. This means that first the parameters $0 < \alpha < 2$ and $0 < \beta < 1$ are fixed and then generalized grey Brownian motion $B_t^{\alpha,\beta}$ is constructed in $L^2(\mu_{\alpha,\beta})$.

3. In the case $\alpha = \beta$ and $0 < \beta \leq 1$, the probability space $(\mathcal{S}'(\mathbb{R}), \mathcal{B}, \mu_{\beta,\beta})$ is called grey noise space and the measure $\mu_{\beta,\beta}$ is called grey noise measure (see [1], [21]).

**Lemma 2.2.2.** For any $\varphi \in \mathcal{S}(\mathbb{R})$ and $n \in \mathbb{N}_0$ we have

$$\int_{\mathcal{S}'(\mathbb{R})} \langle w, \varphi \rangle^{2n+1} d\mu_\beta(w) = 0$$

$$\int_{\mathcal{S}'(\mathbb{R})} \langle w, \varphi \rangle^{2n} d\mu_\beta(w) = \frac{(2n)!}{2^n \Gamma(\beta n + 1)} \mid \varphi \mid^{2n} .$$

**Proof.** A proof can be found in [1].

**Definition 2.2.10.** We consider the generalized stochastic process $X_{\alpha,\beta}$ defined canonically on the $(\mathcal{S}'(\mathbb{R}), \mathcal{B}, \mu_{\alpha,\beta})$, called grey noise by

$$X_{\alpha,\beta}(\varphi) : \mathcal{S}'(\mathbb{R}) \to \mathbb{R}, w \mapsto X_{\alpha,\beta}(\varphi)(w) := \langle w, \varphi \rangle.$$

**Properties**

1. Characteristic function:

$$\mathbb{E}(e^{i\lambda X_{\alpha,\beta}(\varphi)}) := E_\beta(-\lambda^2 \|\varphi\|_\alpha^2),$$

2. Moments:

$$\mathbb{E}(X_{\alpha,\beta}(\varphi))^k = \begin{cases} 0, & k = 2n+1 \\ \dfrac{(2n)!}{\Gamma(\beta n + 1)} \|\varphi\|_\alpha^{2n}, & k = 2n \end{cases}$$

3. For any $f \in H_\alpha$, we have $X_{\alpha,\beta}(f) \in L^2(\mu_{\alpha,\beta})$ and

$$\|X_{\alpha,\beta}(f)\|^2_{L^2(\mu_{\alpha,\beta})} = \frac{2}{\Gamma(\beta + 1)} \|f\|_\alpha^2$$

**Generalized grey Brownian motion definition**

In this subsection we briefly introduce the mathematical definition and the main proprieties of the generalized grey Brownian motion.

**Definition 2.2.11.** The stochastic process

$$\{B_{\alpha,\beta}(t)\}_{t\geq 0} = \{X_{\alpha,\beta}(\mathbf{1}_{[0,t)})\}_{t\geq 0.} \tag{2.2.8}$$

is called generalized (standard) grey Brownian motion.

**Proposition 2.2.6.** [16]

1. $B_{\alpha,\beta}(0) = 0$ a.s. Moreover, for each $t \geq 0$, $\mathbb{E}(B_{\alpha,\beta}(t)) = 0$ and
$$\mathbb{E}(B_{\alpha,\beta}(t)^2) = \frac{2}{\Gamma(\beta+1)} t^{\alpha}. \tag{2.2.9}$$

2. The auto-covariance function is:
$$\mathbb{E}(B_{\alpha,\beta}(t)B_{\alpha,\beta}(s)) = \gamma_{\alpha,\beta}(t,s) = \frac{1}{\Gamma(\beta+1)}(t^{\alpha} + s^{\alpha} - |t-s|^{\alpha}). \tag{2.2.10}$$

3. For any $t, s \geq 0$, the characteristic function of the increments is:
$$\mathbb{E}(e^{iy(B_{\alpha,\beta}(t)-B_{\alpha,\beta}(s))}) = E_{\beta}(-y^2|t-s|^{\alpha}), \quad y \in \mathbb{R}. \tag{2.2.11}$$

**Proposition 2.2.7.** For any $0 < \alpha < 2$ and $0 < \beta \leq 1$, the process $B_{\alpha,\beta}(t), t \geq 0$, is a self-similar with stationary increments process (**H-sssi**), with $H = \alpha/2$.

**Proof.** See [21].

**Remark.** In view of Proposition 2.2.7, $\{B_{\alpha,\beta}(t)\}$ forms a class of **H-sssi** stochastic processes indexed by two parameters $0 < \alpha < 2$ and $0 < \beta \leq 1$. This class includes fractional Brownian motion ($\beta = 1$), grey Brownian motion ($\alpha = \beta$) and Brownian motion ($\alpha = \beta = 1$).

### Basic Properties of the ggBm

#### 2.3.3.1 The p-variation of generalized grey Brownian motion

This subsection is devoted to the study of the p-variation of ggBm. The approach taken is inspired from the one used for the fBm.

**Proposition 2.2.8.** We have the following limit in probability

$$\lim_{n \longrightarrow +\infty} n^{p\frac{\alpha}{2}-1} \sum_{j=1}^{n} \left| B_{\alpha,\beta}\left(\frac{j}{n}\right) - B_{\alpha,\beta}\left(\frac{j-1}{n}\right) \right|^p = \mathbb{E}(|B_{\alpha,\beta}(1)|^p).$$

**Proof.** See [4]

**Proposition 2.2.9.** We have the following limit in probability

$$V_{p,n} := \sum_{j=1}^{n} \left| B_{\alpha,\beta}(\frac{j}{n}) - B_{\alpha,\beta}(\frac{j-1}{n}) \right|^p \xrightarrow[n \longrightarrow +\infty]{} \begin{cases} 0 & a.s. \quad if \quad p\alpha/2 > 1 \\ \infty & a.s. \quad if \quad p\alpha/2 < 1 \\ \mathbb{E}(|B_{\alpha,\beta}(1)|^p) & a.s. \quad if \quad p = 2/\alpha. \end{cases}$$

**Remark.** The ggBm is not a semimartingale. In addition, $B_{\alpha,\beta}$ cannot be of finite variation on $[0,1]$ and by scaling and stationarity of the increment on any interval.

**Proof.** Indeed there is a subsequence such that $V_{p,n}$ converge almost surely to $\infty$ for $p = 1$ and $\alpha \in (0,2)$. If $\alpha \in (1,2)$ we can choose $p \in (2/\alpha, 2)$ such that $V_{p,n}$ converge to 0 for some subsequence. This implies that the quadratic variation of $B_{\alpha,\beta}$ is zero. if $\alpha \in (0,1)$ we can choose $p > 2$ such that $2p/\alpha < 1$ and the p-variation of $B_{\alpha,\beta}$ must be infinite. So, in any case $B_{\alpha,\beta}$ can not be a semimartingale.

#### 2.3.3.2 Characterization of th ggBm

We have seen that the generalized grey Brownian motion (ggBm), is made up off self-similar with stationary increments processes (Prop. 2.2.7) and depends on two real parameters $\alpha \in (0,2)$ and $\beta \in (0,1]$.

The ggBm is defined through the explicit construction of the underline probability space. However, we are now going to show that it is possible to define it in an unspecified probability space. For this purpose, we write down explicitly all the finite dimensional probability density functions. Moreover, we shall provide different ggBm characterizations.

**Proposition 2.2.10.** Let $B_{\alpha,\beta}$ be a ggBm, then for any collection $\{B_{\alpha,\beta}(t_1), ..., B_{\alpha,\beta}(t_n)\}$, the joint probability density function is given by:

$$f_{\alpha,\beta}(x_1, x_2, ..., x_n; \gamma_{\alpha,\beta}) = \frac{(2\pi)^{-\frac{n-1}{2}}}{\sqrt{2\Gamma(1+b)^n \det \gamma_{\alpha,\beta}}} \int_0^\infty \frac{1}{\tau^{n/2}} M_{1/2}\left(\frac{\zeta}{\tau^{1/2}}\right) M_\beta(\tau) d\tau. \quad (2.2.12)$$

with:

$$\zeta = \left(2\Gamma(1+\beta)^{-1} \sum_{i,j=1}^{n} x_i \gamma_{\alpha,\beta}^{-1}(t_i, t_j) x_j\right)^{1/2}, \quad (2.2.13)$$

$$\gamma_{\alpha,\beta}(t_i, t_j) = \frac{1}{\Gamma(1+\beta)}(t_i^\alpha + t_j^\alpha - |t_i - t_j|^\alpha), \qquad i,j = 1, ..., n. \quad (2.2.14)$$

**Proof.** See ([16]).

Using the Kolmogorov extension theorem, the above proposition allows us to define the ggBm in an unspecified probability space. In fact, given a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, the following proposition characterizes the ggBm:

**Proposition 2.2.11.** [16] Let $X(t), t \geq 0$, be a stochastic process, defined in a certain probability space $(\Omega, \mathcal{F}, \mathbb{P})$, such that

1. $X(t)$ has covariance matrix indicated by $\gamma_{\alpha,\beta}$ and finite-dimensional distributions defined by Eq. (2.2.12 ).
2. $\mathbb{E}X^2(t) = \dfrac{2}{\Gamma(1+\beta)} t^{\alpha}$ for $0 < \beta \leq 1$ and $0 < \alpha < 2$.
3. $X(t)$ has stationary increments,

then $X(t)$, $t \geq 0$, is a generalized grey Brownian motion.

In fact condition 2) together with condition 3) imply that $\gamma_{\alpha,\beta}$ must be the ggBm autocovariance matrix Eq. (2.2.10).

**Corollary 2.2.2.** [16] Let $X(t)$, $t \geq 0$, be a stochastic process defined in a certain probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Let $H = \alpha/2$ with $0 < \alpha < 2$ and suppose that

$$\mathbb{E}X(1)^2 = 2/\Gamma(1+\beta).$$

The following statements are equivalent:
i) $X$ is H-**sssi** with finite-dimensional distribution defined by Eq. (2.2.12);
ii) $X$ is a generalized grey Brownian motion with scaling exponent $\alpha/2$ and "fractional order" parameter $\beta$;
iii) $X$ has zero mean, covariance function $\gamma_{\alpha,\beta}(t,s)$, $t, s \geq 0$, defined by Eq. (2.2.10) and finite dimensional distribution defined by Eq. (2.2.12).

#### 2.3.3.3 Representation of ggBm

Up to now, we have seen that the ggBm $B_{\alpha,\beta}(t), t \geq 0$, is an H-sssi process, which generalizes Gaussian processes (it is indeed Gaussian when $\beta = 1$) and is defined only by its autocovariance structure. These properties make us think that $B_{\alpha,\beta}(t)$ may be equivalent to a process $\Lambda_\beta X_\alpha(t), t \geq 0$, where $X_\alpha(t)$ is a Gaussian process and $\Lambda_\beta$ is a suitable chosen independent random variable. In this section we will show that gBm $B_{\alpha,\beta}$ admits different representations involves certain known processes, such as fractional Brownian motion (fBm).

**Theorem 2.2.7.** (**Finite dimensional representation**, [2]) Let $B_{\alpha,\beta}$ be a gBm, then for any collection $X = \{B_{\alpha,\beta}(t_1), \ldots, B_{\alpha,\beta}(t_n)$ has characteristic function given by

$$\mathbb{E}(e^{i(\theta,X)}) = E_\beta\left(-\frac{1}{2}\theta^T \Sigma_\alpha \theta\right), \qquad \theta \in \mathbb{R}$$

and the joint probability density function is given by: $\theta \in \mathbb{R}^n$

$$f_{\alpha,\beta}(\theta, \Sigma_\alpha) = \frac{(2\pi)^{\frac{-n}{2}}}{\sqrt{det \Sigma_\alpha}} \int_0^\infty \tau^{\frac{-n}{2}} e^{-\frac{\theta^T \Sigma_\alpha^{-1} \theta}{2\tau}} M_\beta(\tau) d\tau,$$

where the $M$-Wright density function $M_\beta$ is such that

$$(\mathcal{L} M_\beta)(s) = E_\beta(-s).$$

and

$$\Sigma_\alpha = (t_i^\alpha + t_j^\alpha - |t_i - t_j|^\alpha)_{i,j=1}^n$$

**Proposition 2.2.12.** (**Normal variance mixture**, [2] ) Let $B_{\alpha,\beta}(t), t \geq 0$, be a ggBm, then

$$\{B_{\alpha,\beta}(t), t \geq 0\} \stackrel{d}{=} \{\sqrt{L_\beta} X_\alpha(t), t \geq 0\}, \tag{2.2.15}$$

where $X_\alpha(t)$ is a standard fBm , $L_\beta$ is an independent non negative random variable with probability density function $M_\beta(\tau), \tau \geq 0$.

The representation Eq. (2.2.15) is particularly interesting. In fact, a number of question, in particularly those related to the distribution properties of $B_{\alpha,\beta}(t)$, can be reduced to question concerning the fBm $X_\alpha(t)$.

#### 2.3.3.4 ggBm trajectories

In order to obtain examples of the $B_{\alpha,\beta}(t) = \sqrt{L_\beta} X_\alpha(t)$ trajectories, we just have to simulate the fractional Brownian motion $X_\alpha(t)$. For this purpose (See [16]). Some typical path simulations of $B_{\beta,\beta}(t)$ (shortly $B_\beta(t)$ and $B_{2-\beta,\beta}(t)$), with $\beta = 1/2$ are shown in Figures ((2.1), (2.2)). The first process provides an example of stochastic model for slow-diffusion (short-memory), the second provides a stochastic model for fast-diffusion (long-memory).

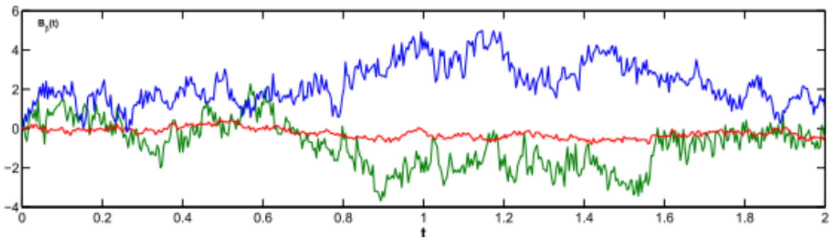

Figure 2.1: $B_\beta(t)$ trajectories in the case $\beta = 0.5$ for $0 \leq t \leq 2$

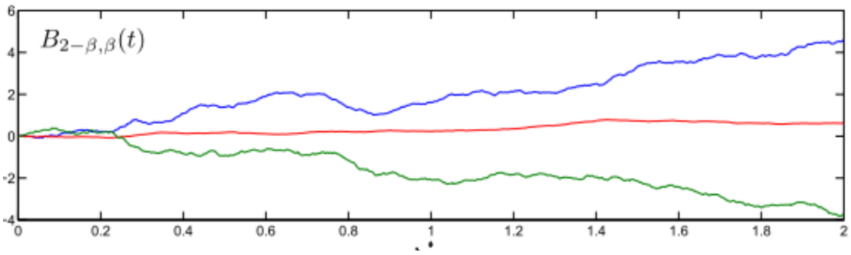


Figure 2.2: $B_{2-\beta,\beta}(t)$ trajectories in the case $\beta = 0.5$ for $0 \leq t \leq 2$.

#### 2.3.3.5 Hölder continuity

**Proposition 2.2.13.** [17] Let $0 < \alpha < 2$ and $0 < \beta < 1$. Then for all $p \in \mathbb{N}$ there exists $K < \infty$ such that $\mathbb{E}(\mid B_t^{\alpha,\beta} - B_s^{\alpha,\beta} \mid^{2p}) = K \mid t - s \mid^{\alpha p}, t, s \geq 0$.

The last proposition ensures that generalized grey Brownian motion has a continuous version. Indeed, choose $p \in \mathbb{N}$ such that $\alpha p > 1$ then the previous proposition provides the estimate $\mathbb{E}((B_t^{\alpha,\beta} - B_s^{\alpha,\beta})^{2p}) \leq k \mid t - s \mid^{1+p}$ with $q = \alpha p - 1 > 0$. This estimate is sufficient to apply Kolmogorov's continuity theorem.

#### 2.3.3.6 Long-range dependency

Because of the stationarity of the increments, the anomalous diffusion appears deeply related to the long-range dependence characterization of $B_{\alpha,\beta}(t)$. We remember that an H-sssi process has long-range dependence (or long memory) if $1/2 < H < 1$. This means that the discrete time process of its increments exhibits long-range correlation [16]. That is, the increments auto-correlation function $r(k)$ tends to zero with a power law as $k$ goes to infinity. Therefore, when $0 < \alpha < 1$ the diffusion is slow and the process has short memory. While when $1 < \alpha < 2$ the diffusion is fast and the process has long memory.

### 2.2.3 Continuous Time Random Walk (CTRW)

Continuous-time random walk (CTRW) is an extension of the random walk. More specifically, it is constructed by introducing a new source of randomness to the random walk. This new source of randomness is waiting time. It was first discussed by Montroll and Weiss(1965), Kenkre and al. (1973), Gorenflo and al. (2007) .

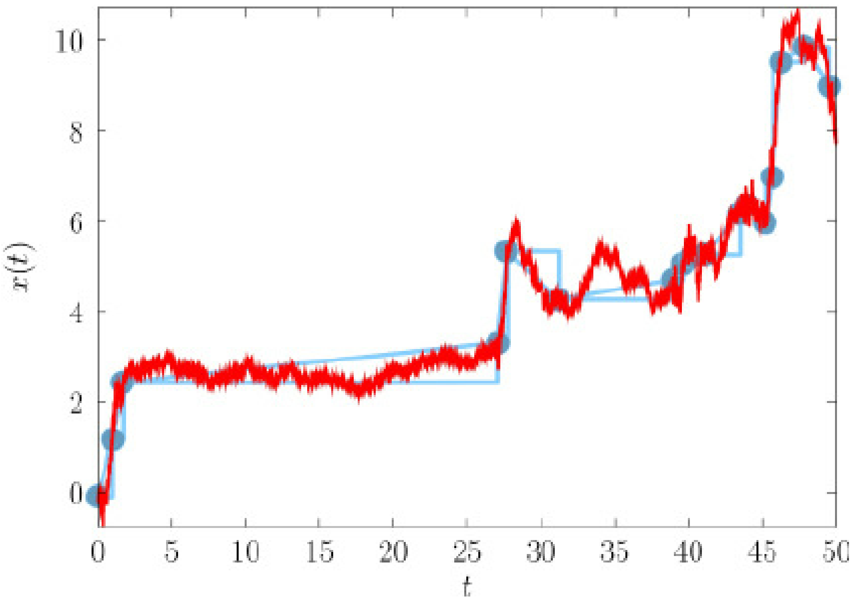


Figure 2.3: Schematic view on a continuous time random walk (CTRW)

**Definition 2.2.12.** A simple formulation of a CTRW is to consider the stochastic process $X(t)$ defined by $X(t) = X_0 + \sum_{i=1}^{N(t)} \Delta X_i$, whose increments $\Delta X_i$ are iid random variables taking values in a domain $\Omega$ and $N(t)$ is the number of jumps in the interval $(0, t)$. The probability for the process taking the value $X$ at time $t$ is then given by

$$P(X, t) = \sum_{n=0}^{\infty} P(n, t) P_n(X).$$

Here $P_n(X)$ is the probability for the process taking the value $X$ after $n$ jumps, and $P(n, t)$ is the probability of having $n$ jumps after time $t$, such that

$$P(n, t) \sim \frac{t^{\alpha-1}}{t^{\alpha} + \frac{\sigma^2 n^2}{2}} = \int_0^{\infty} t^{\alpha-1} e^{-kt^{\alpha}} e^{-\frac{k\sigma^2 n^2}{2}} dk.$$

**Remark.** The kind of diffusion that the CTRW formalism yields depends on the distribution of step increments:

- If the increments are small, then diffusion is normal, and a simple diffusion equation can be derived.

- If the increments are not small, then super as well as sub-diffusion can result, depending on the concrete choice of increment distributions.

- An important property of the CTRW equations is that they are non-local, both in space and time (which is also termed non-Markovian).

**Definition 2.2.13.** The waiting time probability density function with power law tails, i.e., for large $\tau$ is:

$$\phi(\tau) \backsim \frac{1}{\tau^{1+\alpha}}, \alpha > 0.$$

In this case, the first moment of waiting time is divergent for $0 < \alpha < 1$.

**Example 2.2.1.** An example is the heavy-tailed probability density function

$$\phi(\tau) = \begin{cases} 0, & \tau < \tau_0; \\ \alpha \frac{\tau_0^{\alpha}}{\tau^{1+\alpha}}, & \tau > \tau_0. \end{cases} \tag{2.2.16}$$

Here $\tau_0$ is a time scale.

**Properties**

Continuous Time Random Walks (CTRWs) exhibit several important properties that distinguish them from standard random walks. Here are some key properties of CTRWs:

1. Decoupling of time and space: CTRWs decouple temporal and spatial aspects, allowing for more flexible modeling of processes with independent or different mechanisms governing temporal and spatial dynamics.

2. Anomalous diffusion: CTRWs can exhibit subdiffusive or superdiffusive behavior depending on the choice of waiting time and jump length distributions, unlike standard Brownian motion.

3. Long-range correlations and memory effects: CTRWs can capture long-range correlations and memory effects due to broad or heavy-tailed waiting time distributions, resulting in temporally clustered or bursty events common in complex systems.

4. Non stationarity and aging: CTRWs can exhibit non-stationary behavior, allowing for the evolution of statistical properties over time, especially in modeling systems undergoing aging or gradual changes in dynamics.

5. Fractional dynamics: CTRWs can cause fractional dynamics, involving fractional derivatives or calculus, due to power-law tails in the waiting time distribution, causing long-range temporal correlations and memory effects.

**Application: Dynamics of the Asset Prices**

Modeling dynamics of asset prices plays important role in a lot of microeconomics problems. For example, by understanding the behavior of stock prices, one can take good decision for a portfolio [9]. Continuous-time random walk process is a suitable class of process for modeling the behavior of high frequency data.

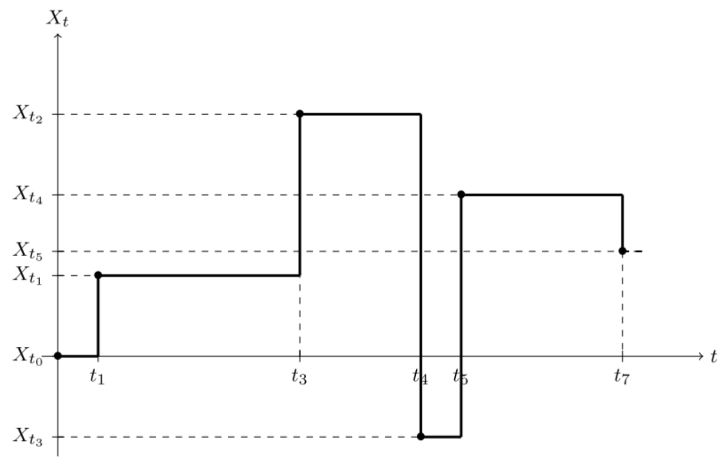


Figure 2.4: A trajectory for the continuous-time random walk process: tick-by-tick price fluctuation.

Figure (2.4) shows a trajectory for the continuous-time random walk. It shows two random variables play important role in the structure of this process: jump magnitude, and waiting time. Unlike the random walk, the waiting time for jumps is not the same during time. It is perfect to describe the behavior of dynamics of The initial setting for implementing the continuous-time random walk for studying the behavior of asset prices is as follows. Denote the waiting times between each trade by $\{j_1, j_2, \cdots, j_n, \cdots\}$. Let $(P_t)_{t\geq 0}$ and $S_t = log(P_t)$ be the price process and log-price of an asset at time $t$. The waiting time random variables are independent and identically distributed. Let $X_1, X_2, \cdots, X_n, \cdots$ be the log return process, more specifically, $X_n$ is given by

$$X_n = S_n - S_{n-1} = log(P_n) - log(P_{n-1}) = log\left(\frac{P_n}{P_{n-1}}\right). \tag{2.2.17}$$

Without loss of generality we assume $X_0 = 0$. Bear in mind that the log-return is more convenient to study the behavior of asset price. Moreover, the log-return random variables are independent and identically distributed. If the random variables $j_n$ and $\Delta X_n$ are independent for each value of $n$, then $X_n$ is called an uncoupled continuous-time random walk process, and if they are dependent, $X_n$ is called a coupled continuous-time random walk process. Let $T_n = j_1 + j_2 + ... + j_n$ be the time $n^{th}$ trade. The number of trades by time $t > 0$ is $N_t = \max\{n : T_n \leq t\}$, and therefore, the log-price at time t is given by $S_{N_t} = log(P_{T_n}) = X_1 + X_2 + ... + X_{N_t}$.

This equation is a subordinated process. More specifically, the calendar time $t$, for the stochastic process $S_t$ is changed with business time, $N_t$. If the waiting times are exponentially distributed, the continuous-time random walk process is a compound Poisson process. Therefore, the continuous-time random process is a Markovian process that belongs to the class of Lévy processes. In this case, the distribution for the log-price is Gaussian and for the price the distribution is log-normal. Some properties for the distribution for a continuous-time random walk process are summarized as follows:

- If the log-returns process has finite variance and $c \to \infty$ , then $c^{\frac{1}{2}} S_{ct} \to B_t$ . $B_t$ is Brownian motion and its probability density function, $f(X,t)$, is the solution of
$$\frac{\partial f(X,t)}{\partial t} = D\frac{\partial^2 f(X,t)}{\partial X^2}, \tag{2.2.18}$$
where $D > 0$.

- If the waiting time random variables have a finite mean such as $\frac{1}{\lambda}$, then $N_t \sim \lambda t$, when $t \to \infty$. Therefore, the the scaling limit of a continuous-time random walk is a Brownian motion and its probability density function satisfies Eq. (2.2.18)

- If the distribution of log-returns is symmetric, with zero mean, and its tail has power-law probability, then the random walk $S_n$ is asymptotically a stable process. More specifically, if $P(|X_n| > r) \sim r^{-\alpha}$, then $c^{-\frac{1}{\alpha}} S_{ct} \to A_t$, where $A_t$ is a stable process. The probability density function for the stable process $A_t$ is the solution
$$\frac{\partial f(X,t)}{\partial t} = D\frac{\partial^\alpha f(X,t)}{\partial |X|^\alpha}, \tag{2.2.19}$$

**Remark.**

- The probability density function for the continuous-time random walk process does not exist in closed-form, it can be obtained in an asymptotic form.

- The compound poisson process is special class of the continuous-time random walk processes where the distribution of the waiting time random variable is exponential.

### 2.2.4 Fractional Itô motion (FIM)

With the notion of Itô SDEs recalled, we introduce the following model: fractional Itô motion FIM, $I_H(t)$ $(t \geq 0)$ , where the subscript $H$ manifests the underlying Hurst exponent. In analogy with fBm, we name FIM in honor of Kioshi Itô the mathematician that invented the white-noise stochastic calculus.

The dynamics of FIM are governed by the Itô SDE

$$\dot{I}_H(t) = |I_H(t)|^{1-\frac{1}{2H}} \dot{B}(t) \tag{2.2.20}$$

Namely, FIM has a zero drift, $\mu(x) = 0$, and a power-law volatility, $\sigma(x) = |x|^{1-\frac{1}{2H}}$. Where $\dot{B}(t)$ is the white noise , we initiate FIM from the spatial origin $I_H(0) = 0$. Hence, integrating Eq. (2.2.20) yields

$$I_H(t) = \int_0^t |I_H(u)|^{1-\frac{1}{2H}} \dot{B}(u) du. \tag{2.2.21}$$

The right-hand side of Eq. (2.2.21) is a running Itô integral.

#### Martingale and Markov property

**Proposition 2.2.14.** [6] A general running Itô integral with an integrand that does not 'look into the future' is a symmetric process and a martingale, hence, in particular, FIM exhibits these properties.

**Proposition 2.2.15.** [6] The FIM is a Markov process and martingale.

#### Self-similarity Property

**Proposition 2.2.16.** [6] FIM is a self-similar process, and the Hurst exponent of FIM takes values in the range $0 < H < 1$. Hence, the diffusivity of FIM is identical to the aforementioned diffusivity of FBM:

1. sub-diffusion in the exponent range $0 < H < 1/2$,
2. super-diffusion in the exponent range $1/2 < H < 1$,
3. regular diffusion at the exponent value $H = 1/2$. Indeed, setting $H = 1/2$ in Eq. (2.2.21) yields BM: $I_{1/2}(t) = B(t)$.

**Proposition 2.2.17.** [6]

The FIM is a process with a continuous trajectory, non-Gaussian dissipation patterns.

### Stationary Processes

Using the fact that FIM is a selfsimilar process with Hurst exponent $H$, as well as the fact that FIM is a martingale, it is shown in the Methods that the FIM increment

$$I_H(t+\Delta) - I_H(t)$$

is a random variable with mean zero and with variance

$$Var[I_H(t+\Delta) - I_H(t)] = Var[I_H(1)].(t+\Delta)^{2H} - t^{2H}. \tag{2.2.22}$$

The variance of Eq. (2.2.22) depends on the starting point $t$, as well as on the length $\Delta$, of the temporal interval $[t, t+\Delta]$. Hence, Eq. (2.2.22) implies that the increments of FIM are not stationary [6].

## Fractional Brownian motion vs fractional Itô motion

In this section we carry on with visual comparisons that examine profound differences between fBm and FIM. comparisons between simulated trajectories of fBm and FIM are offered by ( figure (2.5)) (for sub-diffusion) and by ( figure (2.7)) (for super-diffusion).

- The FIM shares the 'upside' features of fBm: It is a random-motion model which is symmetric and selfsimilar, and whose trajectory is continuous that generalizes BM. Produces both sub-diffusion and super-diffusion. As FIM is a Markov process and a martingale, it circumvents the 'downside' features of fBm: it well applies in the context of stochastic integration.

- As fBm and FIM are selfsimilar processes, they both initiate from the spatial origin. Hence, from a probabilistic perspective, at time 0 both these random motions manifest a unit mass that is placed at the origin. In turn, at a positive time $t$, this unit mass dissipates, and the 'shape of the dissipation' is quantified by a probability density function: the density of the randomvariable $B_H(t)$, in the case of fBm; and the density of the random variable $I_H(t)$, in the case of FIM.

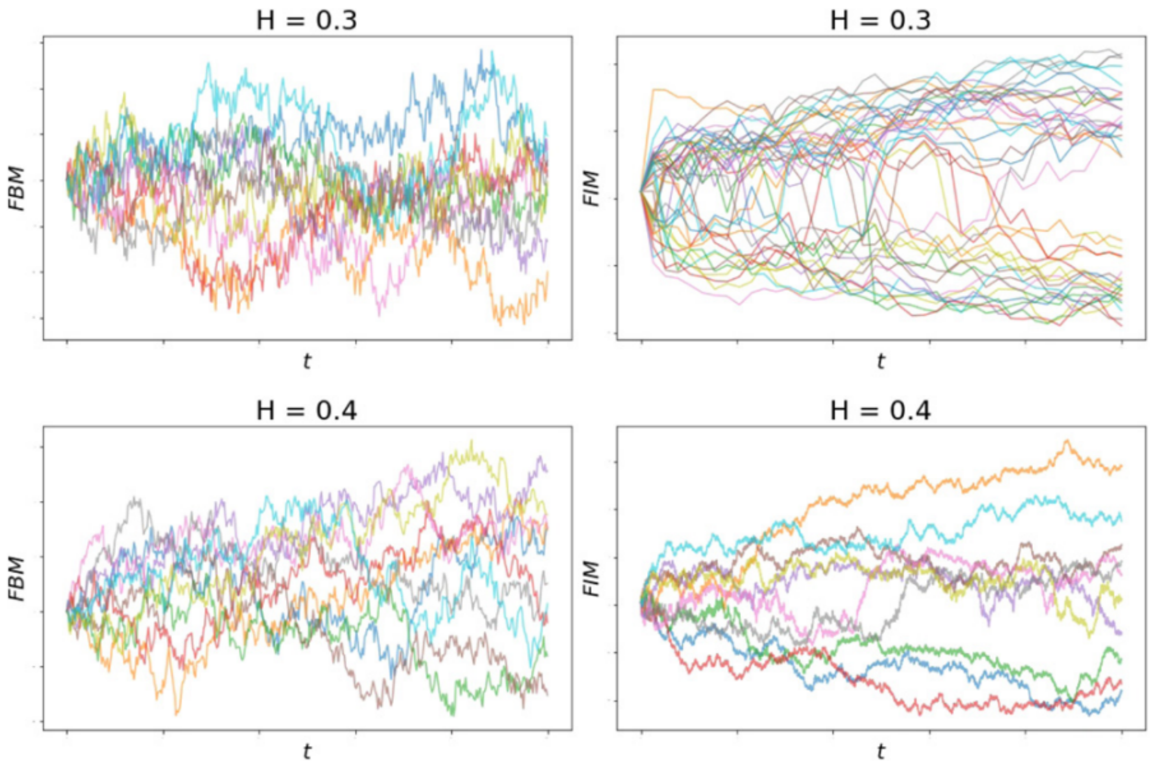


Figure 2.5: Simulated trajectories of sub-diffusive fBm (left panels) and of sub-diffusive FIM (right panels).

The properties of fBm imply that:

- $B_H(t)$ is normal with mean zero and with variance $Var[B_H(t)] = Var[B_H(1)] \cdot t^2H$. Hence, setting $b = Var[B_H(1)]$, the density of the random variable $B_H(t)$ is:

$$\frac{1}{\sqrt{2\pi b}} \cdot \frac{1}{t^H} exp\left(-\frac{x^2}{2bt^{2H}}\right). \tag{2.2.23}$$

This density is a symmetric 'bell curve' (see figure (2.7)): it vanishes at $x \to \pm\infty$ , and it has a unimodal shape the peaks at the spatial origin $x = 0$. We emphasize that the shape of this density is the same for all the values of the Hurst exponent $H$.

- While the density of the random variable $I_H(t)$ is

$$\frac{1}{2H\Gamma(1-H)} \cdot \left(\frac{2H^2}{t}\right)^{1-H} exp\left(-\frac{2H^2}{t}|x|^{1/H}\right)|x|^{1/H-2} \tag{2.2.24}$$

$(-\infty < x < \infty)$. This density is symmetric, and it vanishes at $x \to \pm\infty$. The shape of this density is determined by the value of the Hurst exponent $H$, as follows (see figure (2.7)).

– In the sub-diffusion range, $0 < H < 1/2$ , the density has a bimodal shape: it vanishes at the spatial origin $x = 0$, and it peaks at the spatial points

$$x = \pm\frac{1-2H}{2H^2}t^H;$$

at these points the density's peak height is $c_H/t^H$, where $c_H$ is a constant that depends on the Hurst exponent $H$.

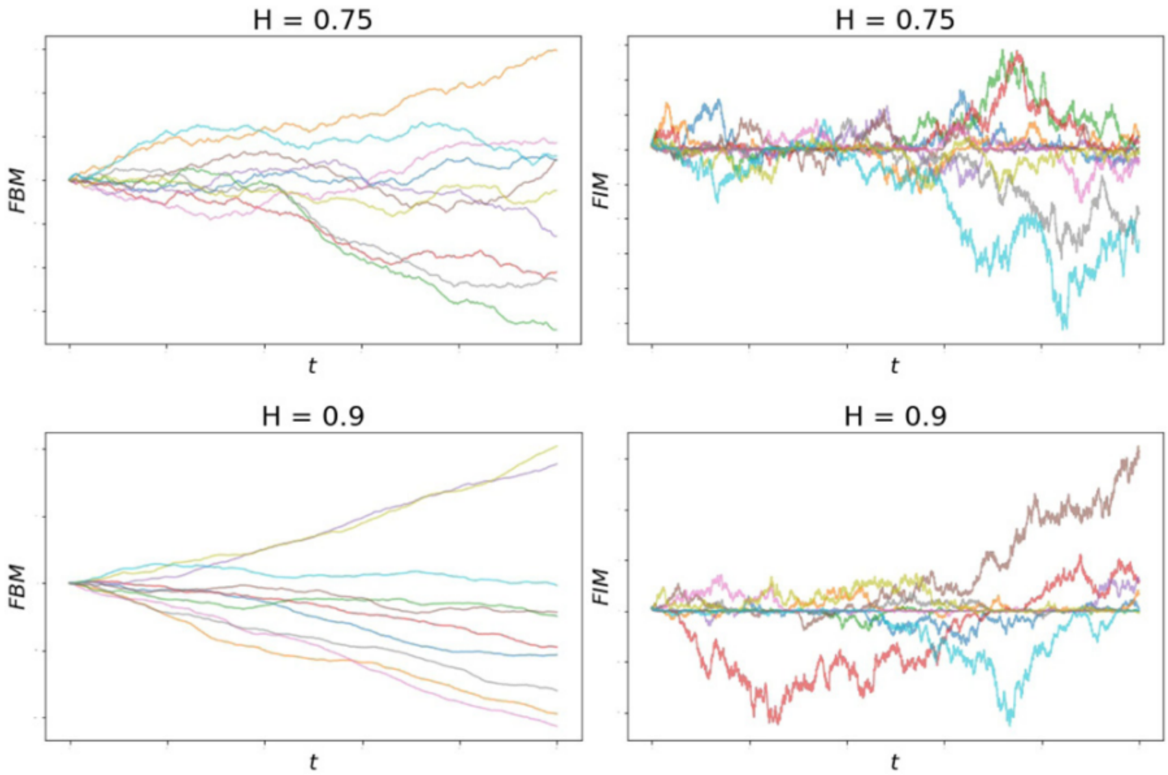


Figure 2.6: Simulated trajectories of super-diffusive fBm(left panels) and of super-diffusive FIM (right panels).

– At the regular-diffusion value, $H = 1/2$, the density is a 'bell curve': it has a uni modal shape that peaks at the spatial origin $x = 0$.

– In the super-diffusion range, $1/2 < H < 1$, the density has a unimodal shape that explodes at the spatial origin $x = 0$.

– The differences between the shape of the Gaussian fBm density of Eq. (2.2.23) and the shape of the non-Gaussian (for $H \neq 1/2$) FIM density of Eq. (2.2.24) are dramatic. On the one hand, changing the Hurst exponent $H$ in the fBm model has no qualitative effect on the shape of the dissipation pattern. On the other hand, changing the Hurst exponent $H$ in the FIM model has a profound qualitative effect on the shape of the dissipation pattern.

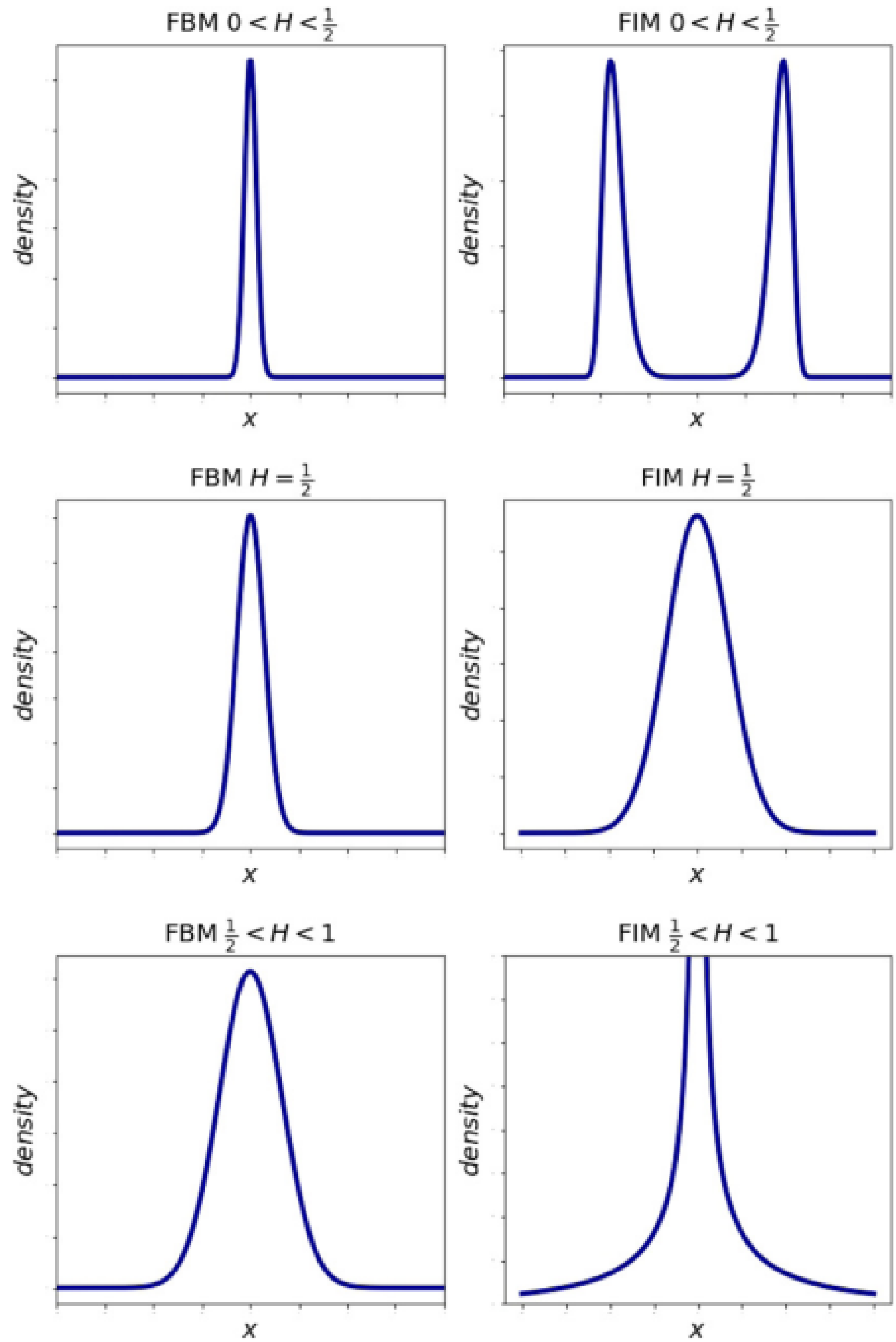


Figure 2.7: Schematic illustrations of the shapes of the FBM and FIM dissipation patterns (for a fixed positive time point t).

Table 2.1: A 'bird's-eye view' comparison between the FBM and FIM models with Hurst exponents $H \neq 1/2$.

| | **BM** | **FBM** | **FIM** |
|---|---|---|---|
| Finite variance | | YES | |
| Symmetric process | | YES | |
| Continuous trajectory | | YES | |
| Selfsimilar process | | YES | |
| Hurst exponent | H = 1/2 | 0 < H < 1 | 0 < H < 1 |
| Gaussian process | YES | YES | NO |
| Markov process | YES | NO | YES |
| Martingale | YES | NO | YES |
| Stationary increments | YES | YES | NO |
| Uncorrelated increments | YES | NO | YES |

Chapter 3

# Fractional anomalous diffusion

In this chapter we will first introduce the basic notions of fractional calculus. The area of mathematics that allows non-integer order integrals and derivatives. Since its to begin with appearance within the late $17^{th}$ century it has ended up well known (particularly among scientists and engineers) because numerous issues are depicted by, and can be fathomed utilizing fractional calculus. Further details on fractional calculus can be found in [11, 19] and references therein.

## 3.1 Fractional calculus

### 3.1.1 Basic definitions of fractional derivatives and Integrals

This section is devoted to review the most important definitions of fractional derivatives and Integrals.

#### 3.2.1.1 Grünwald-Letnikov, 1867-1868.

Grünwald-Letnikov derivative or also named Grünwald-Letnikov differintegral is a basic extension of the natural derivative to fractional one. It was introduced by A. Grünwald in 1867, and then by A. Letnikov in 1868. Hence, it is written as

$$f^{'}(x) = \lim_{h \to 0} \frac{f(x) - f(x-h)}{h},$$

Applying this formula again, we can find the second derivative:

$$\begin{aligned} f''(x) &= \lim_{h\to 0} \frac{f'(x) - f'(x-h)}{h}, \\ &= \lim_{h_1\to 0} \frac{\lim_{h_2\to 0} \frac{f(x+h_2)-f(x)}{h_2} - \lim_{h_2\to 0} \frac{f(x-h_1-h_2)-f(x-h_1)}{h_2}}{h_1}. \end{aligned}$$

By choosing the same value of $h$, i.e. $h_1 = h_2 = h$, the expression simplifies to

$$f''(x) = \lim_{h\to 0} \frac{f(x-2h) - 2f(x-h) + f(x)}{h^2},$$

For the $n^{\text{th}}$ derivative, this procedure can be consolidated into the following summation

$$f^n(x) = D^n f(x) = \lim_{h\to 0} \frac{1}{h^n} \sum_{m=0}^{n} (-1)^m \binom{n}{m} f(x - mh).$$

$$\binom{n}{m} = \frac{n!}{m!(n-m)!}.$$

This expression can be generalized for non-integer values for $n$ with $\alpha \in \mathbb{R}$ provided that the binomial coefficient be understood as using the Gamma Function as $\dfrac{\Gamma(\alpha+1)}{m!\Gamma(\alpha-m+1)}$ in place of the standard factorial. Also, the upper limit of the summation (no longer the integer, $n$) goes to infinity as $\dfrac{t-a}{h}$ (where $t$ and $a$ are the upper and lower limits of differentiation, respectively).

We are left with the generalized form of the **Grünwald-Letnikov** fractional derivative.

$${}_aD^\alpha f(x) = \lim_{h\to 0} \frac{1}{h^\alpha} \sum_{m=0}^{[\frac{x-a}{h}]} (-1)^m \frac{(\alpha-1)!}{m!(\alpha-m+1)!} f(x - mh).$$

For negative $\alpha$, the process will be integration. Therefore, for integration we write

$${}_aD^{-\alpha} f(x) = \lim_{h\to 0} h^\alpha \sum_{m=0}^{[\frac{x-a}{h}]} \frac{\Gamma(\alpha+m)}{m!\Gamma(\alpha)} f(x - mh),$$

or equivalently,

$${}_aD^{-\alpha} f(x) = \lim_{n\to\infty} \left(\frac{n}{x-a}\right)^\alpha \sum_{m=0}^{n} \frac{\Gamma(\alpha+m)}{m!\Gamma(\alpha)} f\left(x - m\left(\frac{x-a}{n}\right)\right).$$

#### 3.2.1.2 Riemann-Liouville, 1832-1847.

The Riemann-Liouville operator is still the most frequently used when fractional integration is performed. It is considered a direct generalization of Cauchy's formula.

We begin by introducing a fractional integral of integer order $n$ in the form of Cauchy formula.

$$ {}_aD_x^{-n}f(x) = \frac{1}{\Gamma(n)}\int_a^x (x-t)^{n-1}f(t)\,dt, $$

It will be shown that the above integral can be expressed in terms of n-multiple integral, that is

$$ {}_aD_x^{-n}f(x) = \int_0^x dx_1 \int_a^{x_1} dx_2 \int_a^{x_2} dx_3 \ldots \int_a^{x_{n-1}} f(t)\,dt. \tag{3.1.1} $$

When $n = 2$, by using the well-known Dirichlet formula, namely

$$ \int_a^b dx \int_a^x f(x,y)dy = \int_a^b dy \int_y^b f(x,y)\,dx, \tag{3.1.2} $$

Eq. (3.1.1) becomes

$$ \begin{aligned} \int_a^x dx_1 \int_a^{x_1} f(t)\,dt &= \int_a^x dt f(t) \int_t^x dx_1 \\ &= \int_a^x (x-t)f(t)\,dt. \end{aligned} \tag{3.1.3} $$

This shows that the two-fold integral can be reduced to a single integral with the help of Dirichlet formula. For $n = 3$, the integral in Eq. (3.1.1) gives

$$ \begin{aligned} {}_aD_x^{-3}f(x) &= \int_a^x dx_1 \int_a^{x_1} dx_2 \int_a^{x_2} f(t)\,dt, \\ &= \int_a^x dx_1 \left[\int_a^{x_1} dx_2 \int_a^{x_2} f(t)\,dt\right]. \end{aligned} \tag{3.1.4} $$

By using the result in Eq. (3.1.3), the integrals within big brackets simplify to yield

$$ {}_aD_x^{-3}f(x) = \int_a^x dx_1 \left[\int_a^{x_1} (x_1-t)f(t)\,dt\right]. $$

If we use Eq. (3.1.2), then the above expression reduces to

$$ {}_aD_x^{-3}f(x) = \int_a^x dt f(t) \int_x^t (x_1-t)dx_1 = \int_a^x \frac{(x-t)^2}{2!}f(t)\,dt. $$

Continuing this process, we finally obtain

$$ {}_aD_x^{-n}f(x) = \frac{1}{(n-1)!}\int_a^x (x-t)^{n-1}f(t)\,dt. \tag{3.1.5} $$

It is evident that the integral in Eq. (3.1.5) is meaningful for any number $n$ provided its real part is greater than zero.

**Definition 3.1.1. (Riemann-Liouville fractional integrals)**
Let $f(x) \in \mathbb{L}(a, b)$, $\alpha > 0$, then

$$ {}_aI_x^{\alpha} f(x) = {}_aD_x^{-\alpha} f(x) = I_{a+}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x \frac{f(t)}{(x-t)^{1-\alpha}} dt, \qquad (3.1.6) $$

and

$$ {}_xI_b^{\alpha} f(x) = {}_xD_b^{-\alpha} f(x) = I_{b-}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_x^b \frac{f(t)}{(t-x)^{1-\alpha}} dt. \qquad (3.1.7) $$

for $x > a$ is called Riemann-Liouville left-sided and right-sided fractional integral, respectively, of order $\alpha$.

**Theorem 3.1.1.** Let $f \in \mathbb{L}_1[a, b]$ and $\alpha > 0$. Then, the integral $I_a^{\alpha} f(x)$ exists for almost every $x \in [a, b]$. Moreover, the function $I_a^{\alpha} f$ itself is also an element of $\mathbb{L}_1[a, b]$.

**proof.** We write the integral in question as

$$ \int_a^x (x-t)^{\alpha-1} f(t) dt = \int_{-\infty}^{+\infty} \phi_1(x-t)\phi_2(t) dt, $$

where

$$ \phi_1(u) = \begin{cases} u^{\alpha-1}, & for \quad 0 < u \leq b-a \\ 0, & else \end{cases} $$

and

$$ \phi_2(u) = \begin{cases} f(u), & for \quad a < u \leq b \\ 0, & else \end{cases} $$

By construction, $\phi_j \in \mathbb{L}(\mathbb{R})$ for $j \in \{1, 2\}$ and thus by a classical result on Lebesgue integration.

**Example 3.1.1.** If $f(x) = (x-a)^{\beta-1}$, then find the value of ${}_aI_x^{\alpha} f(x)$.

We have

$$ {}_aI_x^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1}(t-a)^{\beta-1} dt. $$

If we substitute $t = a + y(x-a)$ in the above integral, it reduces to

$$ \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} (x-a)^{\alpha+\beta-1} $$

where $\beta > 0$. Thus

$$ {}_aI_x^{\alpha} f(x) = \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} (x-a)^{\alpha+\beta-1} $$

Having established these fundamental properties of Riemann-Liouville integral operators, we now come to the corresponding differential operators.

**Definition 3.1.2. (Riemann-Liouville Fractional Derivative)**
Let $(n-1) \leq \alpha < n$. The operator ${}_aD_x^\alpha$, defined by

$$ {}_aD_x^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dt}\right)^n \int_a^x \frac{f(t)}{(x-t)^{\alpha-n+1}} dt, $$

and

$$ {}_xD_b^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dt}\right)^n \int_x^b \frac{f(t)}{(t-x)^{\alpha-n+1}} dt. $$

is called the Riemann-Liouville left-sided and right-sided fractional differential operator, respectively, of order $\alpha$.
For $\alpha = 0$, we set $D^0 := I$, the identity operator.

### 3.2.1.3 Caputo Fractional Derivative, 1967

The Caputo fractional derivative is considered to be an alternative definition for Riemann-Liouville definition, it is introduced by the Italian Mathematician Caputo in 1967.

**Definition 3.1.3.** Let $\alpha > 0$, the Caputo left-sided and right-sided fractional differential operator of order $\alpha$ is given by:

$$ {}_a^CD_x^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x \frac{f^{(n)}(t)}{(x-t)^{\alpha-n+1}} dt, $$

and

$$ {}_x^CD_b^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \int_x^b \frac{f^{(n)}(t)}{(t-x)^{\alpha-n+1}} dt, $$

and

$$ {}_a^CD_x^\alpha f(x) = I_a^{n-\alpha} f^{(n)}(x). $$

### 3.2.1.4 Other definitions of fractional derivative

In the recent years, new definitions of fractional derivative have been introduced in the literature. Interesting examples are Marchaud, Hilfer and Canavati fractional derivatives.

**Definition 3.1.4.** (***Marchaud derivative:1927***) For a function defined on $\mathbb{R}$ and for every $\alpha \in (0,1)$ distinguishing two types of derivatives, respectively from the right and from the left one :

$$D_{+}^{\alpha}f(x) = \frac{\alpha}{\Gamma(1-\alpha)} + \int_{0}^{\infty} \frac{f(x)-f(x-t)}{t^{1+\alpha}}dt,$$

and

$$D_{-}^{\alpha}f(x) = \frac{\alpha}{\Gamma(1-\alpha)} + \int_{-\infty}^{0} \frac{f(x)-f(x+t)}{t^{1+\alpha}}dt.$$

These fractional derivatives are well defined when f is a bounded, locally Hölder continuous function in $\mathbb{R}$.

**Remark.** If we compare the Marchaud derivative with respect to the Riemann-Liouville one, we immediately realize that, in the latter one, the classical derivative operator appears, while, in the first one, it does not. This is one of the key points that Marchaud's definition makes evident. That is, Marchaud derivative avoids applying the classical derivative after an integration in order to define the fractional operator.

**Definition 3.1.5.** (***Hilfer derivative:2000***) Let $\mu \in (0,1)$, $\nu \in [0,1]$, and $f \in L^{1}[a,b]$, $a < t < b$. The Hilfer derivative is defined as

$$(D_{a+}^{\mu,\nu}f)(t) = \left(I_{a+}^{\nu(1-\mu)}\frac{d}{dt}\left(I_{a+}^{(1-\nu)(1-\mu)}f\right)\right)(t);$$

$$(D_{b-}^{\mu,\nu}f)(t) = \left(I_{b-}^{\nu(1-\mu)}\frac{d}{dt}\left(I_{b-}^{(1-\nu)(1-\mu)}f\right)\right)(t).$$

**Remark.** Notice that Hilfer derivatives coincide with Riemann-Liouville derivatives for $\nu = 0$ and with Caputo derivatives for $\nu = 1$.

**Definition 3.1.6.** (***Canavati derivative:2009***) Let $n-1 < \alpha < n, f \in \mathcal{C}^{\alpha}([a,b])$. Then, the Canavati derivative of order $\alpha$ is defined as

$$_{a}^{Can}D_{t}^{\alpha}f(t) = \frac{1}{\Gamma(n-\alpha)} + \frac{d}{dt}\int_{a}^{t} \frac{f^{(n-1)}(\tau)}{(t-\tau)^{\alpha-n+1}}d\tau.$$

## 3.1.2 The basic properties of fractional operator

### 3.2.2.1 Representation

**Lemma 3.1.1.** [19]

- The Riemann Liouville fractional derivative is equivalent to the composition of the same operator ($(n-\alpha)$-fold integration and $n-th$ ordre differentiation) but in reverse ordre i.e

$$_{a}D_{x}^{\alpha}f(x) = D^{n}I_{a}^{n-\alpha}f(x)$$

- Let $n-1<\alpha<n$, $n\in\mathbb{N}$, $\alpha\in\mathbb{R}$ and $f(x)$ be such that ${}^{C}D_{a}^{\alpha}f(x)$ exists. Then,

$$ {}_{a}^{C}D_{x}^{\alpha}f(x)=I_{a}^{n-\alpha}D^{n}f(x). $$

**Proposition 3.1.1.** In general the two operators, Riemann-Liouville and Caputo, do not coincide, i.e,

$$ {}_{a}D_{x}^{\alpha}f(x)\neq {}_{a}^{C}D_{x}^{\alpha}f(x) $$

**proof.** The well-known Taylor series expansion about the point 0 is

$$ \begin{aligned} f(x) &= f(0)+xf^{(1)}(0)+\frac{x^{2}}{2!}f^{(2)}(0)+\frac{x^{3}}{3!}f^{(3)}(0)+...+\frac{x^{n-1}}{(n-1)!}f^{(n-1)}(0)+R_{n-1} \\ &= \sum_{k=0}^{n-1}\frac{x^{k}}{\Gamma(k+1)}f^{(k)}(0)+R_{n-1} \\ R_{n-1} &= \int_{0}^{x}\frac{f^{(n)}(s)(x-s)^{n-1}}{(n-1)!}ds=\frac{1}{\Gamma(n)}\int_{0}^{x}f^{(n)}(s)(x-s)^{n-1}ds \\ &= I^{n}f^{(n)}(x). \end{aligned} $$

Using the linearity property of R-L and representation property of Caputo

$$ {}_{a}^{C}D_{x}^{\alpha}f(x)=I^{n-\alpha}D^{n}f(x). $$

and

$$ \begin{aligned} {}_{a}D_{x}^{\alpha}f(x) &= {}_{a}D_{x}^{\alpha}\left(\sum_{k=0}^{n-1}\frac{x^{k}}{\Gamma(k+1)}f^{(k)}(0)+R_{n-1}\right) \\ &= \sum_{k=0}^{n-1}\frac{{}_{a}D_{x}^{\alpha}x^{k}}{\Gamma(k+1)}f^{(k)}(0)+\ {}_{a}D_{x}^{\alpha}R_{n-1} \\ &= \sum_{k=0}^{n-1}\frac{x^{k-\alpha}}{\Gamma(k+1)}f^{(k)}(0)+\ {}_{a}D_{x}^{\alpha}I^{n}f^{(n)}(x) \\ &= \sum_{k=0}^{n-1}\frac{x^{k-\alpha}}{\Gamma(k+1)}f^{(k)}(0)+I^{n-\alpha}f^{(n)}(x) \\ &= \sum_{k=0}^{n-1}\frac{x^{k-\alpha}}{\Gamma(k+1)}f^{(k)}(0)+\ {}_{a}^{C}D_{x}^{\alpha}f(x). \end{aligned} $$

This means that

$$ {}_{a}D_{x}^{\alpha}f(x)\neq\ {}_{a}^{C}D_{x}^{\alpha}f(x) $$

**Proposition 3.1.2.** The relation between the Riemann-liouville and Caputo fractional derivatives is given by:

$$ {}_{a}^{C}D_{x}^{\alpha}f(x)=\ {}_{a}D_{x}^{\alpha}\left(f(x)-\sum_{k=0}^{n-1}\frac{t^{k}}{k!}f^{(k)}(0)\right). $$

**proof.** The proof result of Proposition 3.1.1 is

$$_aD_x^\alpha f(x) = \sum_{k=0}^{n-1} \frac{x^{k-\alpha}}{\Gamma(k+1)} f^{(k)}(0) + {}_a^C D_x^\alpha f(x)$$

This means that

$${}_a^C D_x^\alpha f(x) = {}_aD^\alpha \left( f(x) - \sum_{k=0}^{n-1} \frac{x^k}{k!} f^{(k)}(0) \right).$$

#### 3.2.2.2 Interpolation

**Lemma 3.1.2.**

- Let $n-1 < \alpha < n$, $n \in \mathbb{N}$, $\alpha \in \mathbb{R}$ and $f(t)$ be such that $D^\alpha f(t)$ exists. Then the following properties for the R-L operator hold:

$$\begin{aligned} \lim_{\alpha \longrightarrow n} D^\alpha f(t) &= f^{(n)}(t), \\ \lim_{\alpha \longrightarrow n-1} D^\alpha f(t) &= f^{(n-1)}(t). \end{aligned}$$

- Let $n-1 < \alpha < n$, $n \in \mathbb{N}$, $\alpha \in \mathbb{R}$ and $f(t)$ be such that ${}^C D^\alpha f(t)$ exists. Then the following properties for the Caputo operator hold:

$$\begin{aligned} \overset{C}{\lim_{\alpha \longrightarrow n}} D^\alpha f(t) &= f^{(n)}(t), \\ \overset{C}{\lim_{\alpha \longrightarrow n-1}} D^\alpha f(t) &= f^{(n-1)}(t) - f^{(n-1)}(0). \end{aligned}$$

**proof.** The proof uses integration by parts.

$$\begin{aligned} {}^c D^\alpha f(t) &= \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{f^{(n)}(s)}{(t-s)^{\alpha+1-n}} ds \\ &= \frac{1}{\Gamma(n-\alpha)} \left( -f^{(n)}(s) \frac{(t-s)^{n-\alpha}}{n-\alpha} \bigg|_{s=0}^{t} - \int_0^t -f^{(n-1)}(s) \frac{(t-s)^{n-\alpha}}{n-\alpha} ds \right) \\ &= \frac{1}{\Gamma(n-\alpha+1)} \left( f^{(n)}(0) t^{n-\alpha} + \int_0^t f^{(n+1)}(s)(t-s)^{n-\alpha} ds \right). \end{aligned}$$

Now, by taking the limit for $\alpha \longrightarrow n$ and $\alpha \longrightarrow n-1$, respectively, it follows

$$\overset{C}{\lim_{\alpha \longrightarrow n}} D^\alpha f(t) = \left( f^{(n)}(0) + f^{(n)}(s) \right) \bigg|_{s=0}^{t} = f^{(n)}(t)$$

and

$$\begin{aligned} \overset{C}{\lim_{\alpha \longrightarrow n-1}} D^\alpha f(t) &= \left( f^{(n)}(0) + f^{(n)}(s)(t-s) \right) \bigg|_{s=0}^{t} - \int_0^t -f^{(n)}(s) ds \\ &= f^{(n-1)}(s) \bigg|_{s=0}^{t} \\ &= f^{(n-1)}(t) - f^{(n-1)}(0). \end{aligned}$$

For the Riemann-Liouville fractional differential operator the corresponding interpolation property reads

$$\lim_{\alpha \longrightarrow n} D^{\alpha} f(t) = f^{(n)}(t),$$
$$\lim_{\alpha \longrightarrow n-1} D^{\alpha} f(t) = f^{(n-1)}(t).$$

#### 3.2.2.3 Non-commutation

**Lemma 3.1.3.**

- Let $n-1 < \alpha < n$, $m, n \in \mathbb{N}$, $\alpha \in \mathbb{R}$ and the function $f(x)$ is such that ${}_aD_x^{\alpha} f(x)$ exists. Then, in general, Riemann Liouville operator is also non-commutative and satisfies

$$D^m \left( {}_aD_x^{\alpha} f(x) \right) = {}_aD_x^{\alpha+m} f(x) \neq {}_aD_x^{\alpha} \left( D^m f(x) \right)$$

- Let $n-1 < \alpha < n$, $m, n \in \mathbb{N}$, $\alpha \in \mathbb{R}$ and the function $f(x)$ is such that ${}_a^CD_x^{\alpha} f(x)$ exists. Then in general

$${}_a^CD_x^{\alpha} \left( D^m f(x) \right) = {}_a^CD_x^{\alpha+m} f(x) \neq D^m \left( {}_a^CD_x^{\alpha} f(x) \right)$$

**proof** Let $\alpha = \dfrac{1}{2}$, $f(x) = 1$, and $m = 1$. using the definition of $D_x^{\alpha}$,

$$D_x^{\frac{1}{2}} D^1(1) = D^{\frac{1}{2}}(0) = 0,$$
$$D_x^{\frac{3}{2}}(1) = -\frac{1}{2\sqrt{(\pi)}} x^{-\frac{3}{2}},$$
$$D_x^{\frac{1}{2}} D^1(1) = 0 \neq D_x^{-\frac{3}{2}}.$$

That means

$$D^{\frac{1}{2}} D^1(1) \neq D^1 D^{\frac{1}{2}}(1).$$

The same proof of Caputo.

#### 3.2.2.4 Composition

- **Fractional integration of a fractional integral**

The Riemann-Liouville fractional integral has the following important property

$${}_aD_t^{-p}({}_aD_t^{-q} f(t)) = {}_aD_t^{-q}({}_aD_t^{-p} f(t)) = {}_aD_t^{-p-q} f(t), \tag{3.1.8}$$

which is called the composition rule for the Riemann-Liouville fractional integrals. Using the definition the proof is quite straightforward

$$\begin{aligned} {}_aD_t^{-p}\left({}_aD_t^{-q}f(t)\right) &= \frac{1}{\Gamma(p)}\int_a^t (t-\tau)^{p-1}({}_aD_t^{-q}f(\tau))d\tau \\ &= \frac{1}{\Gamma(p)}\int_a^t (t-\tau)^{p-1}\left(\frac{1}{\Gamma(q)}\int_a^\tau (\tau-\xi)^{q-1}f(\xi)d\xi\right)d\tau \\ &= \frac{1}{\Gamma(p)\Gamma(q)}\int_a^t\int_a^\tau (t-\tau)^{p-1}(\tau-\xi)^{q-1}f(\xi)\,d\xi\,d\tau. \end{aligned}$$

Changing the order of integration we obtain

$${}_aD_t^{-p}\left({}_aD_t^{-q}f(t)\right) = \frac{1}{\Gamma(p)\Gamma(q)}\int_a^t f(\xi)\int_a^\tau (t-\tau)^{p-1}(\tau-\xi)^{q-1}\,d\tau\,d\xi.$$

We make the substitution $\dfrac{\tau-\xi}{t-\xi} = \zeta$ from which it follows that $d\tau = (t-\xi)\,d\zeta$ and the new interval of integration is $[0,1]$. Now we are able to rewrite the last expression as

$$\begin{aligned} {}_aD_t^{-p}\left({}_aD_t^{-q}f(t)\right) &= \frac{1}{\Gamma(p)\Gamma(q)}\int_a^t f(\xi)\left((t-\xi)^{p+q-1}\int_0^1 (1-\zeta)^{p-1}\zeta^{q-1}d\zeta\right)d\xi \\ &= \frac{1}{\Gamma(p)\Gamma(q)}\int_a^t f(\xi)\left((t-\xi)^{p+q-1}B(p,q)\right)d\xi, \end{aligned}$$

Using identity Eq. (1.1.5) to express the Beta function in terms of the Gamma function we obtain

$$\begin{aligned} {}_aD_t^{-p}\left({}_aD_t^{-q}f(t)\right) &= \frac{1}{\Gamma(p)\Gamma(q)}\frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}\int_a^t f(\xi)(t-\xi)^{p+q-1}\,d\xi \\ &= \frac{1}{\Gamma(p+q)}\int_a^t (t-\xi)^{p+q-1}f(\xi)\,d\xi \\ &= {}_aD_t^{-p-q}f(t). \end{aligned}$$

- **Fractional differentiation of a fractional integral**

An important property of the Riemann-Liouville fractional derivative is

$${}_aD_t^{p}\left({}_aD_t^{-q}f(t)\right) = {}_aD_t^{p-q}f(t), \tag{3.1.9}$$

where $f$ has to be continuous and if $p \geq q \geq 0$, the derivative ${}_aD_t^{p-q}f$ exists. This property is called the composition rule for the Riemann-Liouville fractional derivatives. We shall prove this property, but first we need another property which actually is a special case of the previous one with $q = p$

$${}_aD_t^{p}\left({}_aD_t^{-p}f(t)\right) = f(t), \tag{3.1.10}$$

where $p > 0$ and $t > a$. This implies that the Riemann-Liouville fractional differentiation operator is the left inverse of the Riemann-Liouville fractional integration of the same order $p$. We prove this in the following way.

- First we consider the case $p = n \in \mathbb{N}^*$, then we have

$$\begin{aligned} {}_aD_t^n\left({}_aD_t^{-n}f(t)\right) &= \frac{d^n}{dt^n}\frac{1}{\Gamma(n)}\int_a^t (t-\tau)^{n-1}f(\tau)d\tau \\ &= \frac{d}{dt}\int_a^t f(\tau)d\tau = f(t). \end{aligned}$$

- For the non-integer case we take $k-1 \leq p < k$ and use Eq. (3.1.8) to write

$$ {}_aD_t^{-k}f(t) = {}_aD_t^{-(k-p)}\left({}_aD_t^{-p}f(t)\right).$$

  Now using the definition of the Riemann-Liouville differintegral we obtain

$$\begin{aligned} {}_aD_t^p\left({}_aD_t^{-p}f(t)\right) &= \frac{d^k}{dt^k}\left[{}_aD_t^{-(k-p)}\left({}_aD_t^{-p}f(t)\right)\right] \\ &= \frac{d^k}{dt^k}\left[{}_aD_t^{-k}f(t)\right] = f(t). \end{aligned}$$

- Now we are able to prove Eq. (3.1.9). We consider two cases. First we'll deal with $q \geq p \geq 0$. Then we have

$$ {}_aD_t^p\left({}_aD_t^{-q}f(t)\right) = {}_aD_t^p\left[{}_aD_t^{-p}\left({}_aD_t^{-(q-p)}f(t)\right)\right] = {}_aD_t^{p-q}f(t).$$

  This follows directly from Eq. (3.1.8) and Eq. (3.1.10). Now we will consider the second case in which we have $p > q \geq 0$. Using Eq. (3.1.8) we see that

$$\begin{aligned} {}_aD_t^p\left({}_aD_t^{-q}f(t)\right) &= \frac{d^k}{dt^k}\left[{}_aD_t^{-(k-p)}\left({}_aD_t^{-q}f(t)\right)\right] \\ &= \frac{d^k}{dt^k}\left({}_aD_t^{p-q-k}f(t)\right) = \frac{d^k}{dt^k}\left({}_aD_t^{-(k-(p-q))}f(t)\right) \\ &= {}_aD_t^{p-q}f(t). \end{aligned}$$

  So in both cases we proved Eq. (3.1.9).

**Remark.** The converse of Eq. (3.1.10) is not true, so ${}_aD_t^{-p}\left({}_aD_t^{p}f(t)\right) \neq f(t)$. The proof for this can be found in [19].

#### 3.2.2.5 Semigroup

**Theorem 3.1.2.** For any $f \in C([a,b])$ the Riemann-Liouville fractional integral satisfies

$$I_{a+}^{\alpha}I_{a+}^{\beta}f(x) = I_{a+}^{\alpha+\beta}f(x),$$

for $\alpha > 0, \beta > 0$.

**proof.** The proof is rather direct, we have by definition:

$$I_{a+}^{\alpha} I_{a+}^{\beta} f(x) = \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x \frac{dt}{(x-t)^{1-\alpha}} \int_a^t \frac{f(u)}{(t-u)^{1-\beta}} du,$$

and since $f(x) \in C([a,b])$ we can, by Fubini's theorem, interchange order of integration and by setting $t = u + s(x-u)$, we obtain

$$I_{a+}^{\alpha} I_{a+}^{\beta} f(x) = \frac{B(\alpha,\beta)}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x \frac{f(u)}{(x-u)^{1-\alpha-\beta}} du = I_{a+}^{\alpha+\beta} f(x).$$

#### 3.2.2.6 Linearity

Let $f$ and $g$ are functions for which the given derivatives or integrals operator are defined and $\lambda, \mu \in \mathbb{R}$ are real constants.

$${}_aD_t^p(\lambda f(t) + \mu g(t)) = \lambda \, {}_aD_t^p f(t) + \mu \, {}_aD_t^p g(t).$$

**proof.**

- For Grüunwald-Letnikov fractional derivative, we have:

$$\begin{aligned}
{}_aD_t^p(\lambda f(t) + \mu g(t)) &= \lim_{h\to 0} h^{-p} \sum_{r=0}^{m} (-1)^r \binom{p}{r} (\lambda f(t-rh) + \mu g(t-rh)) \\
&= \lambda \lim_{h\to 0} h^{-p} \sum_{r=0}^{m} (-1)^r \binom{p}{r} f(t-rh) \\
&+ \mu \lim_{h\to 0} h^{-p} \sum_{r=0}^{m} (-1)^r \binom{p}{r} g(t-rh) \\
&= \lambda \, {}_aD_t^p f(t) + \mu \, {}_aD_t^p g(t).
\end{aligned}$$

- For Riemann-Liouville differintegral:

$$\begin{aligned}
{}_aD_t^{-p}(\lambda f(t) + \mu g(t)) &= \frac{1}{\Gamma(p)} \int_a^t (t-\tau)^{p-1} (\lambda f(t) + \mu g(t)) d\tau \\
&= \lambda \frac{1}{\Gamma(p)} \int_a^t (t-\tau)^{p-1} f(\tau) d\tau + \mu \frac{1}{\Gamma(p)} \int_a^t (t-\tau)^{p-1} g(\tau) d\tau \\
&= \lambda \, {}_aD_t^{-p} f(t) + \mu \, {}_aD_t^{-p} g(t).
\end{aligned}$$

#### 3.2.2.7 Zero Rule

It can be proved that if $f$ is continuous for $t \geq a$ then we have

$$\lim_{p\to 0} {}_aD_t^{-p} f(t) = f(t).$$

**proof.** The proof can be found in [19]. Hence, we define

$${}_aD_t^0 f(t) = f(t).$$

#### 3.2.2.8 Product Rule & Leibniz's Rule

If $f$ and $g$ are functions, We know the derivative of their product is given by the product rule

$$(f.g)' = f'.g + f.g'.$$

This can be generalized to

$$(fg)^{(n)} = \sum_{k=0}^{n} \binom{n}{k} f^{(k)} g^{(n-k)},$$

which is also known as the Leibniz rule. In the last expression $f$ and $g$ are n-times differentiable functions.

## 3.2 Application: Anomalous Diffusion in the Human Brain Using Fractional Order Calculus

A new diffusion model has been proposed to describe anomalous diffusion behavior in human brain tissues [24], particularly at high b-values. The model uses fractional order calculus to solve the Bloch-Torrey equation and yields new parameters for describing anomalous diffusion. This study successfully applied the fractional calculus model to analyze diffusion images of healthy human brain tissues in vivo. The model produced spatially resolved maps of diffusion coefficient $D$, fractional order derivative in space $\beta$, and spatial parameter $\mu$, showing notable contrast between white and gray matter due to the varying complexity of tissue structures and microenvironment.

In many biologic tissues, the diffusion-induced MR signal loss deviates from monoexponential decay, exp(-bD) (where $D$ is the diffusion coefficient and $b$ is the b factor), particularly at high b-values (e.g.,$> 1500 sec/mm^2$ for human brain tissues). This phenomenon, sometimes referred to as anomalous diffusion, has been modeled extensively using a biexponential function:

$$S/S_0 = (1-f)exp(-bD_{fast}) + fexp(-bD_{slow}) \tag{3.2.1}$$

where the fast diffusion coefficient $D_{fast}$ can be an order of magnitude larger than the slow diffusion coefficient $D_{slow}$ whose fraction is given by $f$. At relatively low b-values ($e.g., b \leqslant 1000 sec/mm^2$) , the first term in Eq. (3.2.1) dominates, giving a pseudo monoexponential decay reflecting primarily the fast diffusion component. As the b-value

increases, the contribution of the slow diffusion component becomes increasingly important and the deviation from monoexponential decay becomes nonnegligible.
The 'biexponential' behavior has been attributed to tissue heterogeneity manifested by cellular structures, cell membrane, and/or differences between intra- and extracellular spaces. The exact origin of the biexponential decay, however, remains elusive. A prevalent explanation associates the fast and slow diffusion with the extra- and intracellular compartments, respectively, by assuming that higher concentration of macromolecules and presence of subcellular structures (organelles, mitochondria, etc.) can considerably hinder water molecular diffusion in the cell. This seemingly plausible explanation has been used to interpret changes of apparent diffusion coefficients observed in acute cerebral ischemia, epidermoid, arachnoid cyst, gliomas, and other diseases. However, the slow diffusion fraction f, obtained from biexponential fitting, correlates poorly with known cell volume fraction. For example, the cell volume fraction in the gray matter of healthy human brain is typically $\backsim$ 80% .

The biexponential model yields a slow diffusion fraction of only $\backsim$ 40%. In addition, biexponential behavior has been observed from the intracellular compartment alone, further challenging the validity of the intra/extracellular diffusion model. To resolve this discrepancy, Sehy et al. [24], attributed the slow diffusion component to water molecules in the close vicinity of the cell membrane instead of the intracellular space. Although a good correlation has been established between the membrane volume and the slow diffusion fraction, the division of water molecules between the two compartments is somewhat arbitrary since the molecules span a continuum of distribution.

Recognizing the limitations of the biexponential model, several groups have investigated alternative models to describe signals in high b-value diffusion imagin. Jensen et al. [24], used kurtosis to account for nongaussian diffusion observed at high b-values. Pfeuffer et al. Generalized the biexponential decay to a multicompartmental model:

$$S/S_0 = \sum_{i=0}^{n} f_i e^{-bD_i} \tag{3.2.2}$$

where

- $f_i$ is the volume fraction of the $i-th$ compartment and $\sum_{i=0}^{n} f_i = 1$.

Bennett et al. [24], used a stretched exponential model Eq. (3.2.2) to describe the diffusion-induced signal loss:

$$S/S_0 = e^{-(b \times DDC)^{\alpha}} \tag{3.2.3}$$

where

- DDC, coined as distributed diffusion coefficient, is a single number representation of the diffusion coefficient distribution function.
- $\alpha$ is an empiric constant $(0 < \alpha \leqslant 1)$).

The mean-squared displacement of water molecules is linked with the fractal dimension ($H$).

- $H = 1/d_w$.
- $d_w$ is the Brownian motion path ($d_w > 2$ indicates subdiffusion, while $d_w < 2$ corresponds to superdiffusion).

In the stretched exponential formalism was derived by recognizing that first the mean square displacement $\langle r^2(t) \rangle$ of diffusing molecules is related to diffusion time $t$ by Eq.(3.2.4) and second, the dependence of apparent diffusion coefficient on b can be expressed analogously to the dependence of diffusion coefficient on t Eq. (3.2.5),

$$\langle r^2(t) \rangle \propto t^{\alpha} \tag{3.2.4}$$

$$ADC \propto \frac{\langle R^2(b) \rangle}{b} \tag{3.2.5}$$

where

- $\langle R^2(b) \rangle$ is the apparent mean square displacement, analogous to $\langle r^2(t) \rangle$. Equations (3.2.4) and ( 3.2.5) directly lead to the stretched exponential expression described by Eq. (3.2.3).

Fractal models suggest a possible fractional order dynamics in diffusion-induced magnetization changes, as dictated by the Bloch-Torrey equation. Researchers have examined the connection between fractional order dynamics and diffusion by solving the Bloch-Torrey equation using fractional order calculus. The stretched exponential model follows from a fundamental extension of this equation through the application of fractional calculus operators. The model based on fractional calculus yields a new set of parameters to describe anomalous diffusion:

- $D$ diffusion coefficient.
- $\beta$ fractional order derivative in space .
- $\mu$ a spatial parameter.

This study demonstrates that the fractional calculus (FC) model can be successfully applied to analyzing diffusion images of healthy human brain tissues in vivo, producing spatially resolved maps of $D$, $\beta$, and $\mu$.

### 3.2.1 Theory

If $C(x,t)$ represents the concentration of the diffusing species in one dimension, then a fractional order partial differential equation Eq. (3.2.6) emerges from Fickś first law,

$$\frac{\partial C(x,t)}{\partial t^{\alpha}} = \grave{D}\frac{\partial^{2\beta} C(x,t)}{\partial |x|^{2\beta}} \tag{3.2.6}$$

where

- $\grave{D}$ is the generalized diffusion coefficient (note that the units of $\grave{D}$ are $mm^2 b/second$).
- $\alpha$ $(0 < \alpha \leqslant 1)$ is a fractional order derivative with respect to time.
- $\beta$ $(0 < \beta \leqslant 1)$, a fractional order derivative with respect to space.

With this formalism, a fractional order generalization of the Bloch-Torrey equation can be written as

$$\tau^{\alpha-1}\,{}_{0}^{C}D_{\alpha}^{t} M_{XY}(r,t) = \lambda M_{XY}(r,t) + D\mu^{2(\beta-1)}\nabla^{2\beta} M_{XY}(r,t) \tag{3.2.7}$$

$$\lambda = -i\gamma(r,G) \tag{3.2.8}$$

where

- ${}_{0}^{C}D_{\alpha}^{t}$ is the Caputo form of the Riemann-Liouville fractional order derivative in time (see Eq. (3.2.9)).
- $\nabla^{2\beta} = (D_x^{2\beta} + D_Y^{2\beta} + D_Z^{2\beta})$ is a Riesz fractional order Laplacian operator in space.

- $\gamma$ is the gyromagnetic ratio.
- $M_{XY}$ represents the transverse magnetization.
- $\tau^{1-\alpha}$ and $\mu^{2(\beta-1)}$ are fractional order time and space constants, respectively, needed to preserve units (e.g., the units of diffusion coefficient $D$ remain as $mm^{2/sec}$).

The fractional order derivative operator ${}_0^C D_\alpha^t$ can be explicitly expressed as:

$$ {}_0^C D_\alpha^t M_{XY}(r,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\grave{M}_{XY}(r,\tau)}{(t-\tau)^\alpha} d\tau \tag{3.2.9} $$

where

- $M_{XY}(r,t)$ indicates the first order derivative with respect to time.
- $\Gamma(1-\alpha)$ is a gamma function defined as

$$ \Gamma(X) = \int_0^\infty e^{-u} u^{X-1} du \tag{3.2.10} $$

For fractional order dynamics in space (i.e., $a = 1{,}0 < b < 1$), the transverse magnetization was derived for constant, bipolar, Stejskal-Tanner, and twice-refocused diffusion gradients, respectively. The result for the Stejskal-Tanner gradient is given by Eq. (3.2.11).

$$ M_{XY} = M_0 exp\left[-D_{\mu^{2(\beta-1)}}(\gamma G_d \delta)^{2\beta}\left(\Delta - \frac{2\beta-1}{2\beta+1}\delta\right)\right] \tag{3.2.11} $$

where

- $G_d$ is the diffusion gradient amplitude
- $\delta$ and $\Delta$ are the diffusion gradient pulse width and gradient lobe separation, respectively [24].

When $b = 1$. Eq. (3.2.11) reduces to the well-known monoexponential expression $exp(-bD)$ , and the spatial variable m is nullified. In a general case where $b < 1$, $\mu$ becomes active and the conventional definition of $b$ value does not hold. To accommodate these changes, we define a new parameter $b^*$ as follows:

$$ b^* \equiv (\gamma G_d \delta)^2 \left(\Delta - \frac{2\beta-1}{2\beta+1}\delta\right) \tag{3.2.12} $$

With this definition, Eq. (3.2.11) becomes

$$ M_{XY} = M_0 exp\left[-D_{\mu^{2(\beta-1)}}(b^*)^{\beta}\left(\Delta - \frac{2\beta-1}{2\beta+1}\delta\right)^{1-\beta}\right] \tag{3.2.13} $$

If we further define a pseudo diffusion coefficient $D^*$ in Eq. (3.2.14), then Eq. (3.2.13) takes the form of stretched exponential decay (18-20), as described by Eq. (3.2.15).

$$D^* = \left[ D_{\mu^{2(1-\frac{1}{\beta})}} \left( \Delta - \frac{2\beta - 1}{2\beta + 1} \delta \right)^{\frac{1}{\beta} - 1} \right] \tag{3.2.14}$$

$$M_{XY} = M_0 exp \left[ -(D^* \times b^*)^{\beta} \right] \tag{3.2.15}$$

- Note that $D^*$ preserves the nominal units of diffusion coefficient ($mm^{2/sec}$) and is analogous to the distributed diffusion coefficient described by Bennett et al. [24].
- It is also interesting to note that D* becomes identical to $D$ if

  $$\mu^2 = D \left( \Delta - \frac{2\beta - 1}{2\beta + 1} \delta \right),$$

  which can be derived from the equations above.

Although the present study focuses on the diffusion model with fractional order in space described by Eqs. ((3.2.11)-(3.2.15)), for completeness we also present theoretical formulism for the fractional order dynamics in time (i.e., $0 < \alpha < 1$, $b = 1$). With a constant diffusion gradient and an free induction decay (FID) acquisition, the transverse magnetization is given by

$$M_{XY} = M_0 \mathrm{E}_{\alpha} \left[ -i\gamma G_d r \tau (t/\tau)^{\alpha} \right] exp \left[ -B (t/\tau)^{3\alpha} \right] \tag{3.2.16}$$

$$B = \frac{2\Gamma(2-\alpha) D \gamma^2 G_z \tau^3}{3\alpha^2 \Gamma(2\alpha + 1)} \tag{3.2.17}$$

where

- $r$ is a spatial variable along the diffusion gradient direction.
- $\mathrm{E}_{\alpha}$ is the single parameter Mittag-Leffler function. When $\alpha = 1$, Eq. (3.2.16) becomes identical to the classic expression describing diffusion-indced signal attenuation in an FID under the influence of a constant gradient.

## 3.2.2 Materials and method

### Image Acquisition

To demonstrate and evaluate the FC model described above, high b-value diffusion imaging experiments were carried out on five healthy human volunteers, using a $3-T$

*GE* Signa $HD_X$ scanner (General Electric Healthcare, Waukesha, *WI*) equipped with a gradient system capable of a maximal amplitude of 40 $mT/m$ and a maximal slew rate of 150 $T/m/sec$. An eight-channel phased-array head coil was employed to enable parallel imaging (acceleration factor = 2) for improved robustness against image distortion arising from magnetic susceptibility variations. All images were acquired using a customized single-shot echo-planar imaging diffusion sequence. This sequence reduces image distortion caused by eddy currents by dynamically adjusting the imaging gradients (readout, phase encoding, and slice selection), as well as the receiver frequency to offset the eddy current magnetic fields. With this compensation, the maximal image shift and distortion were limited to the subpixel level, as confirmed by a phantom scan. This effective compensation technique allowed us to use the conventional Stejskal-Tanner gradient based upon which Eqs. ((3.2.11)-(3.2.15)) were derived. This simpler gradient waveform features a shorter echo time than the twice-refocused gradient waveforms implemented in commercial diffusion sequences.

Fifteen b-values, ranging from 0 to 4700 $sec/mm^2$, were produced by varying the Stejskal-Tanner diffusion gradient amplitude ($G_d$) while keeping the pulse width ($\delta$) and separation ($\varDelta$) constant ($\varDelta = 55.7$ ms and $\delta = 48.7$ ms). At each b-value, the diffusion-weighting gradient was successively applied along each of the three orthogonal axes to acquire diffusion-weighted images in the axial plane. Trace-weighted images were then computed to remove the effect of diffusion anisotropy, as well as to increase the signal-to-noise ratio (SNR), followed by analysis using the FC diffusion model. The other acquisition parameters were repetition time = 3000 ms, echo time = 112 ms, slice thickness = 4 mm, slice gap = 1.5 mm, field of view = 22 $cm^2$, image matrix size = 256 × 256, number of excitations (NEX) = 8, and the total scan time ≈ 18 min.

**Image Analysis**

Prior to image analysis, the degree of image misregistration caused by head motion was evaluated among the images with different b-values. A pair of images with adjacent b-values was subtracted from each other to detect

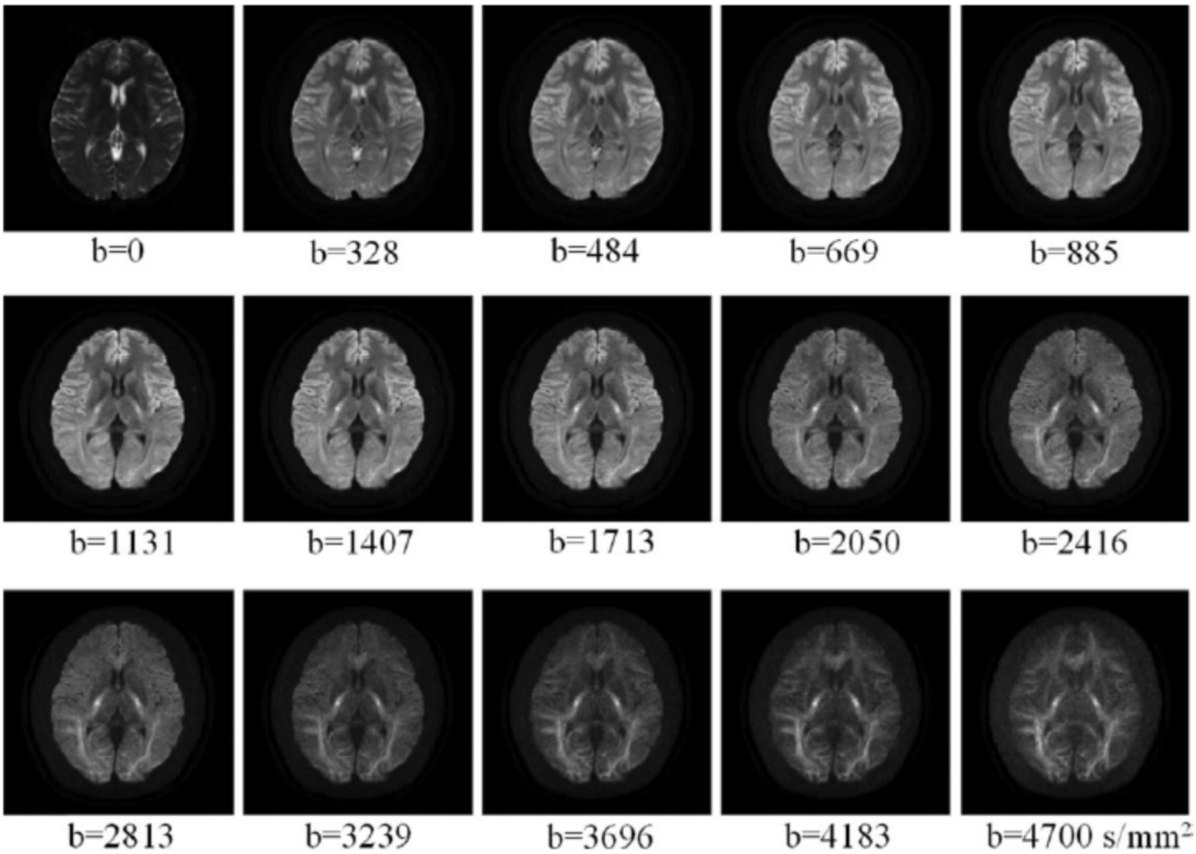


Figure 3.1: A set of representative diffusion-weighted images with different b-values, as shown in the figure. Each frame represents a trace-weighted image obtained by taking the geometric average of the individual diffusion images, with diffusion gradient successively applied along each of the three orthogonal axes.

Relative motion by assessing the width of the edge in the resultant difference image. If substantial edge intensity (i.e., edge width is more than a half of a pixel) was observed, a rigid-body motion correction was performed by applying a linear phase ramp in k-space in the direction along which image shift was detected. The maximal shift observed in all subjects was approximately two pixels, although the motion amplitude was typically well within the subpixel level, which required no correction. Considering the relatively low spatial resolution ($4mm$) in the slice direction, no attempt was made to correct for through-plane motion.

After motion correction, image pixel intensities as a function of $G_d$ were fitted to the FC diffusion model described by Eq. (3.2.11), using a Levenberg-Marquardt nonlinear fitting algorithm. An intensity threshold was set at $\bar{n} + 2\sigma$, where n is the mean noise in the background and s is the standard deviation of noise. Pixel intensities below this threshold were not included in curve fitting. Both n and s were computed from a background region of interest (ROI; $\backsim$ 100 pixels in snnize) free from the Nyquist ghost. The noise followed a Rician distribution.

In the fitting, the initial D value for each pixel was obtained from the data acquired at b-values $< 1000$ $sec/mm^2$, using the classic monoexponential model. The initial $\beta$ values were chosen as $\backsim$ 1, and the initial m values were fitted from Eq. (3.2.11), with $\mu$ being the only variable (the initial values of D and $\beta$ were used in this fitting). After the initial values were determined, the set of diffusion- weighted images was analyzed using Eq. (3.2.11) to yield the final values of D, $\beta$, and $\mu$ on a voxel-by-voxel basis. In addition, the same fitting algorithm was also applied to representative ROIs in gray matter (putamen), white matter (genu of the corpus callosum), and cerebrospinal fluid (CSF). The typical ROI size was $2 \times 2$ pixels. For both pixelwise and ROI analyses, the quality of the fit was measured by $\chi^2$.

### 3.2.3 Result

Figure (3.1) displays a set of representative diffusion-weighted images from a human volunteer with b-values ranging from 0 to 4700 $sec/mm^2$. With an NEX of 8 and a moderate echo time ($112ms$), an SNR greater than 3.5 was achieved in the brain tissues (except for CSF) even at the highest b-value. The SNRs in several selected brain regions are summarized in Table 1. Although images with fewer averages were also attempted, it was found that eight averages were needed to achieve an adequate SNR for reliable and stable fitting results. The problem with head motion during the long acquisition time ($\backsim 18min$) was addressed effectively using the motion correction technique described in the Materials and Methods section.

Table 3.1: SNR in Selected Brain Regions at Two Different b-values.

| | | Caudate | | |
|---|---|---|---|---|
| | **Putamen** | **Nucleus** | **Genu** | **Splenium** |
| $b = 2050 sec/mm^2$ | 8.5 | 10.7 | 13.5 | 14.3 |
| $b = 4700 sec/mm^2$ | 3.5 | 4.6 | 5.7 | 6.5 |

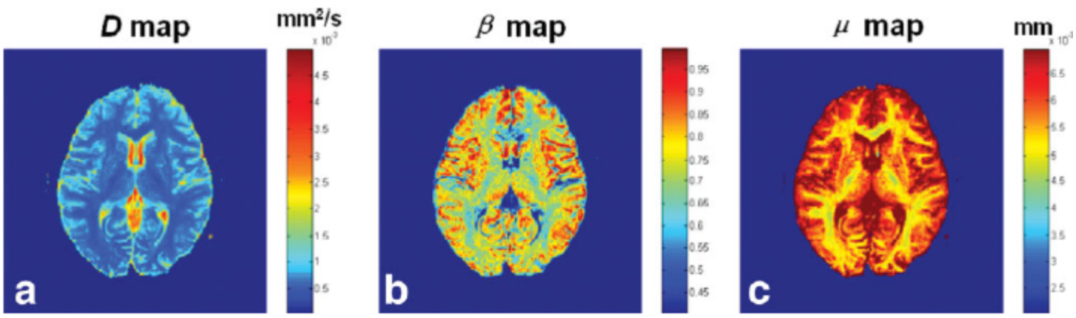


Figure 3.2: Spatially resolved maps based on $D(a)$, $\beta(b)$, and $\mu(c)$ obtained from the images shown in Fig.(3.1). The units and scales are indicated on the right color bar.

Figure (3.2) shows a set of representative maps of D, $\beta$ and $\mu$ obtained from the diffusion-weighted images in Fig.(3.1). The D map (Fig.(3.2) a) closely resembles that obtained using a monoexponential model with a typical value of $0.66 \pm 0.007 \times 10^3$, $0.41 \pm 0.008 \times 10^3$, and $2.72 \pm 0.006 \times 10^3$ $mm^2/sec$ in the putamen, genu, and CSF, respectively (Table 2). The small standard deviations demonstrated the high reliability of the fit. Both the $\beta$ and $\mu$ maps (Fig.(3.2) b, c) exhibited remarkable gray/white matter contrast. The $\beta$ and $\mu$ values in the three representative ROIs (putamen, genu, and CSF) are shown in Table (3.2). In general, the white matter showed substantially lower $\beta$ value (e.g., $0.64 \pm 0.01$ in the genu) than the gray matter (e.g., $0.82 \pm 0.01$ in the putamen), suggesting a larger deviation from the monoexponential model. This result was consistent with the increased diffusion complexity (such as anisotropy) in the white matter comprising primarily axons linked together to form the fiber structures. The CSF exhibited the largest b-value ($0.95 \pm 0.01$; very close to 1.0), reflecting a simpler diffusion process with minimal anomalous diffusion, as expected. The speckles in the $\beta$ map were not caused by noise as they were not accentuated when the SNR was lowered with NEX= 6. In the $\mu$ map (Fig.(3.2) c), the contrast between the white and gray matter was most striking, exhibiting features typically seen in fractional anisotropy maps obtained in diffusion tensor imaging, even though the effects of diffusion anisotropy were suppressed by using diffusion-trace-weighted images to obtain the $\mu$ map. The m values for the three representative ROIs (putamen, genu, and CSF) were found to be $5.88 \pm 0.06$ mm, $4.87 \pm 0.06$ mm, and $7.53 \pm 0.12$ mm, respectively (Table 3.2). The error terms in the gray matter and white matter were comparable, but both were significantly lower than that in the CSF. As detailed in the Discussion section, the increased error in the CSF can be partially attributed to the fact that $\mu$ becomes increasingly unstable when $\beta$ approaches 1 (Eq. (3.2.11)). Although not explicitly shown, the same results were also observed in the other four subjects in the study.

Table 3.2: Diffusion Parameters Obtained From Three Brain Regions, Using the FC Diffusion Model.
$^{a}In$ CSF, only images with $b < 1400\ sec/mm^2$ were used in the fitting.

| | **D** $(\times 10^{-3} mm^2/sec)$ | $\beta$ | $\mu(\mu m)$ | $\chi^2$ |
|---|---|---|---|---|
| Putamen | $0.66 \pm 0.007$ | $0.82 \pm 0.01$ | $5.88 \pm 0.06$ | 0.01 |
| Genu | $0.41 \pm 0.008$ | $0.64 \pm 0.01$ | $4.87 \pm 0.06$ | 0.02 |
| CSF | $2.72 \pm 0.006$ | $0.95 \pm 0.01$ | $7.53 \pm 0.12$ | $0.01^{a}$ |

As an example, the quality of the fractional order curve fits is illustrated in Fig.(3.3), where the signal intensities of the three representative ROIs are plotted as a function of $b^*$ defined in Eq. (3.2.12) (note that the fitting was originally performed with respect to the diffusionweighting gradient amplitude $G_d$, which was later converted to $b^*$ for display). As indicated in Table 2, the fitting errors are rather small, with $\chi^2$ ranging from 0.01 to 0.02. For comparison, the same dataset was also fitted to the biexponential function given by

Eq. (3.2.1) 1. The $\chi^2$ errors of the biexponential fit were four to five times larger. These results were typical for all image pixels and all subjects who were evaluated in this study.

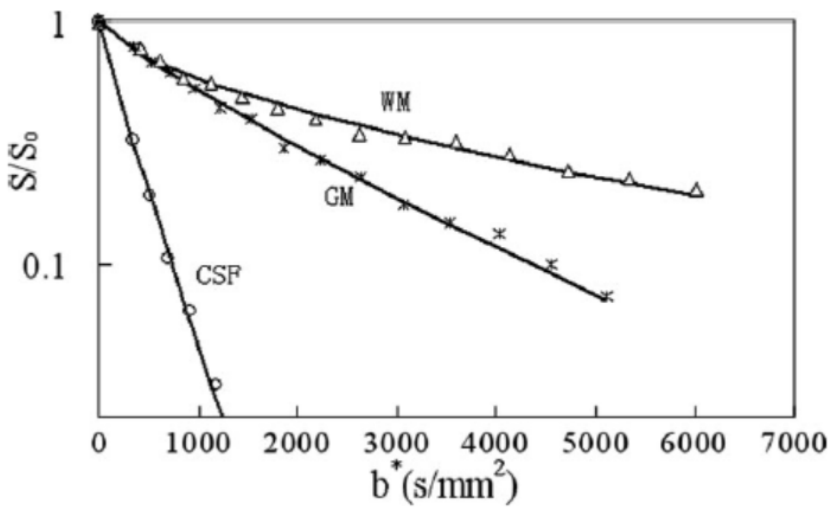


Figure 3.3: Image signal intensity as a function of $b^*$ for three selected ROIs. WM: white matter selected from the genu; GM: gray matter selected from the putamen.

### 3.2.4 Discussion

In this study, a novel model to analyzing anomalous diffusion in human brain tissues in vivo at high b-values up to 4700 $sec/mm^2$ have been applied. This model is based on solutions of fractionalized Bloch-Torrey differential equation with respect to space. The theoretical results demonstrate that the fractional order differential operator yields mathematical expressions similar to those developed by Özarslan, Bennett , Hall and Barrick [24], without relying on fractals or empiric information. Fractionalization of the Laplacian in the Bloch-Torrey equation produces two additional parameters: the operational order parameter $\beta$ (dimensionless) and the unitpreserving space constant $\mu$ (in units of micrometers). As shown by Eq. (3.2.15), $\beta$ is directly related to the exponent in the stretched exponential model and serves as a parameter describing the fractional order dynamics associated with anomalous diffusion in biologic tissues.

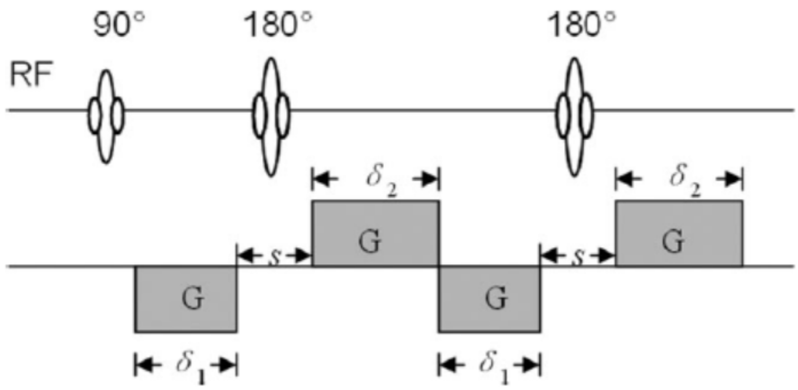


Figure 3.4: A sequence diagram of the diffusion-weighting module with twice-refocused spin echo.

Previous studies on phantoms and biologic tissues have shown that a decrease in $\beta$ value strongly correlates with increased structural complexity. This observation was further substantiated in the present study, where white matter was found to consistently exhibit lower $\beta$ values than the gray matter not only in the selected ROIs but also in virtually all pixels in the major white-matter tracts. This result suggests a connection between the phenomenological stretched exponential and the fractional order dynamics assumed here for describing anomalous diffusion using the fractionalized Bloch-Torrey equation. The $\beta$ value employed in the model also naturally distinguishes simple diffusion (e.g., monoexponential diffusion) from anomalous diffusion. In the fluid environment of CSF where conventional diffusion processes (instead of anomalous diffusion) are expected, $\beta$ gives a significantly higher value (ranging from 0.94 to 1.0) than those in the brain parenchyma.

Unlike $\beta$, which can also be derived from fractals, $\mu$ is unique to the FC diffusion model. Although $\mu$ was introduced as a parameter to preserve the nominal units of diffusion coefficient, it appears to provide a measure of diffusion environment with a surprisingly high contrast between the white and gray matter (Fig.(3.2) c). Previous studies on Sephadex with different pore sizes found that $m$ was inversely related to the mean free length of diffusing molecules. This trend, however, was not observed in the brain tissues. Instead, the smaller $\mu$ values in the white matter as compared to the gray matter suggested a correlation with the reduced mean free length because of tightly packed axonal structures. In the CSF where the diffusion process is least restricted, the largest

$\mu$ value was observed despite an elevated error Table ((3.2)). To use the $\mu$ map for tissue characterization, however, caution must be exercised because $\mu$ values become increasing unstable as $\beta$ approaches 1.0 (Eq. (3.2.11)). This phenomenon was seen in the CSF ($\beta \approx 1$) where $\mu$ values exhibited large variations, ranging from 5.9 mm to 8.7 mm. For white matter and gray matter in which $\beta$ was typically less than 0.8, $\mu$ values were very stable, as shown by the small standard deviations in Table (3.2).

Introduced as mathematical parameters, both $\beta$ and $\mu$ have shown good correlations with physical entities such as tissue structures and the microenvironment in which water diffusion becomes anomalous. The biophysical interpretation of $\beta$ and $\mu$ needs to be further explored through simulations and well-controlled experiments. The exact relationship between $\beta$ or $\mu$ and tissue structures may provide us with valuable insights into anomalous diffusion in tissue, perhaps revealing new features of the tissue microenvironment. Even with limited and preliminary results on $\beta$ and $\mu$, the FC diffusion model appears to suggest a fundamentally different approach to exploring tissue structures through diffusion measurements. Instead of focusing on changes in the diffusion coefficient or the multicompartmental feature of diffusion process, the FC model emphasizes the fractional order dynamics associated with diffusion environmental changes that can be related to experimentally measurable parameters $\beta$ and $\mu$. The microenvironmental changes in tissues are the reasons for the observed changes in apparent diffusion coefficient. With the FC diffusion model, we may have a more direct access to the tissue microenvironmental changes than what is typically inferred from apparent diffusion coefficients using the existing approaches.

Unlike other diffusion models, the diffusion coefficient in Eq. (3.2.11) is decoupled from the parameters relating to the tissue microenvironment and thus reflects the diffusion process in a pure physical sense without being substantially influenced by structures. This property was further preserved in the fitting algorithm, in which the initial $D$ value was determined from the low b-values ($b < 1000\ sec/mm^2$) where the nominal diffusion process is dominant. Once the initial diffusion coefficient was determined, the final $D$ value did not vary substantially, even when data with substantially higher$b$ values were employed in the fitting. This result suggests that the diffusion coefficient in the FC model may reflect an intrinsic physical property not substantially influenced by diffusion environment.

The highest b-value employed in this study was limited to 4700 $sec/mm^2$ due to the maximal gradient strength available ($40mT/m$) and SNR considerations. b-values beyond 4700 $sec/mm^2$ were attempted, but the low SNR (e.g., SNR $< 3$) led to unreliable nonlinear fitting. Even at $b = 4700$ $sec/mm^2$, a large number of signal averages was needed to achieve an adequate SNR, resulting in long acquisition times (i.e., 18 min for 15 b-values).

# Conclusion

The concept of diffusion plays a fundamental role in the understanding of our surrounding, specially in those systems in which the motion of particles cannot be completely described by a deterministic theory. For a long time, most stochastic processes where associated to a Brownian (or normal)-like behaviour. However, in recent years, we have seen how many of the systems of study diverge from it. In order to explain such divergence, other models that currently form what we now know as the anomalous diffusion theory; inspired and closely related to Brownian motion have been proposed.

The main point of this master thesis was to present the main concepts behind normal and anomalous diffusion stochastic processes. Starting from the different regimes of diffusion, namely normal, subdiffusive and superdiffusive. then studying the mean anomalous diffusion stochastic processes, discussing first their formal characteristics, and properties such as Grey Brownian motion (GBM), fractional Brownian motion (fBm), Continuous-time random walk (CTRW) and fractional Itô motion (FIM). and last as a practical application, a new mathematical approach-fractional order calculus-to describe anomalous diffusion in human brain tissues have been used. The result, based on fractional order calculus, yields a diffusion model that features two new parameters: the fractional order parameter $\beta$ (dimensionless) and the unit-preserving space constant $\mu$ (in units of $\mu m$). Spatially resolved maps based on $\beta$ and $\mu$ showed notable contrast between white and gray matter. The contrast observed in $\beta$ and $\mu$ maps appears to correlate with the underlying tissue structures and micro-environment. Although the biophysical basis of $\beta$ and $\mu$ remains elusive, these parameters can potentially characterize molecular diffusion beyond what the apparent diffusion coefficient can offer and may lead to a new way to investigate tissue structural changes in disease progression, intervention, and regression.

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