# APPLICATION OF FRACTIONAL CALCULUS TO THE ANALYSIS OF LAPLACE TRANSFORMED DATA

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**ABSTRACT**

This paper describes a novel method using fractional calculus to estimate non-integer moments of a random variable from the measured Laplace transform of its probability density function. We demonstrate that the $\omega$-th moment ($\omega \in \mathbb{R}$) of the random variable can be directly obtained by a linear transformation of the data. When $\omega > 0$, computation of moments corresponds to fractional integration of the data. When $\omega \le 0$, computation of moments corresponds to fractional differentiation.

## 1. INTRODUCTION

Fitting exponentials to measured data is a well-known ill-conditioned problem in science and engineering. It involves solving for non-negative amplitude $f_T$ from the measured multi-exponential decay in the time-domain $M(t)$

$$M(t) = \int_0^\infty e^{-t/T} f_T(T) dT + \varepsilon(t). \tag{1}$$

Here $\varepsilon(t)$ is the measurement error modeled as additive, white, Gaussian noise with known variance. In eqn. (1), the measured data $M(t)$ is a Laplace transform of the amplitudes $f_s(s) \equiv T^2 f_T(T)$, where we set $s = 1/T$. Traditionally, the inverse Laplace transform is used to estimate the amplitudes $f_T(T)$ from the measured data. The time constants $T$ are often assumed to be a continuum. Without loss of generality, the corresponding non-negative amplitude $f_T(T)$ is considered to be the probability density function of variable $T$.

Our study is guided by nuclear magnetic resonance (NMR) applications in biological systems and porous media where experimental protocols have been developed to measure data represented by eqn. (1). In these applications, the time constant $T$ corresponds to the characteristic relaxation time for loss of energy by protons in hydrocarbons or water present in pores of a rock or in the bulk fluid. The amplitude $f_T(T)$ at any given $T$ is proportional to the number of protons relaxing at that rate. The mean, width and some of the moments of $T$ are used to infer information about the rock and/or fluid [1, 2]. Although our work is motivated by NMR applications, the sum-of-exponentials model is widely used in a number of disciplines including acoustics [3], diffusion tomography [4], imaging [5] and optics [6].

It is well known in the literature that the inverse Laplace transform is an ill-conditioned problem: small changes in the measured data due to noise can result in widely different $f_T(T)$ [7, 8]. In theory, there are infinitely many solutions for $f_T(T)$. The classical approach to the problem involves choosing the "smoothest" solution $f_T(T)$ that fits the data. This smooth solution is often estimated by minimization of a cost function $Q$ with respect to the underlying $f$ [9, 10],

$$Q = \|M - Kf\|^2 + \alpha \|f\|^2, \tag{2}$$

where $M$ is the measured data, $K$ is the matrix of the discretized kernel $e^{-t/T}$ and $f$ is the discretized version of the underlying density function $f_T(T)$ in eqn. (1). The first term in the cost function is the least squares error between the data and the fit from the model in eqn. (1). The second term denoting Tikhonov regularization, incorporates smoothness in the expected solution of the density function.

The mathematical definition of smoothness as well as the value of $\alpha$ are subjective. The parameter $\alpha$ denotes the compromise between the fit to the data and an *a priori* expectation of the density function. When $\alpha$ is too small, the inversion problem is unstable. Small changes in the data (due to additive noise) result in widely different estimates for $f_T(T)$. When $\alpha$ is too large, the solution does not sufficiently take the measured data into account. In this case, the estimated density function $f_T(T)$ is stable, but results in poor fit to the data. In the literature, there are a wide variety of recipes to choose $\alpha$, including the "L" curve method, generalized and ordinary cross validation, predictive mean square error and self-consistency methods [11, 12, 13]. These different methods provide different values of $\alpha$ and result in different solutions $f_T(T)$, all of which provide reasonable fits to the data.

Often, the density function of $T$ may itself not be of direct interest. Instead it is used to derive a second set of parameters such as specific moments of $T$, which are used to provide insight into the underlying physical process. For example, the negative 0.4-th moment of relaxation time is related empirically to the irreducible water-saturation in rocks. Similarly, the 0.2-th moment of relaxation time is found to be a good predictor of rock permeability [2]. The average chain length of a hydrocarbon is related to the 0.8-th moment of relaxation time [14].

The $\omega$-th moment of $T$ is defined as,

$$\langle T^\omega \rangle \equiv \int_0^\infty T^\omega f_T(T) dT, \quad \omega \in \mathbb{R}. \tag{3}$$

In this manuscript, we demonstrate that the $\omega$-th moment of $T$ can be obtained directly from a linear transformation of the

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data,

$$\langle T^{\omega}\rangle = \frac{(-1)^n}{\Gamma(\mu)}\int_0^{\infty} t^{\mu-1}\left[\frac{d^nM(t)}{dt^n}\right]dt \tag{4a}$$

$$\omega = \mu - n, \quad \text{with} \begin{cases} n = 0 & \text{if} \quad \omega > 0 \\ n = [-\omega]+1 & \text{otherwise.} \end{cases} \tag{4b}$$

where $\Gamma()$ represents the Gamma function and $[\omega]$ refers to the integral part of the number $\omega$. The contribution of variable $\omega$ is in two parts: a real number $\mu$ and an integer $n$ where the mathematical operator $t^{\mu-1}$ operates on the $n$-th derivative of the data. Eqn. (4) obviates the use of the ill-conditioned Laplace transform to compute the moments. In the next section, we provide a derivation of eqn. (4) from the perspective of fractional calculus. We demonstrate that when $\omega > 0$, eqn. (4) corresponds to fractional integration of the data. When $\omega \le 0$, the operation corresponds to fractional differentiation.

A practical application of this work is in computation of moments from NMR relaxation data obtained from fluids in porous media [15].

## 2. MOMENT ESTIMATION USING FRACTIONAL CALCULUS

From eqn. (1), it is seen that integer moments of $T$ can be obtained by integration or differentiation of the data. For example,

$$\langle T\rangle = \int_0^{\infty} M(t)dt \tag{5a}$$

$$\left\langle \frac{1}{T}\right\rangle = \left|\frac{dM}{dt}\right|_{t=0} \tag{5b}$$

$$\left\langle \frac{1}{T^2}\right\rangle = \left|\frac{d^2M}{dt^2}\right|_{t=0} \tag{5c}$$

This leads one to naturally consider fractional calculus to obtain the $\omega$-th moment of $T$ when $\omega$ is not restricted to be an integer and can take on a real value.

The Liouville fractional integral denoted by ${}_{-\infty}D_x^{-\omega}$ of a function $g()$ is defined as, [16]

$${}_{-\infty}D_x^{-\omega}(g) \equiv \frac{1}{\Gamma(\omega)}\int_{-\infty}^{x}(x-t)^{\omega-1}g(t)dt, \; \omega > 0. \tag{6}$$

Fractional derivatives are defined by applying differentiation a whole number of times to fractional integral. Let $\omega \le 0$ and $n$ be the smallest integer greater than $-\omega$. Let $\mu = n + \omega, 0 < \mu \le 1$. Fractional derivatives are defined as (eqn (6.1), Chapter 2, [16])

$${}_{-\infty}D_x^{-\omega}(g) \equiv {}_{-\infty}D_x^{n}\left[{}_{-\infty}D_x^{-\mu}g(x)\right], \; \omega < 0. \tag{7}$$

The notation ${}_{-\infty}D_x^{-\omega}$ unifies integration and differentiation into a single entity, sometimes referred to as 'differintegration'. When $\omega > 0$, ${}_{-\infty}D_x^{-\omega}$ denotes a fractional integral and when $\omega \le 0$, it denotes fractional differentiation. Fractional calculus has so far been a largely theoretical subject with applications in problems where the governing equation is a fractional differential equation in time.

Consider an exponential function, $g(x) = e^{ax}, a > 0, x \in [-\infty \; 0]$. In this classical textbook example, it has been shown that (eqn (6.9), Chapter 1, [16])

$${}_{-\infty}D_x^{-\omega}e^{ax} = a^{-\omega}e^{ax}, \;\; \omega \in \mathbb{R}. \tag{8}$$

Since fractional differentiation and integration are linear operations, when applied to a sum of exponentials in eqn. (1), we get,

$${}_{-\infty}D_0^{-\omega}(M(-t)) = \langle T^{\omega}\rangle, \;\; \omega \in \mathbb{R}. \tag{9}$$

To prove eqn. (4), let us first consider the case of fractional integration with $\omega > 0$. Let $t_1 = -t$ and $g(t_1) = M(t)$. From eqn. (6),

$${}_{-\infty}D_0^{-\omega}(g) = \frac{1}{\Gamma(\omega)}\int_{-\infty}^{0}(-t_1)^{\omega-1}g(t_1)dt_1, \quad \omega > 0. \tag{10}$$

Reversing the time-axis on the right-hand side of eqn. (10) yields

$${}_{-\infty}D_0^{-\omega}(M(-t)) = \frac{1}{\Gamma(\omega)}\int_0^{\infty} t^{\omega-1}M(t)dt, \quad \omega > 0. \tag{11}$$

From eqn. (9) and (11), we get,

$$\langle T^{\omega}\rangle = \frac{1}{\Gamma(\omega)}\int_0^{\infty} t^{\omega-1}M(t)dt, \quad \omega > 0. \tag{12}$$

Next, consider the case of fractional differentiation with $\omega \le 0$. Let $\omega = \mu - n$, where $n = [-\omega]+1$.

*Case 1: Let* $-1 < \omega \le 0$. In this case, $n = 1$ and $\mu = \omega + 1$. From the definition of fractional differentiation in eqn. (7), we get,

$${}_{-\infty}D_x^{-\omega}(M(-t)) = \frac{1}{\Gamma(\mu)}\frac{d}{dx}\left[\int_{-\infty}^{x}(x-t)^{\mu-1}M(-t)dt\right]. \tag{13}$$

The next step is to interchange the integral and differential operators in eqn. (13). This can be done by applying the general form of Leibniz integration rule given as,

$$\frac{d}{dx}\int_{a(x)}^{b(x)} g(x,t)dt = g(x,b(x))b'(x) - g(x,a(x))a'(x) + \int_{a(x)}^{b(x)}\frac{\partial}{\partial x}g(x,t)dt. \tag{14}$$

However, in order to avoid artificial singularities that result from the direct application of Leibniz rule, we first apply integration by parts to the integral between the square brackets of eqn. (13) to get

$${}_{-\infty}D_x^{-\omega}(M(-t)) = \frac{1}{\Gamma(\mu+1)}\frac{d}{dx}\left[\int_{-\infty}^{x}(x-t)^{\mu}\frac{dM(-t)}{dt}dt\right] \tag{15}$$

where we use the property that $M(t)$ vanishes exponentially as $t \to \infty$. Applying Leibniz integration rule to eqn. (15), we obtain,

$$ {}_{-\infty}D_x^{-\omega}(M(-t)) = \frac{1}{\Gamma(\mu)} \int_{-\infty}^{x} (x-t)^{\mu-1} \frac{dM(-t)}{dt} dt. \quad (16) $$

When $x = 0$, using eqn. (9) and reversing the time-axis we get,

$$ \langle T^{\omega} \rangle = \frac{-1}{\Gamma(\mu)} \int_{0}^{\infty} t^{\mu-1} \frac{dM(t)}{dt} dt. \quad (17) $$

*Case 2: Let* $-2 < \omega \leq -1$. In this case $n = 2$ and $\mu = \omega + 2$. From the definition of fractional differentiation in eqn. (7), we get,

$$ {}_{-\infty}D_x^{-\omega}(M(-t)) = \frac{1}{\Gamma(\mu)} \frac{d^2}{dx^2} \left[ \int_{-\infty}^{x} (x-t)^{\mu-1} M(-t) dt \right]. \quad (18) $$

Applying the integration by parts twice to eqn. (18) followed by Leibniz rule, we obtain,

$$ {}_{-\infty}D_x^{-\omega}(M(-t)) = \frac{1}{\Gamma(\mu)} \int_{-\infty}^{x} (x-t)^{\mu-1} \left( \frac{d^2M(-t)}{dt^2} \right) dt. \quad (19) $$

When $x = 0$, using eqn. (9) and reversing the time-axis we get,

$$ \langle T^{\omega} \rangle = \frac{1}{\Gamma(\mu)} \int_{0}^{\infty} t^{\mu-1} \frac{d^2M(t)}{dt^2} dt. \quad (20) $$

*Case 3: Let* $\omega \leq 0$. Let $n = [-\omega] + 1$ and $\mu = n + \omega$. In this case, from eqn. (7), we get,

$$ {}_{-\infty}D_x^{-\omega}(M(-t)) = \frac{1}{\Gamma(\mu)} \frac{d^n}{dx^n} \left[ \int_{-\infty}^{x} (x-t)^{\mu-1} M(-t) dt \right]. \quad (21) $$

By induction from cases (1) and (2), we can deduce that

$$ {}_{-\infty}D_x^{-\omega}(M(-t)) = \frac{1}{\Gamma(\mu)} \int_{-\infty}^{x} (x-t)^{\mu-1} \left( \frac{d^nM(-t)}{dt^n} \right) dt. \quad (22) $$

When $x = 0$, using eqn. (9) and reversing the time-axis we get,

$$ \langle T^{\omega} \rangle = \frac{(-1)^n}{\Gamma(\mu)} \int_{0}^{\infty} t^{\mu-1} \frac{d^nM(t)}{dt^n} dt. \quad (23) $$

## 3. SIMULATION RESULTS

In this section, we present simulation results on a non-smooth distribution $f_T(T)$, shown in Fig. 1(A). Simulated data are generated from this distribution using eqn. (1) and corrupted with additive Gaussian zero-mean noise with standard deviation $\sigma_\varepsilon$. One such data set is shown in Fig. 1(B). Fractional moments were estimated using eqn. (4) described in this manuscript. Estimated moments are compared with the true moments in Fig. 1(C). The errorbars on the estimated moments are obtained from analyzing data with multiple realizations of noise. The simulation results obtained on this models are representative of results seen on other models.

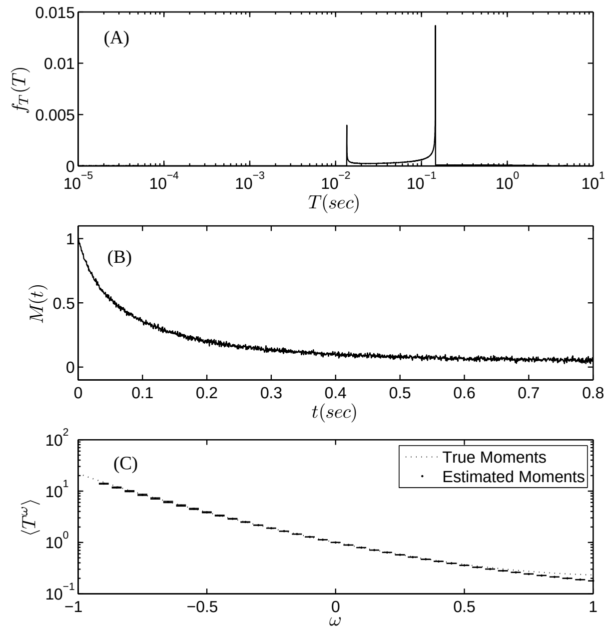


Figure 1: (A) A complex $f_T(T)$ is considered. (B) Data simulated from this model with additive white Gaussian noise with $\sigma_\varepsilon = 0.01$. One realization of the data is shown. (C) Moments are estimated from the data using eqn. (4). The mean and error-bar of estimated moments are obtained from 100 different noise realizations and compare well with the true moments.

## 4. SUMMARY

Traditional methods of computing moments involves solving the inverse Laplace transform for the probability density function, which is a well-known mathematically ill-conditioned problem. Often, regularization or prior information about the expected density function is incorporated to make the problem better conditioned. However, the choice of a regularization functional as well as the weight given to prior information are non-unique and are well-known drawbacks of the transform.

This paper describes a novel method using fractional calculus to estimate moments of a random variable from the measured Laplace transform of its probability density function. The moments are obtained from a simple, straightforward linear transformation of the data. Further, we have demonstrated that when $\omega > 0$, computation of moments corresponds to fractional integration of the data. When $\omega \leq 0$, computation of moments corresponds to fractional differentiation.

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