Random Diffusivity from Stochastic Equations: Two Models in Comparison for Brownian Yet Non-Gaussian Diffusion.

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1. Introduction

2. A set of stochastic equations for random diffusivity
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2 A set of stochastic equations for random diffusivity

3 Generalised grey Brownian motion with random diffusivity
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3. Generalised grey Brownian motion with random diffusivity

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Introduction

Brownian Yet Non-Gaussian Diffusion

1. linear trend of the MSD;
2. non Gaussian PDF.


Not well described by standard models for anomalous diffusion (CTRWs, fBM). Other models have been proposed:
Correlated random walks (Codling, E. A. et al. 2008, J. R. Soc. Interface, 5);
Superstatisical Brownian motion (Beck, C. 2006, Prog. Theor. Phys. Suppl, 162);
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- Biological systems

- Materials with glassy dynamics
  (Chaudhuri, P. et al. 2007, Phys. Rev. Lett., 99);

- Ecological processes
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- Diffusing Diffusivities
Stochastic Equations for Random Diffusivity: Assumptions

\[ D(t) = y_2(t) \, dy = a(y) \, dt + \sigma \, dW(t). \]

\[ a(y) \] can be defined through the distribution of \( y(t) \) by means of:

\[ a(y) = \sigma^2 \frac{dy}{y(y)} \] (1)

Given the \( Y = g(X) \), for sufficiently good functions \( g(x) \), we have:

\[ p_Y(y) = p_X(g^{-1}(y)) \bigg| \frac{dy}{g^{-1}(y)} \] (2)

An ad hoc set of stochastic equations for \( D(t) \) can be built:

\[ p_D(D) \rightarrow p_y(y) \rightarrow a(y). \]
Stochastic Equations for Random Diffusivity: Assumptions

\[
\begin{aligned}
D(t) &= y^2(t) \\
\end{aligned}
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Stochastic Equations for Random Diffusivity: Assumptions

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\( a(y) \) can be defined through the distribution of \( y(t) \) by means of:

\[
a(y) = \frac{\sigma^2}{2 p_y(y)} \frac{dp_y(y)}{dy}. \tag{1}
\]
\[
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\end{align*}
\]

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p_Y(y) = p_X(g^{-1}(y)) \left| \frac{d}{dy}g^{-1}(y) \right|.
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Stochastic Equations for Random Diffusivity: Assumptions

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\begin{align*}
D(t) &= y^2(t) \\
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Given the \(Y = g(X)\), for sufficiently good functions \(g(x)\), we have:

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An \textit{ad hoc} set of stochastic equations for \(D(t)\) can be built

\[
p_D(D) \xrightarrow{\text{Eq. \(2\)}} p_y(y) \xrightarrow{\text{Eq. \(1\)}} a(y).
\]
Stochastic Equations for Random Diffusivity: Definition

\[
\gamma \eta, \eta \left( D \right) = \eta D^{\star} \Gamma \left( \frac{\nu}{\eta} \right) D^{\nu} - 1 e^{-\left( \frac{D}{D^{\star}} \right) \eta},
\]

\[
\left\langle D_n \right\rangle = D^{\star} \Gamma \left( \frac{\nu + n}{\eta} \right) \Gamma \left( \frac{\nu}{\eta} \right),
\]

where \( D^{\star} = y^2 \), \( \nu \) and \( \eta \) are positive constants.

\[
\begin{align*}
dy &= \sigma^2 \frac{2}{y^{\nu - 1} - 2 \eta \left( \frac{y}{y^{\star}} \right)^2 \eta} dt + \sigma dW(t) \\
D(t) &= y^2(t),
\end{align*}
\]

For \( \nu = 0.5 \) and \( \eta = 1 \) we obtain an Ornstein-Uhlenbeck (OU) process for the variable \( y(t) \).

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Stochastic Equations for Random Diffusivity: Definition

\[ \gamma_{\nu,\eta}^{\text{gen}}(D) = \frac{\eta}{D^\nu \Gamma(\nu/\eta)} D^{\nu-1} e^{-(D/D_*)^\eta}, \quad \langle D^n \rangle = D_*^{n} \frac{\Gamma\left(\frac{\nu+n}{\eta}\right)}{\Gamma\left(\frac{\nu}{\eta}\right)}, \]

where \( D_* = y_*^2 \), \( \nu \) and \( \eta \) are positive constants.
\[ \gamma_{\nu,\eta}^{\text{gen}}(D) = \frac{\eta}{D_* \Gamma(\nu/\eta)} D^{\nu - 1} e^{-\left(D/D_*\right)^\eta}, \quad \langle D^n \rangle = D_*^n \frac{\Gamma\left(\frac{\nu + n}{\eta}\right)}{\Gamma\left(\frac{\nu}{\eta}\right)}, \]

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\[ \gamma_{\nu,\eta}^{\text{gen}}(D) = \frac{\eta}{D^* \Gamma(\nu/\eta)} D^{\nu-1} e^{-\left(D/D^*\right)^\eta}, \quad \langle D^n \rangle = D^* \frac{\Gamma\left(\frac{\nu+n}{\eta}\right)}{\Gamma\left(\frac{\nu}{\eta}\right)}, \]

where \( D^* = y^2 \), \( \nu \) and \( \eta \) are positive constants.

\[
\begin{align*}
\frac{dy}{dt} &= \frac{\sigma^2}{2y} \left[ 2\nu - 1 - 2\eta \left( \frac{y}{y^*} \right)^{2\eta} \right] dt + \sigma \, dW(t) \\
D(t) &= y^2(t),
\end{align*}
\]
Stochastic Equations for Random Diffusivity: Definition

\[ \gamma_{\nu, \eta}^{\text{gen}}(D) = \frac{\eta}{D_\star \Gamma(\nu/\eta)} D^{\nu-1} e^{-(D/D_\star)^\eta}, \quad \langle D^n \rangle = D_\star^n \frac{\Gamma(\nu+n)}{\Gamma(\nu/\eta)}, \]

where \( D_\star = y_\star^2 \), \( \nu \) and \( \eta \) are positive constants.

\[ \begin{align*}
\frac{dy}{dt} &= \frac{\sigma^2}{2y} \left[ 2\nu - 1 - 2\eta \left( \frac{y}{y_\star} \right)^{2\eta} \right] dt + \sigma \, dW(t) \\
D(t) &= y^2(t),
\end{align*} \]

For \( \nu = 0.5 \) and \( \eta = 1 \) we obtain an Ornstein-Uhlenbeck (OU) process for the variable \( y(t) \).
Numerical evaluation of the correlation time by means of:

\[ \tau_{\text{corr}} = \frac{1}{\text{ACF}(0)} \int_0^\infty \text{ACF}(\tau) \, d\tau; \]

exponential fit:

\[ \text{ACF}(\tau) = \text{ACF}(0) e^{-\tau/\tau_{\text{corr}}}. \]
Numerical evaluation of the correlation time by means of:
computation of the integral:
\[ \tau_{\text{corr}} = \frac{1}{\int_0^\infty ACF(\tau) d\tau}; \]
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Numerical evaluation of the correlation time by means of:

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Numerical evaluation of the correlation time by means of:

- computation of the integral: $\tau_{\text{corr}} = \frac{1}{\text{ACF}(0)} \int_0^\infty \text{ACF}(\tau) d\tau$;
- exponential fit: $\text{ACF}(\tau) = \text{ACF}(0) e^{-\tau/\tau_{\text{corr}}}$.
It is possible to define ggBM model through the stochastic representation

\[ X_{ggBM} = \sqrt{\Lambda} X_g, \]

where \( \Lambda \) is an independent non-negative random variable and \( X_g \) is a Gaussian process.

The PDF of the stochastic variable \( X_{ggBM} \) can be evaluated by means of the integral

\[ P_{ggBM}(x, t) = \int_0^{\infty} p_{X_g}(x \lambda^{1/2}) \, p_{\Lambda}(\lambda) \, d\lambda \]

where \( p_{X_g} \) and \( p_{\Lambda} \) are the distributions of \( X_g \) and \( \Lambda \) respectively.

It is possible to define $ggBM$ model through the stochastic representation

$$X_{ggBM} = \sqrt{\Lambda} X_g,$$

where $\Lambda$ is an independent non-negative random variable and $X_g$ is a Gaussian process.

Generalised Grey Brownian Motion: Definition

It is possible to define ggBM model through the stochastic representation

\[ X_{\text{ggBM}} = \sqrt{\Lambda} X_g, \]

where \( \Lambda \) is an independent non-negative random variable and \( X_g \) is a Gaussian process.

The PDF of the stochastic variable \( X_{\text{ggBM}} \) can be evaluated by means of the integral

\[
P_{\text{ggBM}}(x, t) = \int_0^\infty p_{X_g} \left( \frac{x}{\lambda^{1/2}} \right) p_\Lambda(\lambda) \frac{d\lambda}{\lambda^{1/2}}
\]

where \( p_{X_g} \) and \( p_\Lambda \) are the distributions of \( X_g \) and \( \Lambda \) respectively.

Particles diffusing in Brownian fashion in a complex random environment properties independent on the diffusing particles and represented by a random diffusivity.

$$X^{ggBM} = \sqrt{2D(t)}W(t), \quad W(t) = \int_0^t \xi(s)ds.$$ 

Assuming a generalised Gamma distribution for the random diffusivity $$\gamma^{gen}_{\nu,\eta}(D) = \eta D^{\nu}\Gamma(\nu/\eta)D^{\nu-1}e^{-D/D^*}\eta,$$

$$\langle D^n \rangle = D^n\Gamma(\nu+n\eta)/\Gamma(\nu\eta),$$ where $$D^*, \nu, \eta$$ are positive constants.

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Generalised Grey Brownian Motion & Random Diffusivity

- Particles diffusing in Brownian fashion in a complex random medium;

\[ \text{X} \text{ggBM} = \sqrt{2D(t)}W(t), \quad W(t) = \int_0^t \xi(s) \, ds. \]

Assuming a generalised Gamma distribution for the random diffusivity \( \gamma_{\text{gen}} \nu, \eta \):

\[ D = \eta D^\nu \Gamma(\nu/\eta)D^{\nu-1}e^{-\frac{D}{D^\nu}}\eta, \]

where \( D^\nu, \nu \) and \( \eta \) are positive constants.

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- Particles diffusing in Brownian fashion in a complex random medium;
- environment properties independent on the diffusing particles and represented by a random diffusivity.
Generalised Grey Brownian Motion & Random Diffusivity

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Generalised Grey Brownian Motion & Random Diffusivity

- Particles diffusing in Brownian fashion in a complex random medium;
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X_{ggBM} = \sqrt{2 D(t)} W(t), \quad W(t) = \int_0^t \xi(s) ds.
\]

Assuming a generalised Gamma distribution for the random diffusivity

\[
\gamma^{\text{gen}}_{\nu, \eta}(D) = \frac{\eta}{D^\nu \Gamma(\nu/\eta)} D^{\nu-1} e^{-\left(\frac{D}{D_*}\right)^\eta}, \quad \langle D^n \rangle = D_*^n \frac{\Gamma\left(\frac{\nu+n}{\eta}\right)}{\Gamma\left(\frac{\nu}{\eta}\right)},
\]

where \(D_*\), \(\nu\) and \(\eta\) are positive constants.
Generalised Grey Brownian Motion & Random Diffusivity

\[ \langle x^2 \rangle_{\text{ggBM}}(t) = \int_{-\infty}^{\infty} x^2 f_{\text{ggBM}}(x, t) \, dx = 2t \int_{0}^{\infty} D \gamma_{\text{gen}, \nu, \eta}(D) \, dD = 2\langle D \rangle_{\text{st}}. \]

\[ \langle x^2 \rangle_{\text{ggBM}}(t) \sim 0.40 t \]

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Generalised Grey Brownian Motion & Random Diffusivity

\[ f_{\text{ggBM}}(x, t) = \int_0^\infty G\left(\frac{x}{\sqrt{D}}, t\right) p_D(D) \frac{dD}{\sqrt{D}} = \int_0^\infty \gamma_{\nu, \eta}^\text{gen}(D) G(x, t|D) dD \]
\[ f_{ggBM}(x, t) = \int_0^\infty G \left( \frac{x}{\sqrt{D}}, t \right) p_D(D) \frac{dD}{\sqrt{D}} = \int_0^\infty \gamma_{\nu, \eta}^{\text{gen}}(D) G(x, t|D) dD \]

\[ \simeq \frac{1}{\Gamma(\nu/\eta) \sqrt{4\pi D_\star t}} \left( \frac{x^2}{4D_\star t} \right)^{\frac{2\nu-\eta-1}{2(\eta+1)}} \exp \left[ -\frac{\eta + 1}{\eta} \eta^{\frac{1}{\eta+1}} \left( \frac{x^2}{4D_\star t} \right)^{\frac{\eta}{\eta+1}} \right]. \]
Generalised Grey Brownian Motion & Random Diffusivity

\[ f_{ggBM}(x, t) = \int_0^\infty G \left( \frac{x}{\sqrt{D}}, t \right) p_D(D) \frac{dD}{\sqrt{D}} = \int_0^\infty \gamma_{\nu, \eta}^{gen}(D) G(x, t | D) dD \]

\[ \approx \frac{1}{\Gamma(\nu/\eta)\sqrt{4\pi D_* t}} \left( \frac{x^2}{4D_* t} \right)^{\frac{2\nu-\eta-1}{2(\eta+1)}} \exp \left[ -\frac{\eta+1}{\eta} \frac{1}{\eta+1} \left( \frac{x^2}{4D_* t} \right) \right]. \]
Generalised Grey Brownian Motion & Random Diffusivity

\[ f_{ggBM}(x, t) = \int_0^\infty G \left( \frac{x}{\sqrt{D}}, t \right) p_D(D) \frac{dD}{\sqrt{D}} = \int_0^\infty \gamma_{\nu, \eta}^{\text{gen}}(D) G(x, t | D) dD \]

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Generalised Grey Brownian Motion & Random Diffusivity

\[
f_{\text{ggBM}}(x, t) = \int_0^\infty G \left( \frac{x}{\sqrt{D}}, t \right) p_D(D) \frac{dD}{\sqrt{D}} = \int_0^\infty \gamma_{\nu, \eta}^{\text{gen}}(D) G(x, t|D) dD
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\[
\approx \frac{1}{\Gamma(\nu/\eta)\sqrt{4\pi D_* t}} \left( \frac{x^2}{4D_* t} \right)^{2\nu-\eta-1/2} \left( \eta + \frac{1}{\eta} \right)^{1/\eta+1} \exp \left[ -\frac{\eta + 1}{\eta} \left( \frac{x^2}{4D_* t} \right)^{\eta/(\eta+1)} \right].
\]

\[
\langle x_{\text{ggBM}}^2(t) \rangle = \int_{-\infty}^{+\infty} x^2 f_{\text{ggBM}}(x, t) dx
\]

\[
= 2t \int_0^\infty D \gamma_{\nu, \eta}^{\text{gen}}(D) dD = 2 \langle D \rangle_{st} t.
\]
A minimal model for Diffusing Diffusivities

\[ \text{DD}(t) = \int_0^t \sqrt{2D(s)} \xi(s) \, ds, \]

\[ D(t) = Y_2(t), \]

\[ t \ll \tau_D \quad \text{Brownian yet non-Gaussian Diffusion.} \]

\[ t \gg \tau_D \quad \text{Gaussian Diffusion.} \]

A minimal model for Diffusing Diffusivities

\[ X_{DD}(t) = \int_0^t \sqrt{2D(s)} \xi(s) \, ds, \]
\[ D(t) = Y^2(t), \]
\[ Y(t) \text{ \(n\)-dimensional OU process.} \]

A minimal model for Diffusing Diffusivities

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\[ Y(t) \] n-dimensional OU process.

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Brownian yet non-Gaussian Diffusion.

A minimal model for Diffusing Diffusivities

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A generalise minimal model for Diffusing Diffusivities

\[
\begin{aligned}
X_{\text{DD}}(t) &= \int_0^t \sqrt{2D(s)} \xi(s) ds, \\
D(t) &= y^2(t), \\
dy &= \frac{\sigma^2}{2y} \left[ 2\nu - 1 - 2\eta \left( \frac{y}{y_*} \right)^{2\eta} \right] dt + \sigma \, dW(t).
\end{aligned}
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A generalise minimal model for Diffusing Diffusivities

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For \( t \ll \tau_{corr} \)

\[ f_{DD}^{ST}(x, t) \approx \int_0^{+\infty} p_D(D) G(x, t|D) dD \]

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A generalised minimal model for Diffusing Diffusivities

\[
\begin{align*}
X_{DD}(t) &= \int_0^t \sqrt{2D(s)} \xi(s) ds, \\
D(t) &= y^2(t), \\
dy &= \frac{\sigma^2}{2y} \left[ 2\nu - 1 - 2\eta \left( \frac{y}{y_*} \right)^{2\eta} \right] dt + \sigma \ dW(t).
\end{align*}
\]

For \( t \ll \tau_{\text{corr}} \)

\[
f_{DD}^{ST}(x, t) \sim \int_0^{+\infty} p_D(D) G(x, t|D) dD
\]
A generalise minimal model for Diffusing Diffusivities

\[
\begin{cases}
X_{DD}(t) = \int_0^t \sqrt{2D(s)} \xi(s) ds, \\
D(t) = y^2(t), \\
dy = \frac{\sigma^2}{2y} \left[ 2\nu - 1 - 2\eta \left( \frac{y}{y^*} \right)^{2\eta} \right] dt + \sigma \ dW(t).
\end{cases}
\]

For \( t \ll \tau_{corr} \)

\[
f_{DD}^{ST}(x, t) \simeq \int_0^{+\infty} p_D(D) G(x, t|D) dD
\]

For \( t \gg \tau_{corr} \)

\[
f_{DD}^{LT}(x, t) \simeq \frac{1}{\sqrt{4\pi \langle D \rangle_{st} t}} \exp \left( -\frac{x^2}{4\langle D \rangle_{st} t} \right)
\]
A generalise minimal model for Diffusing Diffusivities

\[
X_{\text{DD}}(t) = \int_0^t \sqrt{2D(s)} \xi(s) ds,
\]
\[
D(t) = y^2(t),
\]
\[
dy = \frac{\sigma^2}{2y} \left[ 2\nu - 1 - 2\eta \left( \frac{y}{y_*} \right)^{2\eta} \right] dt + \sigma \, dW(t).
\]

For \( t \ll \tau_{\text{corr}} \)

\[
f^{ST}_{\text{DD}}(x, t) \sim \int_0^{+\infty} p_D(D) G(x, t|D) dD
\]

For \( t \gg \tau_{\text{corr}} \)

\[
f^{LT}_{\text{DD}}(x, t) \sim \frac{1}{\sqrt{4\pi\langle D \rangle_{st} t}} \exp \left( -\frac{x^2}{4\langle D \rangle_{st} t} \right)
\]
A generalise minimal model for Diffusing Diffusivities

For $t \ll \tau_{corr}$

$$
\langle x^2_{DD}(t) \rangle_{ST} = \int_{-\infty}^{+\infty} x^2 f_{ST, DD}(x, t) \, dx = 2t \langle D \rangle_{st}.
$$

For $t \gg \tau_{corr}$

$$
\langle x^2_{DD}(t) \rangle_{LT} = \int_{-\infty}^{+\infty} x^2 f_{LT, DD}(x, t) \, dx = \int_{-\infty}^{+\infty} x^2 G(x, t | \langle D \rangle_{st}) \, dx = 2\langle D \rangle_{st}.
$$

$\eta = 1.3, \nu = 0.5$

FIT $\sim 0.41 t$
A generalise minimal model for Diffusing Diffusivities

For $t \ll \tau_{\text{corr}}$

\[
\langle x_{DD}^2(t) \rangle_{ST} = \int_{-\infty}^{+\infty} x^2 f_{DD}^{ST}(x, t) dx
\]

\[= 2t \int_{0}^{\infty} D \gamma_{\nu, \eta}^{\text{gen}}(D) dD = 2 \langle D \rangle_{st} t.\]
A generalise minimal model for Diffusing Diffusivities

For $t \ll \tau_{\text{corr}}$

\[
\langle x_{\text{DD}}^2(t) \rangle_{\text{ST}} = \int_{-\infty}^{+\infty} x^2 f_{\text{DD}}^{ST}(x, t) \, dx \\
= 2t \int_{0}^{\infty} D \gamma_{\nu, \eta}^{\text{gen}}(D) \, dD = 2 \langle D \rangle_{\text{st}} \, t.
\]

For $t \gg \tau_{\text{corr}}$

\[
\langle x_{\text{DD}}^2(t) \rangle_{\text{LT}} = \int_{-\infty}^{+\infty} x^2 f_{\text{DD}}^{LT}(x, t) \, dx \\
= \int_{-\infty}^{+\infty} x^2 G(x, t | \langle D \rangle_{\text{st}}) \, dx = 2 \langle D \rangle_{\text{st}} \, t.
\]
A generalise minimal model for Diffusing Diffusivities

For $t \ll \tau_{\text{corr}}$

$$\langle x_{DD}^2(t) \rangle_{ST} = \int_{-\infty}^{+\infty} x^2 f_{DD}^{ST}(x, t) dx$$

$$= 2t \int_{0}^{\infty} D \gamma_{\nu, \eta}^{\text{gen}}(D) dD = 2 \langle D \rangle_{st} t.$$

For $t \gg \tau_{\text{corr}}$

$$\langle x_{DD}^2(t) \rangle_{LT} = \int_{-\infty}^{+\infty} x^2 f_{DD}^{LT}(x, t) dx$$

$$= \int_{-\infty}^{+\infty} x^2 G(x, t|\langle D \rangle_{st}) dx = 2 \langle D \rangle_{st} t.$$
The Two Models in Comparison

Generalised grey Brownian motion (ggBM)

\[ X_{\text{ggBM}}(t) = \sqrt{2D(t)} W(t), \]

\[ X_{t+1}^{\text{ggBM}} = \sqrt{2D_{t+1}} W_{t+1}. \]

Diffusing Diffusivities (DD)

\[ X_{\text{DD}}(t) = \int_0^t \sqrt{2D(s)} \xi(s) \, ds, \]

\[ X_{t+1}^{\text{DD}} = X_t^{\text{DD}} + \sqrt{2D_t} dW_t. \]

\[ \eta = 1.3, \nu = 0.5 \]

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The Two Models in Comparison

Generalised grey Brownian motion (ggBM)

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\[ X_{ggBM}^{t+1} = \sqrt{2D^{t+1}} W^{t+1}. \]

Diffusing Diffusivities (DD)

\[ X_{DD}(t) = \int_0^t \sqrt{2D(s)} \xi(s) \, ds, \]
\[ X_{DD}^{t+1} = X_{DD}^t + \sqrt{2D^t} \, dW^t. \]
The Two Models in Comparison

**Generalised grey Brownian motion (ggBM)**

\[ X_{ggBM} = \sqrt{2D(t)} \, W(t), \]
\[ X_{ggBM}^{t+1} = \sqrt{2D_{t+1}} \, W^{t+1}. \]

**Diffusing Diffusivities (DD)**

\[ X_{DD}(t) = \int_0^t \sqrt{2D(s)}\xi(s)ds, \]
\[ X_{DD}^{t+1} = X_{DD}^t + \sqrt{2D_t} \, dW^t. \]

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The Two Models in Comparison

In common: non-Gaussian dynamics for short times; ubiquitous linear trend of the variance.

Not in common: DD approaches a standard diffusion at long times; ggBM does not display changes in its trend.

$$K = 3\Gamma(\nu + 2\eta)/\Gamma(\nu\eta)$$

$$\eta = 1.3, \nu = 0.5$$

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<table>
<thead>
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\[
K = 3^{\eta} \Gamma(\nu+2^{\eta}) \Gamma(\nu^{\eta}) \Gamma(\nu^{1+\eta})^2
\]
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Conclusions

Broad spectrum of distributions for the random diffusivity that allows us to reproduce a broad spectrum of distributions for the particles displacement also.

Proposal of two models suitable for different physical and/or biological systems exhibiting Brownian yet non-gaussian diffusion.

Development, generalisation and comparison of two models already known in literature.

Introduction of non equilibrium initial condition for the diffusivity dynamics.

Possibility to generalise the study to fractional Gaussian noise, introducing thus an anomalous spreading.

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