Generalised Langevin Equation with Lévy distribution

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Introduction

Generalised Lagevin equation (GLE)

$$\frac{\mathrm{d}V(t)}{\mathrm{d}t} = -\int_0^t V(t)K(t-s)\mathrm{d}s + F(t)$$

is one of the most powerful and used models of non-equilibrium statistical physics, which

- can model phenomena such as normal, sub- and superdiffusion,
- is the most strict derivation of other popular models such as Ornstein-Uhlenbeck process and fractional Brownian motion,
- has a strict derivation, which links many phenomenological models with statistical mechanics.

But, in the most studied approach, GLE is thought to be equation describing Gaussian process. This assumption is not without a cause, as it corresponds to the model of environment in thermal equilibrium. i.e. having Gibbs equlibrium distribution, which is usually Gaussian.

Here we want to give insight into non-Gaussian, Lévy case, which may appear in the case of non-equlibrium environment.

Hamiltonian approach

From the point of view of statistical mechanics, GLE results from the system of equations decribing the evolution of the harmonic heat bath

$$\frac{\mathrm{d}}{\mathrm{d}t}X = \frac{P}{m} = V,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}P = -\mathcal{V}'(X) + \sum_{k=1}^{\infty} m_k\gamma_k q_k,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}q_k = \frac{p_k}{m_k},$$
$$\frac{\mathrm{d}}{\mathrm{d}t}p_k = -m_k\omega_k^2 q_k + m_k\gamma_k X,$$

where the randomness is contained in the random initial conditions $q_k(0)$ and $p_k(0)$ which we assume to have Lévy distribution. The coordinates of interest $X(t)$ and $V(t)$ are therefore the solution of the set of random ordinary differential equations with Lévy distribution.

Transforming the above, we obtain the form of the stochastic force, which acts in the GLE equation

$$F(t) = \mathrm{Re}\sum_{k=1}^{\infty} m_k\gamma_k \left(q_k(0) + \frac{\mathrm{i}p_k(0)}{m_k\omega_k}\right)\mathrm{e}^{\mathrm{i}\omega_k t}.$$

Note that this is an example of infinitely divisible harmonic process. For i.i.d $q_k(0), p_k(0)$ the above sum is convergent if $(m_k\gamma_k)_k$ and $(1/(m_k\omega_k))_k$ are in ℓ^2 for L^2 Lévy variables, or ℓ^α for α-stable variables.

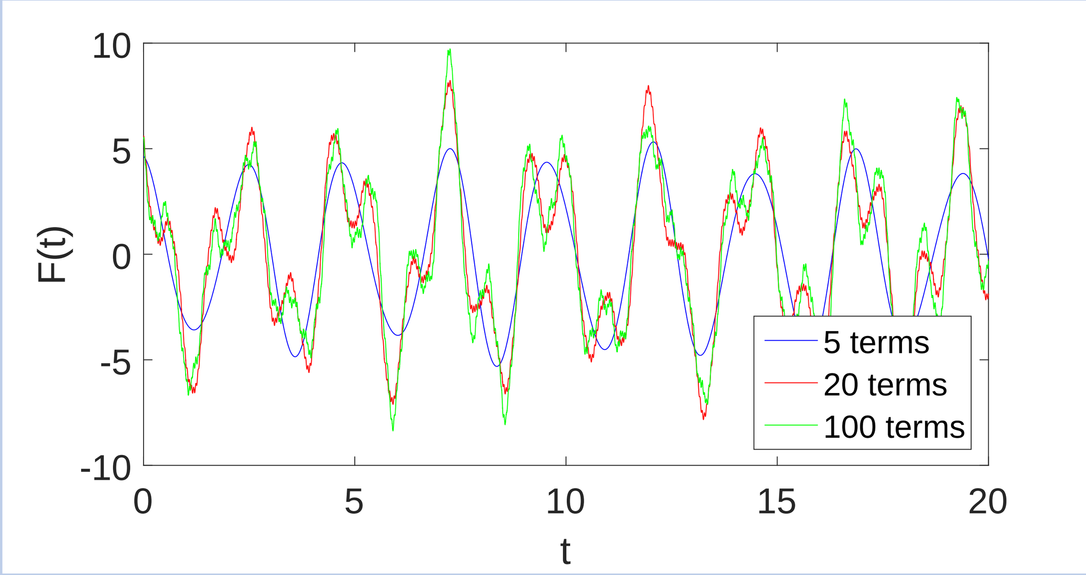

Figure: Harmonic process $F(t)$ with $\alpha = 1.2$ stable $p_k(0), q_k(0)$ and power-law distributed $m_k\gamma_k$ and ω_k for various truncation of the harmonic sum.

Harmonizable process

The stochastic force $F(t)$ can be effectively regarded as infinitely divisible harmonizable process

$$F(t) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}\omega t}\Lambda(\mathrm{d}\omega),$$

where Λ is some infinitely divisible random measure. Taking real part can be omitted if Λ is taken to be antisymmetrical: $\Lambda(\mathrm{d}\omega) = \overline{\Lambda}(-\mathrm{d}\omega)$. In the case of harmonic process, the measure Λ is concentrated on points ω_k, but for real systems these points are scattered so densely, that in practical purposes can be considered dense. In such case we can write $\Lambda(\mathrm{d}\omega) = \rho(\omega)\mathrm{d}L(\omega)$, where $\mathrm{d}L$ are increments of Lévy process and ρ is a spectral density, which must belong to L^α space for α-stable process and to L^2 for second-order process; the integral for $F(t)$ is understood in the respective sense.

The processes of these class are noticeably different from the most used models. For example, the main infinitely divisible anomalous diffusion process

$$L_d(t) = \int_{\mathbb{R}} \left((t-s)_+^d - (-s)_+^d\right)\mathrm{d}L(s)$$

is a basis for the most used model of force $F(t)$, which is considered to be increments of L_d: $F(t) = \mathrm{d}L_d(t)$, understood in the weak sense. But, the harmonizable process

$$X_d(t) = \int_{\mathbb{R}} \frac{\mathrm{e}^{\mathrm{i}\omega t} - 1}{|\omega|^{d+1}}\mathrm{d}L(\omega).$$

has the same second-order properties (if it has moments) as L_d, and at the same time different full memory structure (e.g. codifference). The hamiltonian approach indicates harmonizable process is a correct choice, in the case above corresponding to spectral density $\rho(\omega) = \omega^{-d}$.

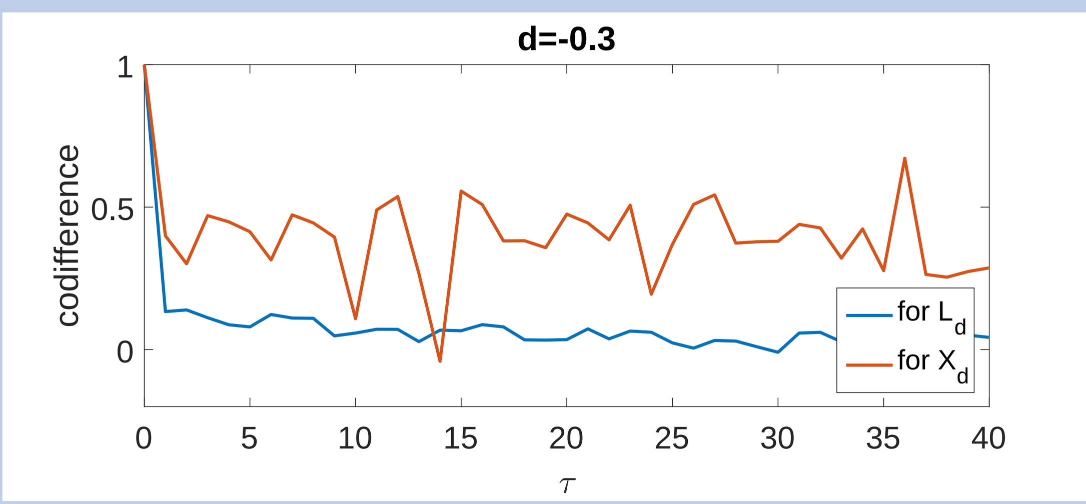

Figure: Comparison of codifferences for L_d and X_d increments, $d = -0.3$.

Solution of GLE

The Generalised Langevin Equation which fallows from previous consideration can be understood as stochastic Volterra integro-differential equation

$$\mathrm{d}V(t) = -\int_0^t V(t)K(t-s)\mathrm{d}s\mathrm{d}t + \mathrm{d}\tilde{F}(t),$$

where $\mathrm{d}\tilde{F}(t) = F(t)\mathrm{d}t$ and kernel K is given by

$$K(t) = \sum_{k=1}^{\infty} m_k \frac{\gamma_k^2}{\omega_k^2}\cos(\omega_k t).$$

The existence of solution $V(t)$ depends mainly on the regularity of kernel K. If the operator given by the convolution with K is a contraction in a proper Banach space, the solution exists in the sense of corresponding metrics. One of the possible sufficient conditions is $\max_{s:\, s<t}|tK(t-s)| < 1$, which guarantees existence of solution for α-stable,$\alpha > 1$, stochastic force.

However, in practical applications there is more use of weaker mild solution which is given by

$$V(t) = \int_0^t G(t-s)\mathrm{d}\tilde{F}(t),$$

where the Green's function G is a solution of the distributional equation

$$G'(t) = -\int_0^t G(s)K(t-s)\mathrm{d}s + \delta(t);$$

δ denotes Dirac delta distribution. This equation is solvable for bounded K, e.g. by means of Laplace transform. Given function G, the sufficient condition for existence of the mild solution is $\hat{G}\rho \in L^\alpha$ ($\hat{G}$ is Fourier transform of G).

Summary

- the physical heat bath model can describe the infinitely divisible diffusion processes
- the processes with the most physical significance under GLE theory are harmonic and harmonizable processes
- the existence of solution requires few subsequent technical assumptions, so it is better to consider GLE equation case-by-case

References

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- S. Kou, X. Xie; *Generalized Langevin Equation with Fractional Gaussian Noise: Subdiffusion within a Single Protein Molecule*; Physical Review Letters 93/18 (2004).

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