Generalized Langevin Equations Driven by Fractional Brownian Noise

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1 Introduction

Generalized Langevin equations have been extensely used in the domain of anomalous diffusion [**?**], where families with power law kernels have been extensely studied and applied. A special emphasis is given on the long term behaviour of the solution of these equations, that is clearly subdiffusive.

In this work we choose to work with noise driven by fractional Brownian motion due to technical reasons explicited further in the text. In this case, we were able to put together a toolbox that allow to find a good number of exact results, specially with relation to diffusion.

The tools of fractional calculus and notation used are exposed in Section II. We follow by defining in Section III the necessary pre-requisites concerning fractional Brownian motion, and some results are derived. Finally, in Section IV, we deal with the results related to the generalized Langevin equation, specially the exact formulas linked to anomalous diffusion.

2 Fractional Calculus

2.1 Basic definitions

As a technical requisite that simplify many of the relations in this subject, we will need many properties of the fractional calculus. To begin, we define the fundamental monomials:

$$p_\alpha(t) = \frac{t^\alpha}{\Gamma(\alpha + 1)}$$

We start by defining forward fractional integral for $\alpha > 0$ by:

$$J^{\alpha}_{a+}f(t) = \frac{1}{\Gamma(\alpha)}\int_a^t \frac{f(u)}{(t-u)^{1-\alpha}}du = -\int_a^t f(u)\, dp_{\alpha}(t-u)$$

and also the backwards fractional integral of same order:

$$J^{\alpha}_{b-}f(t) = \frac{1}{\Gamma(\alpha)}\int_t^b \frac{f(u)}{(u-t)^{1-\alpha}}du = \int_t^b f(u)\, dp_{\alpha}(t-u).$$

These two integrals can be seen as adjoints with respect to the standard inner product in $[a,b]$, as we have:

$$\int_a^b g(t)J^{\alpha}_{a+}f(t)dt = \int_a^b f(t)J^{\alpha}_{b-}g(t)dt.$$

One of the most important features of fractional derivatives is the semi-group property, that translates our intuition that quantity of integrals is extensive:

$$J^{\alpha}_{a+}J^{\beta}_{a+} = J^{\alpha+\beta}_{a+}.$$

Given these integrals we define one of the most common alternatives for a fractional derivative, the Riemann-Liouville (RL) one, that is given for $0 \leq \alpha < 1$ by:

$$D^{\alpha}_{a+}f(t) = \frac{d}{dt}J^{1-\alpha}_{a+}f(t)$$

and analogously for the backwards integral. We define also another fractional derivative, the Caputo (C) one:

$$D^{\alpha *}_{a+}f(t) = J^{1-\alpha}_{a+}\frac{d}{dt}f(t)$$

that can be seen as an adjoint for the Riemann-Liouville derivative:

$$\int_a^b g(t)D^{\alpha}_{a+}f(t)dt = -\int_a^b f(t)D^{\alpha *}_{b-}g(t)dt.$$

If we are interested in higher order derivatives we may differentiate more times, giving an even bigger quantity of possible derivatives, but this case is not important for this project. If $a = 0$, are going to use the more familiar notation:

$$D^{\alpha}_{0+}f(t) = \frac{d^{\alpha}f(t)}{dt^{\alpha}}$$

As we consider here functions that are defined only on times that are bigger than 0, Fourier transform is not avaible, and we must recur to the Laplace transform. It has a very simple relation with fractional integrals and derivatives by:

$$\widehat{\frac{d^\alpha f}{dt^\alpha}}(s) = s^\alpha \hat{f}(s), \quad \widehat{J^\alpha f}(s) = s^{-\alpha}\hat{f}(s).$$

Finally, the most important properties of fractional integrals and derivatives are given by their effect on fundamental monomials:

$$I^\beta p_\alpha(t) = p_{\alpha+\beta}(t), \quad \forall \alpha, \beta \in \mathbb{R}$$

$$D^\beta p_\alpha(t) = p_{\alpha-\beta}(t), \quad \forall \alpha \in \mathbb{R}/\{1-\beta\}, \beta \in \mathbb{R}$$

$$D^{\beta *} p_\alpha(t) = p_{\alpha-\beta}(t), \quad \forall \alpha \in \mathbb{R}^*, \beta \in \mathbb{R}$$

2.2 Approximation properties of fractional derivatives

In the same way that usual derivatives give the best integer order polynomial approximation to a function, fractional derivatives can be shown to have similar properties. The first important property of this type is the generalized fundamental theorem of calculus for $0 \leq \alpha \leq 1$:

$$I^\alpha_{a+} D^{\alpha *}_{a+} f(t) = f(t) - f(a), \quad D^\alpha_{a+} I^\alpha_{a+} f(t) = f(t).$$

A simple approximation on the first equation gives that:

$$f(t) = f(a) + D^{\alpha *}_{a+} f(w)\, p_\alpha(t-a)$$

for some $a \leq w \leq t$.

2.3 Some important functions and relations

In order to start the discussion of these equations, we define the generalized fractional exponential:

$$e^{\lambda;t}_{\alpha;\beta} = \sum_{k=0}^{\infty} \lambda^k p_{\alpha k+\beta}(t)$$

When β is hidden, we take it for 0 and when $\alpha = 1$ it reduces to the usual exponential. It can be written in terms of the Mittag-Leffler function as:

$$e^{\lambda;t}_{\alpha;\beta} = t^\beta E_{\alpha,\beta+1}(\lambda t^\alpha)$$

We can use the assymptotic expansion of Mittag-Leffler functions [P, HMS], to find that for positive λ we have:

$$e^{\lambda;t}_{\alpha;\beta} = \frac{1}{\alpha}\exp(\lambda^{1/\alpha}t) - \sum_{n=1}^{N-1}\lambda^{-n}p_{\beta-n\alpha}(t) + O\left(t^{\beta-N\alpha}\right).$$

and in the negative case we have:

$$e^{\lambda;t}_{\alpha;\beta} = -\sum_{n=1}^{N-1}\lambda^{-n}p_{\beta-n\alpha}(t) + O\left(t^{\beta-N\alpha}\right).$$

for the same case.

2.4 Some fractional differential equations

One of the most important FDE's that are found with a certain frequence is the eigenvalue equation:

$$D^{\alpha*}_{0+}f(t) = \lambda f(t).$$

Its solution is given by multiples of the fractional exponential:

$$f(t) = e^{\lambda,t}_{\alpha}$$

from where we see the importance of the functions defined before.

To finish this introduction, we analyse the generalized Abel equation of second order [GM], that will be fundamental to the analysis of the Langevin equation:

$$f(t) = \frac{\lambda}{\Gamma(1-\alpha)}\int_0^t \frac{f(u)}{(t-u)^{\alpha}} + g(t).$$

This equation can be written in terms of fractional operators as:

$$(I - \lambda J^{1-\alpha})f(t) = g(t)$$

which can be solved by inverting the operator on the left, that gives:

$$f(t) = \sum_{k=0}^{\infty}\lambda^k J^{k(1-\alpha)}g(t)$$

Developping and calculating each term, we can write this solution as a convolution of the fractional exponential with the inhomogeneous term:

$$f(t) = g(t) + \dot{e}_{\alpha}(t,\lambda) * g(t)$$

where the dot represents differentiation with respect to t. Or, if g is regular enough, we get:

$$f(t) = g(0)e_\alpha(t,\lambda) + \int_0^t e_\alpha^{\lambda;t-u}\, dg(u)$$

where the last term must be seen as a Stieltjes integral.

3 Fractional Brownian Motion

3.1 Definition and basic properties

A gaussian process $B^\alpha = \{B_t^\alpha,\, t \geq 0\}$ is called a *fractional brownian motion* (*fBm*) [N] of parameter $\alpha \in (0,2)$ if it has mean zero and is self similar:

$$B_{at} \approx a^{\alpha/2} B_t$$

It can be shown that it happens if its covariance function is given by a multiple of:

$$\mathbb{E}(B_t^\alpha B_s^\alpha) = \frac{1}{2}\left(p_\alpha(t) + p_\alpha(s) - p_\alpha(|t-s|)\right).$$

For $\alpha = 1$ classical brownian motion is recovered. Direct application of this definition gives the following property:

$$\mathbb{E}[(B_t^\alpha - B_s^\alpha)^2] = p_\alpha(|t-s|).$$

Property (2) shows that we can already classify fBm's in two types. For $\alpha > 1$, diffusion is in average faster than in the classical brownian motion, that is, motion is *superdiffusive*. Otherwise, if $\alpha < 1$, motion is *subdiffusive*.

3.2 Stochastic integrals with relation to fBm

In this section we will not bother to define the stochastic integral of processes, as these are not relevant for this paper and have lots of sophistications. We will restrict ourselves to the integration of functions.

We define the Stratonovich stochastic integral of a function F by:

$$B_t^\alpha(F) = \int_0^t F_u\, dB_u^\alpha = \lim_{|P|\to 0} \sum_k \bar{F}_{t_k}\left(B_{t_{k+1}}^\alpha - B_{t_k}^\alpha\right)$$

where we defined:

$$\bar{F}_{t_k} = \frac{F_{t_{k+1}} + F_{t_k}}{2}$$

and the limit is taken in the mean square sense. We will not enter into details of the mathematical properties of this definition, as they are complicated to be treated formally.

Our main goal with this definition is to find an equivalent formula for the Itô isometry [AN]. For it, start by discretizing the formula:

$$\langle B_t^\alpha(F) B_t^\alpha(G) \rangle = \sum_{i,j} \bar{F}_{t_i} \bar{G}_{t_j} \langle [B_{t_i} - B_{t_{i-1}}][B_{t_j} - B_{t_{j-1}}] \rangle.$$

As a further step, we divide the sum into two parts:

$$\sum_{i,j} = \sum_{i=j} + \sum_{i \neq j}$$

and we study each case separately. We find that:

$$\begin{aligned} 2\langle (B_{t+dt} - B_t)(B_{s+ds} - B_s) \rangle &= p_\alpha(|t - s + dt|) + p_\alpha(|t - s - ds|) \\ &\quad - p_\alpha(|t - s + dt - ds|) - p_\alpha(|t - s|) \end{aligned}$$

Taking $t > s$ and doing a second order expansion of each term, we get:

$$\langle dB_t \, dB_s \rangle = \frac{1}{2} p_{\alpha-2}(t - s) \, ds \, dt$$

For $t = s$ we get to first order symbolically:

$$\langle dB_t \, dB_t \rangle = p_{\alpha-1}(0) \, dt$$

Using these results, we can write the former sum as:

$$\sum_i \bar{F}_{t_i} \bar{G}_{t_i} p_{\alpha-1}(0) \, dt_j + \frac{1}{2} \sum_{i \neq j} \bar{F}_{t_i} \bar{G}_{t_j} p_{\alpha-2}(t_i - t_j) \, dt_i \, dt_j$$

In the case where $F = G$, we transform further this equation to the form:

$$\begin{aligned} &\sum_i \left(\bar{F}_{t_i} \bar{F}_{t_i} p_{\alpha-1}(0) \, dt_j + \sum_{i > j} \bar{F}_{t_i} \bar{F}_{t_j} p_{\alpha-2}(t_i - t_j) \, dt_i \, dt_j \right) \to \\ &\to \int_{t_0}^t F_u \frac{d}{du} \int_{t_0}^u F_s p_{\alpha-1}(u - s) \, ds \, du \end{aligned}$$

using the formula:

$$\frac{d}{dt}\int_a^t F(t,u)\,du = F(t,t) + \int_a^t \partial_t F(t,u)\,du$$

that gives finally the closed formula for the correlation of two stochastic integrals in terms of fractional Riemann-Liouville derivatives:

$$\langle B_t^\alpha(F)^2\rangle = \int_{t_0}^t F_u \cdot D_{t_0+}^{1-\alpha} F_u\,du$$

Using the same method (or the polarization formula) it is simple to prove the analogous inner product formula:

$$\langle B_t^\alpha(F) B_t^\alpha(G)\rangle = \frac{1}{2}\int_{t_0}^t [G_u \cdot D_{t_0+}^{1-\alpha} F_u + F_u \cdot D_{t_0+}^{1-\alpha} G_u]\,du$$

When meeting the applications in the next sections, the first formula will be useful specilly in its dual form using Caputo derivatives:

$$\langle B_t^\alpha(F)^2\rangle = F_t \cdot I_{t_0+}^{\alpha} F_t - \int_{t_0}^t F_u \cdot D_{t-}^{(1-\alpha)*} F_u\,du$$

It is important to notice that everywhere here, is we meet a derivative of order $1-\alpha$ for $\alpha > 1$, then we mean the standard fractional integral of same type and of order $\alpha - 1$.

4 Fractional Brownian Noise

4.1 Langevin equation

The linear response theory of non-equilibrium statistical mechanics says that if we have a generalized Langevin equation of the form

$$m\frac{dv_t}{dt} = -\int_0^t K(t-u)v_t\,du + \xi_t$$

then by the fluctuation-dissipation theorem, the memory kernel is completely determined by the covariance of the noise using the relation:

$$\langle \xi_t, \xi_u\rangle = k_B T K(t-u)$$

In the case of the fBm, we calculate this memory kernel from the definition on the previous section:

$$\begin{aligned}\langle \xi_t, \xi_u \rangle &= \frac{\partial}{\partial t}\frac{\partial}{\partial u}\langle B_t, B_u \rangle \\ &= p_{\alpha-2}(|t-u|)\Theta(t-u) + 2p_{\alpha-1}(|t-u|)\delta(t-u).\end{aligned}$$

Integrating and integrating memory in the Stratonovich sense (which gives half of the weight of a delta function on the extremities of the interval) , we can write the Langevin equation as:

$$m\frac{dv_t}{dt} = -\frac{\eta^2}{k_B T}\frac{d}{dt}\int_0^t p_{\alpha-1}(t-u)v_u\, du + \eta\xi_t$$

because there is only half of correlation on t. Using the tools from fractional calculus from the first section, we can rewrite this equation as:

$$m\frac{dv_t}{dt} = -\frac{\eta^2}{k_B T}\frac{d^{1-\alpha}v_t}{dt^{1-\alpha}} + \eta\xi_t$$

which we will write from here as:

$$\frac{dv_t}{dt} = \lambda\frac{d^{1-\alpha}v_t}{dt^{1-\alpha}} + \eta\xi_t.$$

to improve readability.

It is interesting to note that in terms of Itô integrations, we would have lacked the delta into the formulation, which is not a problem for $\alpha > 1$, but which cause a divergence when $\alpha < 1$. Altough it is yet possible to work symbolically with an equation of this type, the formulation here disappears with this problem while being equally well treatable.

4.2 Solution of the Langevin equation and properties

In order to obtain the solution of this equation, we start by writing it on form more friendly to the tools we already met before, namely:

$$v_t = \lambda J^\alpha v(t) + v_0 + \eta B_t$$

which results from simple integration of the Langevin equation. This is an Abel equation of the second kind, so it can be solved as before:

$$v_t = v_0\, e_\alpha^{\lambda;t} + \eta\int_0^t e_\alpha^{\lambda;t-u}\, dB_u.$$

We notice that because of the fact that we are integrating simple functions, it is not a problem to write this solution as an stochastic integral like that. Integrating once more, we get:

$$x_t = x_0 + v_0\, e_{\alpha;1}^{\lambda;t} + \eta \int_0^t e_{\alpha;1}^{\lambda;t-u}\, dB_u.$$

In order to obtain the diffusive behaviour of this solution, we study the mean square displacement, which can be divided into two parts, an stochastic one due to noise, and a deterministic one due to friction:

$$\left\langle (x_t - x_0)^2 \right\rangle = \left(v_0 \cdot e_{\alpha,1}^{\lambda;t}\right)^2 + \eta^2 \left\langle \left(\int_0^t e_{\alpha;1}^{\lambda;t-u}\, dB_u \right)^2 \right\rangle$$

The second term can be calculated using the formulas obtained from the sections before, which gives us with a little calculation and using the properties of fractional exponentials:

$$\begin{aligned}
\left\langle (x_t - x_0)^2 \right\rangle &= \left(v_0 \cdot e_{\alpha,1}^{\lambda;t}\right)^2 - \frac{\eta^2}{\lambda} \int_0^t e_{\alpha,1}^{\lambda;t-u} \left(1 - e_{\alpha}^{\lambda;t-u}\right) du \\
&= \left(v_0 \cdot e_{\alpha,1}^{\lambda;t}\right)^2 - \frac{\eta^2}{\lambda} \int_0^t e_{\alpha,1}^{\lambda;u} \left(1 - e_{\alpha}^{\lambda;u}\right) du \\
&= \left(v_0^2 - \frac{\eta^2}{2\lambda}\right) \cdot \left(e_{\alpha,1}^{\lambda;t}\right)^2 - \frac{\eta^2}{\lambda} \cdot e_{\alpha,2}^{\lambda;t}
\end{aligned}$$

Using the assymptotic properties of fractional exponentials, we find that for a long time t, we will get a principal term of order:

$$\left\langle (x_t - x_0)^2 \right\rangle \approx t^{2-\alpha}$$

which is a classic power subdiffusion. It is interesting to note that a noise that is more positively correlated (bigger α) gives a slower diffusion in the long term.

4.3 Mixed noise

Now we study the case where the noise is mixed, that is, $B_t = \eta_\alpha B_t^\alpha + \eta_\beta B_t^\beta$, where both terms are independent. In this case, we obtain the equation:

$$m v_t = -\frac{\eta_\alpha^2}{k_B T} I^\alpha v_t - \frac{\eta_\beta^2}{k_B T} I^\beta v_t + \eta_\alpha B_t^\alpha + \eta_\beta B_t^\beta$$

which we will reduce to the simplified form:

$$v_t = \lambda_\alpha I^\alpha v_t + \lambda_\beta I^\beta v_t + \eta_\alpha B_t^\alpha + \eta_\beta B_t^\beta$$

In order to obtain the inverse of the linear operator we have, we are going to use the following formula:

$$\frac{1}{1-x-y} = \sum_{i,j=0}^{\infty} \binom{i+j}{i} x^i y^j$$

In this way we can define the function given by:

$$e_{\alpha,\beta;\gamma}^{\lambda_\alpha,\lambda_\beta;t} = \sum_{n,m} \binom{n+m}{n} \lambda_\alpha^n \lambda_\beta^m p_{n\alpha+m\beta+\gamma}(t)$$

Using this definition and using similar methods that those used before, we can write the general solution of the equation as:

$$v_t = v_0 \cdot e_{\alpha,\beta}^{\lambda_\alpha,\lambda_\beta;t} + \int_0^t e_{\alpha,\beta}^{\lambda_\alpha,\lambda_\beta;t-u} \, dB_u$$

or, integrating once more:

$$x_t = x_0 + v_0 \cdot e_{\alpha,\beta;1}^{\lambda_\alpha,\lambda_\beta;t} + \int_0^t e_{\alpha,\beta;1}^{\lambda_\alpha,\lambda_\beta;t-u} \, dB_u$$

which has a form similar from the solution before. We can find the mean square deplacement of this solution using the isometry formulas form before, using the fact that the noises are independant, that is:

$$\langle B_t(F)^2 \rangle = \langle B_t^\alpha(F)^2 \rangle + \langle B_t^\beta(F)^2 \rangle$$

and using the same procedure as before, we find that:

$$\left\langle (x_t - x_0)^2 \right\rangle = \left(v_0 \cdot e_{\alpha,\beta;1}^{\lambda_\alpha,\lambda_\beta;t} \right)^2 - \eta_\alpha^2 \int_0^t e_{\alpha,\beta;1}^{\lambda_\alpha,\lambda_\beta;u} \cdot e_{\alpha,\beta;\alpha}^{\lambda_\alpha,\lambda_\beta;u} du - \eta_\beta^2 \int_0^t e_{\alpha,\beta;1}^{\lambda_\alpha,\lambda_\beta;u} \cdot e_{\alpha,\beta;\beta}^{\lambda_\alpha,\lambda_\beta;u} du$$

This solution is less well treatable than the ones from the simple noise case, but which can be solved with a deeper study about the properties of the mixed exponential, which is out of the scope of this work.

4.4 Discussion about the solution

One of the biggest interests of the knowledge of the exact form and behaviour of these solutions is to be able to know how to estimate parameters in a certain dynamical model. This estimation is generally connected to a global quantity that characterizes the dynamics of this system.

In this case, it is important to remark that these solutions are not stationary in general, that is, the behavior of $x_t - x_s$ and the one of x_{t-s} is very distinct, at least when considering short time intervals. That means that the most usual quantity used to characterize the system, the averaged mean square deplacement [G]:

$$\mathcal{M}(t,h) = \frac{1}{t-h} \int_0^{t-h} (x_{u+h} - x_u)^2 \, du$$

as a cumulative statistics that is typical of stationary increment process is not the best possible characteristic to be studied.

As an example, for a system whose dynamics follow a exponential:

$$x_t = e^{\lambda t}$$

it is possible to correct this measure by a renormalization in time, for example:

$$\mathcal{M}'(t,h) = \frac{1}{t-h} \int_0^{t-h} e^{-\lambda u} (x_{u+h} - x_u)^2 \, du$$

that respects the form of the general solution. In the case found here, because of the complicated algebraical properties of fractional exponentials, this study is more complicated and a very important next step for the effective estimation of parameters in this kind of dynamics.

5 Conclusion

In first place, we remark the points of this work which are new. In the domain of fractional calculus, only the notation for the exponentials have been introduced, but made in a way that facilitates the symbolic work greatly, allowing to work with the present equations as if they were more usual ones.

For fractional brownian motion, the formula for the correlation of two stochastic integrals of functions is new in the sense that it expands formulas already found for $\alpha > 1$ to the case $\alpha < 1$. This development was possible only in a symbolic matter and is difficult to formalize (due to singulatities).

The form of the Langevin equation used here is different from the one used in most works of physics, so what is shown is that the results are very similar to the case that is treated usually. The equations for mixed noise and its mean square deplacement are original also, even if they do not go as much as far than that.

Even if there are no breakthroughs in this project, it serves as a good reference that connects strongly the literatures of fractional calculus, fractional brownian motion and generalized Langevin equations, as works in these areas have lots of exchanges between then, but almost never in a common language that is at the same time practical to use and representative of the behavior of solutions.

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