

# Sim.DiffProc: A Package for Simulation of Diffusion Processes in R

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## Abstract

The **Sim.DiffProc** package provides a simulation of diffusion processes and the differences methods of simulation of solutions for stochastic differential equations (SDEs) of the Itô's type, in financial and actuarial modeling and other areas of applications, for example the stochastic modeling and simulation of pollutant dispersion in shallow water using the attractive center, and the model of two diffusions in attraction, which can modeling the behavior of two insects, one attracts the other. The simulation of the processes of diffusion, through stochastic differential equations to allow simulated a random variable  $\tau_c$  "first passage time" of the particle through a sphere of radius  $c$ , two methods are used in the estimation problem of the probability density function of a random variable  $\tau_c$  the histograms and the kernel methods. The R package **Sim.DiffProc** is introduced, providing a simulation and estimation for the stationary distribution of the stochastic process that describes the equilibrium of some dynamics.

*Keywords:* attractive model, diffusion process, simulations, stochastic differential equation, stochastic modeling, R language.

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## 1. Introduction

Stochastic differential equations (SDEs) are a natural choice to model the time evolution of dynamic systems. These equations have a variety of applications in many disciplines and can be a powerful tool for the modeling and the description of many phenomena. Examples of these applications are physics, astronomy, economics, financial mathematics, geology, genetic analysis, ecology, neurology, biology, biomedical sciences, epidemiology, political analysis and social processes, and many other fields of science and engineering. The stochastic differential equations, with slight notational variations, are standard in many books with applications in different fields see [Rolski, Schmidli, Schmidt, and Teugels \(1998\)](#); [Franck \(2009\)](#); [Allen \(2007\)](#); [Stefano \(2008\)](#); [Douglas and Peter \(2006\)](#) to name only a few.

The first is to recall the theory and implement methods for the simulation of paths of diffusion processes  $\{X_t, t \geq 0\}$  solutions to stochastic differential equations (SDEs), the sense that only SDEs with Gaussian noise  $B_t$  are considered i.e., processes for which the writing

$$\frac{dX_t}{dt} = \mu(\theta, t, X_t) + \sigma(\vartheta, t, X_t)B_t$$

With the gaussian noise  $B_t$  is the formal derivative of the standard Wiener process  $W_t$  (i.e.,  $B_t = \frac{dW_t}{dt}$ ), the write formally for the process  $\{X_t, t \geq 0\}$  is

$$dX_t = \mu(\theta, t, X_t)dt + \sigma(\vartheta, t, X_t)dW_t,$$

with some initial condition  $X_0$ .

We seek to motivate further interest in this specific field by introducing the **Sim.DiffProc** package (Boukhetala and Guidoum 2011a) (Simulation of Diffusion Processes) for use with the statistical programming environment R (R Development Core Team 2011); freely available on the Comprehensive R Archive Network (CRAN) at <http://CRAN.R-project.org/package=Sim.DiffProc>. There exist a graphical user interface (GUI) for some functions for **Sim.DiffProc** package, the R package **Sim.DiffProcGUI** (Boukhetala and Guidoum 2011b) a freely available at <http://CRAN.R-project.org/package=Sim.DiffProcGUI>.

This work is organized as follows. Section 2 gives a simulation for some very popular stochastic differential equations models (trajectory of the Brownian motion, Ornstein-Uhlenbeck process), and present the different numerical methods (schemes) of simulation of SDEs (See Peter and Eckhard 1995), simulation the random variable  $X_t$  at time  $t$  by a simulated diffusion processes used the numerical methods and estimate the stationary distribution for  $X_t$  by histograms and kernel methods. Section 3 the diffusion processes are used to modeling the behavior of the dispersal phenomenon and dynamic models for insects orientation, two important models can be indicated. The graphical user interface (GUI) for **Sim.DiffProc** package are provided in Section 4.

## 2. Diffusion processes

We consider the model as the parametric Itô stochastic differential equation

$$dX_t = \mu(\theta, t, X_t)dt + \sigma(\vartheta, t, X_t)dW_t, \quad t \geq 0, X_0 = \zeta \quad (1)$$

Where  $\{W_t, t \geq 0\}$  is a standard Wiener process,  $\mu : \Theta \times [0, T] \times \mathbb{R} \rightarrow \mathbb{R}$ , called the drift coefficient, and  $\sigma : \Xi \times [0, T] \times \mathbb{R} \rightarrow \mathbb{R}^+$ , called the diffusion coefficient, are known functions except the unknown parameters  $\theta$  and  $\vartheta$ ,  $\Theta \subset \mathbb{R}$ ,  $\Xi \subset \mathbb{R}$  and  $E(\zeta^2) < \infty$ , the estimation problems for the parameters  $\theta$  and  $\vartheta$  can be seen in some papers (Boukhetala 1984, 1995), (Brodeau and Breton 1979). The drift coefficient is also called the trend coefficient or damping coefficient or translation coefficient. The diffusion coefficient is also called volatility coefficient. Under global Lipschitz and the linear growth conditions on the coefficients  $\mu$  and  $\sigma$ , there exists a unique strong solution of the above Itô SDEs, called the diffusion process or simply a diffusion, which is a continuous strong Markov semimartingale. The drift and the diffusion coefficients are respectively the instantaneous mean and instantaneous standard deviation of the process. All over the text, the stochastic differential equation (1), they are supposed to be measurable.

**Assumption 1: (Global Lipschitz)** For all  $x, y \in \mathbb{R}$  and  $t \in [0, T]$ , there exists a constant  $K < \infty$  such that

$$|\mu(t, x) - \mu(t, y)| + |\sigma(t, x) - \sigma(t, y)| < K|x - y|.$$

**Assumption 2: (Linear growth)** For all  $x, y \in \mathbb{R}$  and  $t \in [0, T]$ , there exists a constant  $C < \infty$  such that

$$|\mu(t, x)| + |\sigma(t, x)| < C(1 + |x|),$$

The linear growth condition controls the behaviour of the solution so that  $X_t$  does not explode in a finite time.

## 2.1. Simulation of Stochastic Differential Equations SDEs

In this section, we present some of the well-known and widely used diffusion process solutions to the stochastic differential equation. There are two main objectives in the simulation of the trajectory of a process solution of a stochastic differential equation, either interest is in the whole trajectory or in the expected value of some functional of the diffusion process (moments, distributions, etc) which usually are not available in explicit analytical form. Numerical Methods are usually based on discrete approximations of the continuous solution to a stochastic differential equation. The following examples use the **Sim.DiffProc** package for simulation some diffusion process.

To install the **Sim.DiffProc** package on your version of R, type the following line in the R console.

```
R> install.packages("Sim.DiffProc")
```

If you don't have enough privileges to install software on your machine or account, you will need the help of your system administrator. Once the package has been installed, you can actually use it by loading the code with

```
R> library(Sim.DiffProc)
```

A short list of help topics, corresponding to most of the commands in the package, is available by typing

```
R> library(help = "Sim.DiffProc")
```

### *Simulation of the trajectory of the Brownian motion*

Simulation of the trajectory of the Brownian motion: The very basic ingredient of a model describing stochastic evolution is the so-called Brownian motion or Wiener process. There are several alternative ways to characterize and define the Wiener process  $W = \{W_t, t \geq 0\}$ , and one is the following: it is a Gaussian process with continuous paths and with independent increments such that  $W(0) = 0$  with probability 1,  $E(W_t) = 0$ , and  $\text{VAR}(W_t - W_s) = t - s$  for all  $0 \leq s < t$ . In practice, what is relevant for our purposes is that  $W(t) - W(s) \sim N(0, t - s)$ . Given a fixed time increment  $\Delta t > 0$ , one can easily simulate a trajectory of the Wiener process in the time interval  $[t_0, T]$ . Indeed, for  $W_{\Delta t}$  it holds true that

$$W(\Delta t) = W(\Delta t) - W(0) \sim N(0, \Delta t) \sim \sqrt{\Delta t} \cdot N(0, 1)$$

and the same is also true for any other increment  $W(t + \Delta t) - W(t)$ ; i.e.,

$$W(t + \Delta t) - W(t) \sim N(0, \Delta t) \sim \sqrt{\Delta t} \cdot N(0, 1)$$

For  $i = 0, 1, \dots, N - 1$ , with initial deterministic value  $x_0$ . Usually the time increment  $\Delta t = t_{i+1} - t_i$  is taken to be constant (i.e.,  $\Delta t = (T - t_0)/N$ )

```
R> BMN(N = 10000, t0 = 0, T = 1, C = 1)
```

```
R> BMN2D(N = 10000, t0 = 0, T = 1, x0 = 0, y0 = 0, Sigma = 1)
```

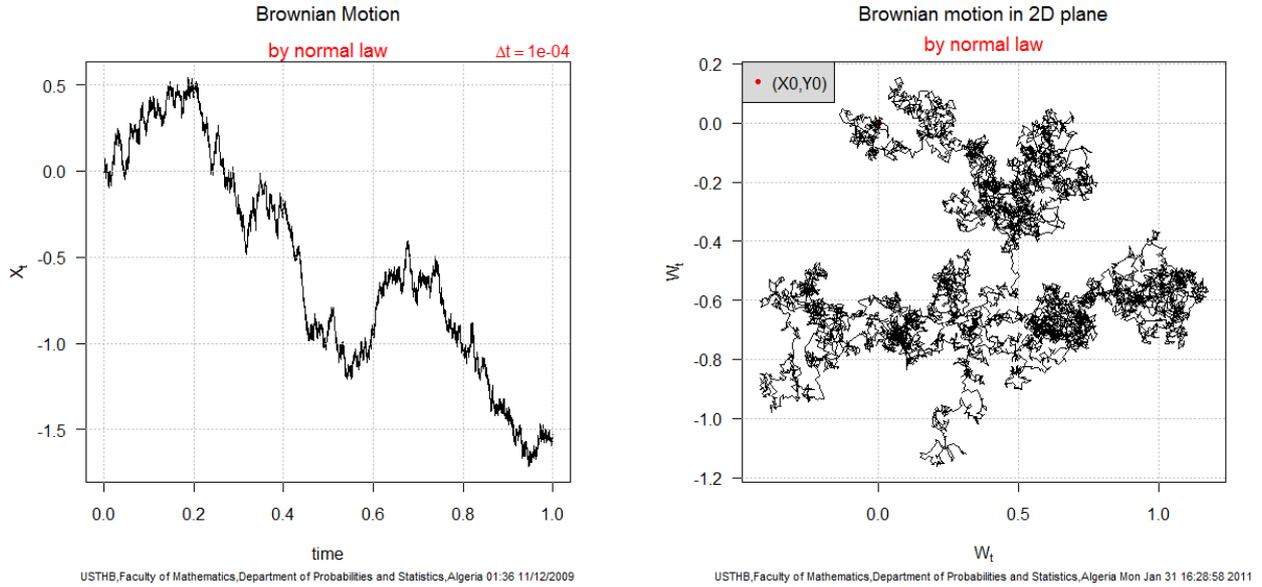


Figure 1: Simulation examples to illustrate the trajectory of the Brownian motion used the function BMN, and 2-dimensional Brownian motion used BMN2D.

### Simulation a Ornstein-Uhlenbeck or Vasicek process

The Ornstein-Uhlenbeck or Vasicek process is the unique solution to the following stochastic differential equation

$$dX_t = r(\theta - X_t)dt + \sigma dW_t, \quad X_0 = x_0, \quad (2)$$

where  $\sigma$  is interpreted as the volatility,  $\theta$  is the long-run equilibrium value of the process, and  $r$  is the speed of reversion. As an application of the Itô lemma, we can show the explicit solution of (2) by choosing  $f(t, x) = xe^{rt}$ , we obtain

$$X_t = \theta + (x_0 - \theta)e^{-rt} + \sigma \int_{t_0}^t e^{-r(t-s)} dW_s$$

It can be seen that for  $\theta = 0$  the trajectory of  $X_t$  is essentially a negative exponential perturbed by the stochastic integral. One way of simulating trajectories of the Ornstein-Uhlenbeck process is indeed via the simulation of the stochastic integral.

```
R> HWV(N = 1000, t0 = 0, T = 10, x0 = -5, theta = 0, r = 1, sigma = 0.5)
R> HWVF(N = 1000, M = 100, t0 = 0, T = 10, x0 = -5, theta = 0, r = 1,
        sigma = 0.5)
```

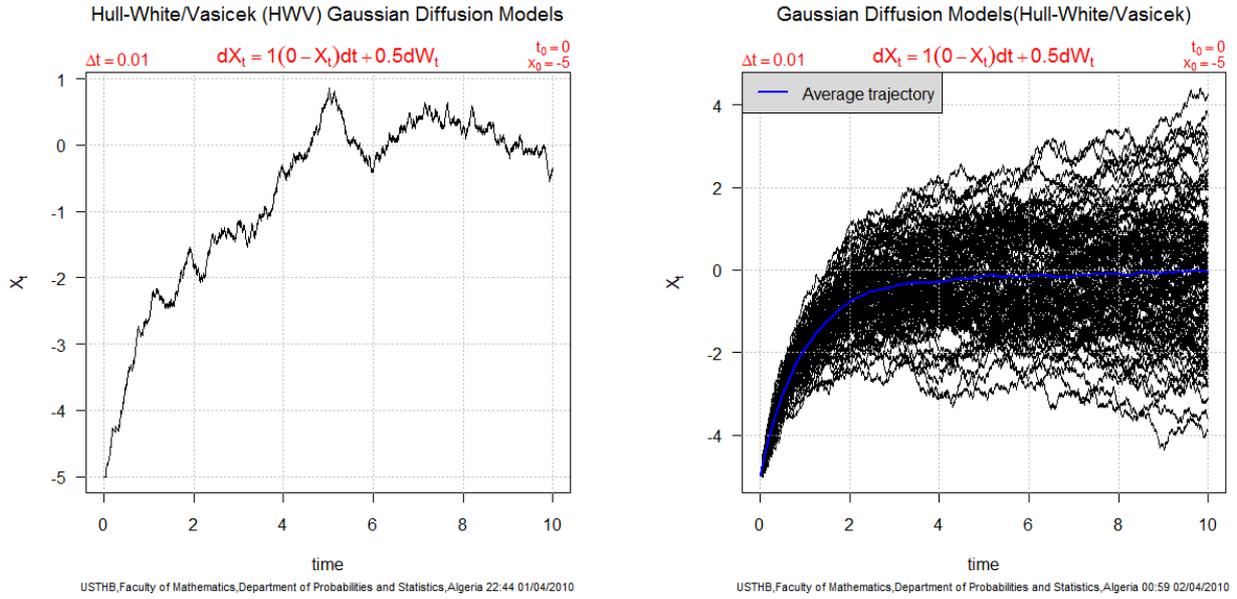


Figure 2: Simulated path of the Ornstein-Uhlenbeck process  $dX_t = -X_t dt + 0.5dW_t$  used the function HWV, and 100 trajectories of the  $dX_t = -X_t dt + 0.5dW_t$  used HWVF.

We sketch some very popular SDEs models and example of simulations :

Models	Expressions	R code
Arithmetic Brownian Motion	$dX_t = \theta dt + \sigma dW_t$	ABM
Geometric Brownian Motion	$dX_t = \theta X_t dt + \sigma X_t dW_t$	GBM
Cox-Ingersoll-Ross	$dX_t = (r - \theta X_t) dt + \sigma \sqrt{X_t} dW_t$	CIR
Constant Elasticity of Variance	$dX_t = \mu X_t dt + \sigma X_t^\gamma dW_t$	CEV
Radial Ornstein-Uhlenbeck	$dX_t = (\theta X_t^{-1} - X_t) dt + \sigma dW_t$	ROU
Chan-Karloyi-Logstaff-Sanders	$dX_t = (r + \theta X_t) dt + \sigma X_t^\gamma dW_t$	CKLS
Hyperbolic Diffusion	$dX_t = -\theta X_t (1 + X_t^2)^{-0.5} dt + \sigma dW_t$	Hyproc
Jacobi diffusion	$dX_t = -\theta (X_t - 0.5) dt + \sqrt{\theta X_t (1 - X_t)} dW_t$	JDP

Table 1: Some parametric families of SDEs models.

### Example of use

In particular, it is possible to generate  $M$  independent trajectories of the same process with one single call of the function by just specifying a value for  $M$

```
R> ABM(N = 1000, t0 = 0, T = 1, x0 = 0, theta = 3, sigma = 2)
R> GBM(N = 1000, T = 1, t0 = 0, x0 = 1, theta = 2, sigma = 0.5)
R> CIR(N = 1000, M = 1, t0 = 0, T = 1, x0 = 1, theta = 0.2, r = 1,
```

```

sigma = 0.5)
R> CEV(N = 1000, M = 1, t0 = 0, T = 1, x0 = 1, mu = 0.3, sigma = 2,
gamma = 1.2)
R> ROU(N = 1000, M = 1, T = 1, t0 = 0, x0 = 1, theta = 0.05)
R> CKLS(N = 1000, M = 1, T = 1, t0 = 0, x0 = 1, r = 0.3, theta = 0.01,
sigma = 0.1, gamma = 0.2)
R> Hyproc(N = 1000, M = 1, T = 100, t0 = 0, x0 = 3, theta = 2)
R> JDP(N = 1000, M = 1, T = 100, t0 = 0, x0 = 0, theta = 0.05)

```

## 2.2. Numerical Methods for SDEs

The idea is the following given an Itô process  $\{X_t, 0 \leq t < T\}$  solution of the stochastic differential equation

$$dX_t = f(X_t)dt + g(X_t)dW_t, \quad X_0 = x_0, \quad (3)$$

where  $W_t$  represents the standard Wiener process and initial value  $x_0$  is a fixed value. In many literatures, whose partial list can be seen in the references of the present paper, numerical schemes for SDE (3) were proposed, which recursively compute sample paths (trajectories) of solution  $X_t$  at step-points. Numerical experiments for these schemes can be seen in some papers (Greiner, Strittmatter, and Honerkamp 1988), (Kloeden and Platen 1989), (Saito and Mitsui 1993).

In the following, we present numerical schemes. They adopt an equidistant discretization of the time interval  $[t_0, T]$  with stepsize

$$\Delta t = \frac{(T - t_0)}{N}, \quad \text{for fixed natural number } N.$$

Furthermore,

$$t_n = n\Delta t, n \in \{1, 2, \dots, N\}.$$

denotes the  $n$ -th step-point. We abbreviate  $X_n = X_{t_n}$ .

The following three random variables will be used in the  $(n + 1)$  time step of the schemes:

$$\begin{aligned} \Delta W_n &= W_{t_{n+1}} - W_{t_n}, \\ \Delta Z_n &= \int_{t_n}^{t_{n+1}} \int_{t_n}^s dW_r ds, \\ \Delta \bar{Z}_n &= \int_{t_n}^{t_{n+1}} \int_{t_n}^s dr dW_s. \end{aligned}$$

They are obtained as sample values of normal random variables using the transformation (Saito and Mitsui 1993)

$$\begin{aligned} \Delta W_n &= \xi_{n,1}(\Delta t)^{1/2}, \\ \Delta Z_n &= \frac{1}{2} \left( \xi_{n,1} + \frac{\xi_{n,2}}{\sqrt{3}} \right) (\Delta t)^{3/2}, \\ \Delta \bar{Z}_n &= \frac{1}{2} \left( \xi_{n,1} - \frac{\xi_{n,2}}{\sqrt{3}} \right) (\Delta t)^{3/2}. \end{aligned}$$

and, together with them, we further use  $\Delta\widetilde{W}_n = \xi_{n,2}(\Delta t)^{1/2}$ , where  $\xi_{n,1}, \xi_{n,2}$  are mutually independent  $N(0, 1)$  random variables.

### Numerical schemes

Euler-Maruyama scheme (Maruyama 1955):

$$X_{n+1} = X_n + f_n\Delta t + g_n\Delta W_n \quad (4)$$

Milstein scheme (Milstein 1974):

$$X_{n+1} = X_n + f_n\Delta t + g_n\Delta W_n + \frac{1}{2}g'_n g_n((\Delta W_n)^2 - \Delta t) \quad (5)$$

Milstein Second scheme (Milstein 1974):

$$\begin{aligned} X_{n+1} = & X_n + f_n\Delta t + g_n\Delta W_n + \frac{1}{2}g'_n g_n((\Delta W_n)^2 - \Delta t) + f'_n g_n \Delta Z_n \\ & + \left(g'_n f_n + \frac{1}{2}g''_n g_n^2\right) \Delta \bar{Z}_n + \frac{1}{6}(g_n'^2 g_n + g_n'' g_n^2)((\Delta W_n)^3 - 3\Delta t \Delta W_n) \end{aligned} \quad (6)$$

Taylor scheme (Kloeden and Platen 1989):

$$\begin{aligned} X_{n+1} = & X_n + f_n\Delta t + g_n\Delta W_n + \frac{1}{2}g'_n g_n((\Delta W_n)^2 - \Delta t) + f'_n g_n \Delta Z_n \\ & + \left(g'_n f_n + \frac{1}{2}g''_n g_n^2\right) \Delta \bar{Z}_n + \frac{1}{6}(g_n'^2 g_n + g_n'' g_n^2)((\Delta W_n)^3 - 3\Delta t \Delta W_n) \\ & + \frac{1}{2} \left(f'_n f_n + \frac{1}{2}f''_n g_n^2\right) (\Delta t)^2 \end{aligned} \quad (7)$$

Heun scheme (McShane 1974):

$$X_{n+1} = X_n + \frac{1}{2}[F_1 + F_2]\Delta t + \frac{1}{2}[G_1 + G_2]\Delta W_n, \quad (8)$$

where

$$\begin{aligned} F_1 &= F(X_n), & G_1 &= g(X_n), \\ F_2 &= F(X_n + F_1\Delta t + G_1\Delta W_n), & G_2 &= g(X_n + F_1\Delta t + G_1\Delta W_n), \\ F_x &= \left[f - \frac{1}{2}g'g\right](x). \end{aligned}$$

Improved 3-stage Runge-Kutta scheme (Saito and Mitsui 1993):

$$\begin{aligned} X_{n+1} = & X_n + \frac{1}{4}[F_1 + 3F_3]\Delta t + \frac{1}{4}[G_1 + 3G_3]\Delta W_n \\ & + \frac{1}{2\sqrt{3}} \left[f'_n g_n - g'_n f_n - \frac{1}{2}g''_n g_n^2\right] \Delta t \Delta \widetilde{W}_n, \end{aligned} \quad (9)$$

where

$$\begin{aligned} F_1 &= F(X_n), & G_1 &= g(X_n), \\ F_2 &= F\left(X_n + \frac{1}{3}F_1\Delta t + \frac{1}{3}G_1\Delta W_n\right), & G_2 &= g\left(X_n + \frac{1}{3}F_1\Delta t + \frac{1}{3}G_1\Delta W_n\right), \\ F_3 &= F\left(X_n + \frac{2}{3}F_2\Delta t + \frac{2}{3}G_2\Delta W_n\right), & G_3 &= g\left(X_n + \frac{2}{3}F_2\Delta t + \frac{2}{3}G_2\Delta W_n\right), \\ F_x &= \left[f - \frac{1}{2}g'g\right](x). \end{aligned}$$

### Example of use

The following examples for different methods of simulation of SDEs use the `snsdde` function

```
snsdde(N, M, T = 1, t0, x0, Dt, drift, diffusion, Output = FALSE,
       Methods = c("SchEuler", "SchMilstein", "SchMilsteinS",
                  "SchTaylor", "SchHeun", "SchRK3"))
```

with SchEuler (4), SchMilstein (5), SchMilsteinS (6), SchTaylor (7), SchHeun (8), SchRK3 (9).

Consider for example the stochastic process  $\{X_t, t \geq 0\}$  solution of

$$dX_t = (\mu t X_t - X_t^3)dt + \sigma dW_t, \quad X_0 = x_0,$$

For this process,  $f(X_t) = (\mu t X_t - X_t^3)$  and  $g(X_t) = \sigma$ . Suppose we fix an initial value  $X_0 = 0$  and the set of parameters  $\mu = 0.03$  and  $\sigma = 0.1$ . The following algorithm can be used to simulate one trajectory of the process  $X_t$  using the Euler algorithm (figure 3), and 100 trajectories used Milstein scheme (figure 4)

```
R> f_x <- expression( 0.03 * t * x - x^3 )
R> g_x <- expression( 0.1 )
R> snsdde(N = 1000, M = 1, t0 = 0, x0 = 0, Dt = 0.1, drift = f_x,
         diffusion = g_x, Methods = "SchEuler")
R> output <- data.frame(time,X)
R> output

 1      0.0  0.000000e+00
 2      0.1  3.162278e-02
 3      0.2  6.324555e-06
.      .      .
.      .      .
.      .      .
1000  99.9 -1.716814e+00
1001 100.0 -1.756944e+00

R> snsdde(N = 1000, M = 100, t0 = 0, x0 = 0, Dt = 0.1, drift = f_x,
         diffusion = g_x, Methods = "SchMilstein")
```

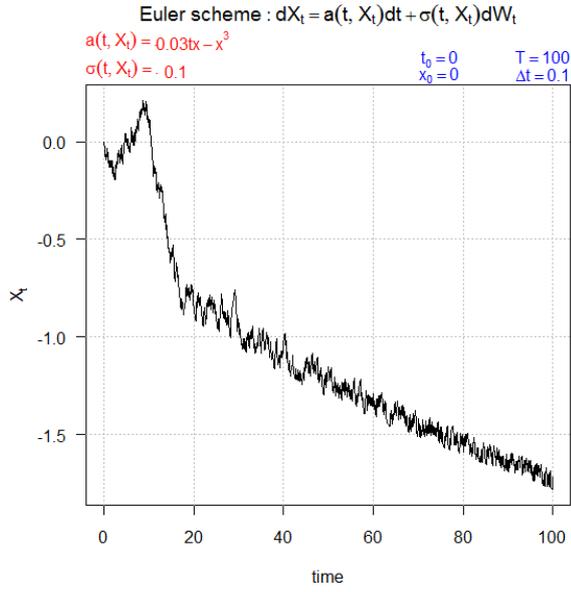


Figure 3: Simulated one trajectory of the process  $dX_t = (0.03tX_t - X_t^3)dt + 0.1dW_t$  used Euler algorithm.

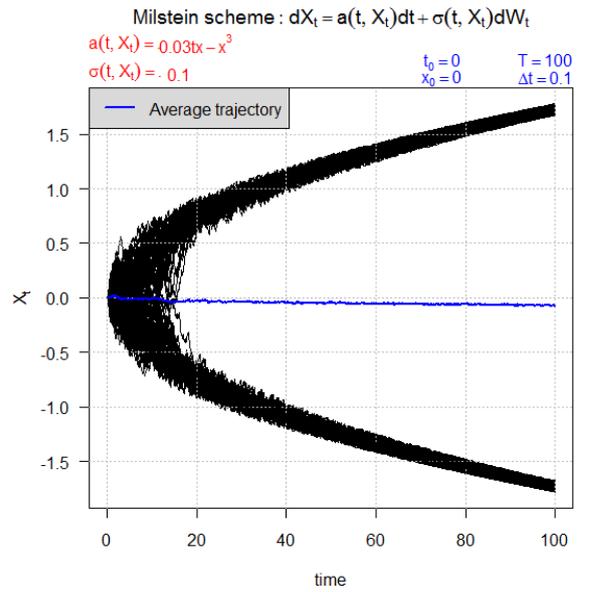


Figure 4: Simulated 100 trajectories of the process  $dX_t = (0.03tX_t - X_t^3)dt + 0.1dW_t$  used Milstein scheme.

### 2.3. Stationary distribution in the SDEs models

The stationary distribution of the stochastic process that describes the equilibrium of some dynamics. For these disciplines, the interest is in the shape of the stationary distributions and the statistical indexes related to them (mean, mode, etc.). The stochastic differential equations usually have a linear drift of the form  $f(x) = r(\theta - x)$  with  $r > 0$ . For this reason, the models are called linear feedback models. The diffusion coefficient  $g(x)$  may be constant, linearly depending on  $x$ , or of polynomial type, leading, respectively, to Gaussian, Gamma, or Beta stationary distributions.<sup>1</sup>

#### *Type N model (Normal Distribution)*

For this model, we have:

Drift coefficient:	$f(X_t) = r(\theta - X_t), r > 0.$
Diffusion coefficient:	$g(X_t) = \sqrt{2\sigma}, \sigma > 0.$
Sde:	$dX_t = r(\theta - X_t)dt + \sqrt{\sigma}dW_t.$
Stationary density:	$\pi(x) = \frac{1}{\sqrt{2\pi\delta}} \exp\left(-\frac{(x - \theta)^2}{2\delta}\right), \delta = \frac{\sigma}{r}.$
Statistics:	mean, mode = $\theta$ , variance = $\delta$ .

<sup>1</sup>These correspond to the following Pearson family of distributions: Gamma = type III, Beta = type I, and Gaussian = limit of type I, III, IV, V, or VI.

*Type G model (Gamma Distribution)*

For this model, we have:

Drift coefficient:	$f(X_t) = r(\theta - X_t), r > 0.$
Diffusion coefficient:	$g(X_t) = \sqrt{\sigma X_t}, \sigma > 0.$
Sde:	$dX_t = r(\theta - X_t)dt + \sqrt{\sigma X_t}dW_t.$
Stationary density:	$\pi(x) = \left(\frac{x}{\delta}\right)^{-1+\frac{\theta}{\delta}} \frac{e^{-\frac{x}{\delta}}}{\Gamma\left(\frac{\theta}{\delta}\right)}, \delta = \frac{\sigma}{2r}.$
Statistics:	mean = $\theta$ , mode = $\theta - \delta$ , variance = $\delta\theta$ .

*Type B model (Beta Distribution)*

For this model, we have:

Drift coefficient:	$f(X_t) = r(\theta - X_t), r > 0.$
Diffusion coefficient:	$g(X_t) = \sqrt{\sigma X_t(1 - X_t)}, \sigma > 0.$
Sde:	$dX_t = r(\theta - X_t)dt + \sqrt{\sigma X_t(1 - X_t)}dW_t.$
Stationary density:	$\pi(x) = \frac{\Gamma\left(\frac{1}{\delta}\right)}{\Gamma\left(\frac{\theta}{\delta}\right)\Gamma\left(\frac{1-\theta}{\delta}\right)} x^{-1+\frac{\theta}{\delta}}(1-x)^{-1+\frac{1-\theta}{\delta}}, \delta = \frac{\sigma}{2r}.$
Statistics:	mean = $\theta$ , mode = $\frac{\theta - \delta}{1 - 2\delta}$ , variance = $\frac{\theta(1 - \theta)}{1 + \delta}.$

*Example of use*

simulation  $M$ -sample ( $M = 100$ ) for the random variable  $X_t$  at time  $t$  by a simulated diffusion processes, using the function `AnaSimX`.

```
AnaSimX(N, M, t0, Dt, T = 1, X0, v, drift, diff, Output = FALSE,
        Methods = c("Euler", "Milstein", "MilsteinS", "Ito-Taylor",
                   "Heun", "RK3"))
```

Consider for example the stochastic process the type  $N : dX_t = 2(1 - X_t)dt + dW_t$ .

```
R> r      = 2
R> theta = 1
R> sigma = 1
R> f_x   <- expression(r * (theta - x))
R> g_x   <- expression(sqrt(sigma))
R> AnaSimX(N = 1000, M = 100, t0 = 0, Dt = 0.01, T = 10, X0 = -6, v = 7,
           drift = f_x, diff = g_x, Methods = "Euler")
```

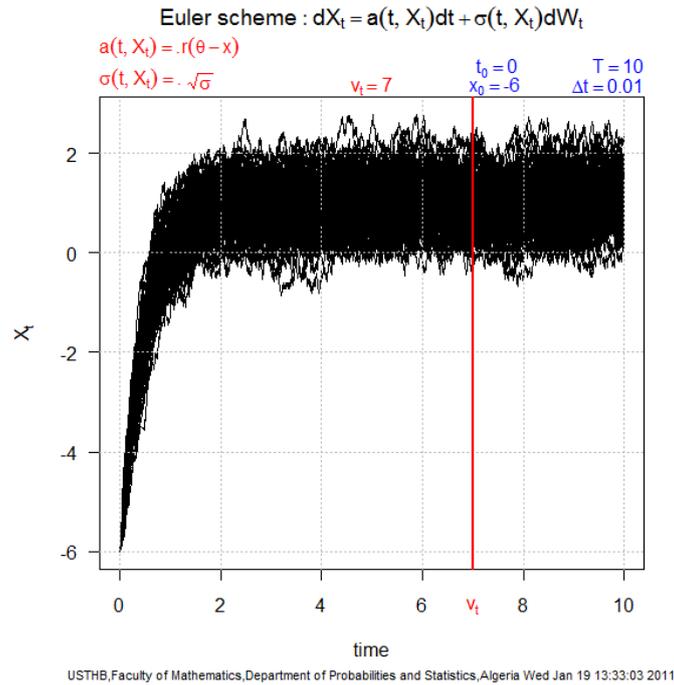


Figure 5: Simulation 100-samples of the random variable  $X_t$  at time  $v_t = 7$  by a simulated 100 trajectories of  $dX_t = 2(1 - X_t)dt + dW_t$ , used Euler algorithm, with  $X_0 = -6$ .

R> X

[1]	0.42457787	0.89022987	0.53798985	0.85601970	0.87574259
[6]	0.13023321	0.78466182	1.67646649	1.86814912	0.91651605
[11]	0.40458587	1.25308171	0.50399329	1.02546173	1.02647338
[16]	0.26630316	1.15195695	0.66666422	0.85174517	0.76239199
[21]	0.44828044	0.27588758	1.01659444	0.99617363	1.00829577
[26]	0.86676310	0.64266320	0.26960628	0.98420215	0.67478779
[31]	0.87145246	1.27619465	0.77522554	0.94704303	1.42153343
[36]	0.98755623	0.77789867	0.08774791	1.16267498	0.84184574
[41]	1.03631156	0.57812454	0.88114625	1.11535893	1.40388370
[46]	1.16252625	0.87735322	1.55669661	1.30152170	1.02433169
[51]	1.23616081	1.51367164	1.61080710	0.99608594	0.59199640
[56]	1.35987961	1.81565309	0.93158510	1.24933297	0.94759695
[61]	0.90637034	0.28367297	1.06232243	0.39463121	0.95167687
[66]	0.68991567	0.52513906	0.82081028	1.11318080	1.25055621
[71]	0.76350645	1.29918398	0.32224426	0.75747775	1.05616919
[76]	1.13505537	1.37253188	0.84595736	1.23985729	1.06338587
[81]	1.20910711	1.54841177	0.94479993	1.52138324	0.93499736
[86]	1.50113064	0.43927942	-0.09752953	0.99846875	1.69256126
[91]	-0.24466704	1.31776649	0.77478081	0.65812555	0.98086811
[96]	1.34704883	1.24507068	-0.27647792	0.92965613	0.67631369

```
R> summary(X)
```

```
      Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
-0.2765  0.6865  0.9459  0.9235  1.2160  1.8680
```

Estimate parameters of the normal distribution by the method of maximum likelihood. The function `Ajdnorm` needs as input the random variable  $X$ , and Initial values for optimizer (mean, sd) with the confidence level required. two methods are used of estimation for the stationary distribution, the histograms used the function `hist_general`, and the kernel methods by used `Kern_general`.

```
hist_general(Data, Breaks, Law = c("exp", "Gamma", "chisq", "Beta",
    "fisher", "student", "weibull", "Normlog", "Norm"))
Kern_general(Data, bw, k, Law = c("exp", "Gamma", "chisq", "Beta",
    "fisher", "student", "weibull", "Normlog", "Norm"))
```

```
R> Ajdnorm(X, starts = list(mean = 1, sd = 1), leve = 0.95)
```

```
Profiling...
```

```
$summary
```

```
Maximum likelihood estimation
```

```
Call:
```

```
mle(minuslogl = lik, start = starts)
```

```
Coefficients:
```

```
      Estimate Std. Error
mean 0.9285440 0.04218993
sd    0.4197845 0.02983209
```

```
-2 log L: 109.0828
```

```
$coef
```

```
      mean      sd
0.9285440 0.4197845
```

```
$AIC
```

```
[1] 113.0828
```

```
$vcov
```

```
      mean      sd
mean 1.779990e-03 -1.799151e-10
sd   -1.799151e-10 8.899539e-04
```

```
$confint
```

```
      2.5 %      97.5 %
```

```
mean 0.8450425 1.0120456
sd    0.3674690 0.4858145
```

```
R> hist_general(Data = X, Breaks = 'Sturges', Law = "Norm")
R> Kern_general(Data = X, bw = "Bcv", k="gaussian", Law = "Norm")
```

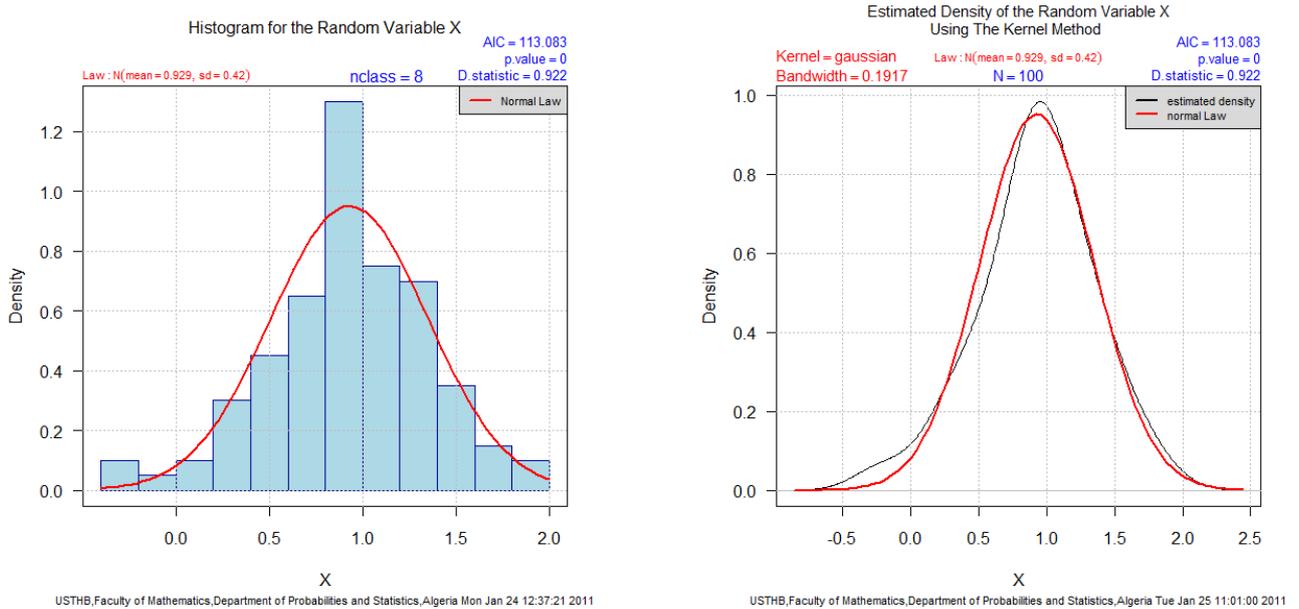


Figure 6: Estimation stationary distribution used histograms and kernel methods.

### 3. Attractive models

The problem of dispersion is a very complex phenomenon in many problems dealing with environment, biology, physics, chemistry, etc . . . , the dynamical behavior of such phenomenon is a random process, often hard to modeling mathematically. This problem, have been proposed by many authors (Hadelar, de Mottoni, and Schumacher 1980), (Helland 1983), (Heemink 1990), (Boukhetala 1994, 1996). For many dispersal problems, the diffusion processes are used to modeling the behavior of the dispersal phenomenon. For example, two important models can be indicated, the first is proposed by Boukhetala (1996), and describes the dispersion of a pollutant on an area of shallow water (attractive model for one diffusion process), the second model is the two diffusions processes in attraction proposed by Boukhetala (1998a) (attractive model for two diffusions processes), which describes the dynamical behavior of a two insects, one attracts the other.

#### 3.1. Attractive model for one diffusion process

Consider a shallow water area with depth  $L(x, y, z, t)$ , horizontal  $U_w(x, y, z, t)$  and  $V_w(x, y, z, t)$ ,  $S_w(x, y, z, t)$  the velocities of the water in respectively the  $x$ -,  $y$ - and  $z$ - directions, and

$U_a(x, y, z)$ ,  $V_a(x, y, z)$ ,  $S_a(x, y, z)$  the velocities of a particle caused by an attractive mechanism. Let  $(X_t, Y_t, Z_t)$  be the position of a particle injected in the water at time  $t = t_0$  at the point  $(x_0, y_0, z_0)$ .

For a single particle, we propose the following dispersion models family (Boukhetala 1996):

$$\begin{cases} dX_t = \left( -U_a + U_w + \frac{\partial L}{\partial x} D + \frac{\partial D}{\partial x} \right) dt + \sqrt{2D} dW_t^1 \\ dY_t = \left( -V_a + V_w + \frac{\partial L}{\partial y} D + \frac{\partial D}{\partial y} \right) dt + \sqrt{2D} dW_t^2 \\ dZ_t = \left( -S_a + S_w + \frac{\partial L}{\partial z} D + \frac{\partial D}{\partial z} \right) dt + \sqrt{2D} dW_t^3 \end{cases}, t \in [0, T] \quad (10)$$

with:

$$U_a = \frac{Kx}{\left(\sqrt{x^2 + y^2 + z^2}\right)^{s+1}}, \quad V_a = \frac{Ky}{\left(\sqrt{x^2 + y^2 + z^2}\right)^{s+1}}, \quad S_a = \frac{Kz}{\left(\sqrt{x^2 + y^2 + z^2}\right)^{s+1}}.$$

and  $s \geq 1$ ,  $K > 0$ ,  $W_t^1$  and  $W_t^2, W_t^3$  are Brownian motions.

$U_w(x, y, z, t)$  and  $V_w(x, y, z, t)$ ,  $S_w(x, y, z, t)$  are neglected and the dispersion coefficient  $D(x, y, z)$  is supposed constant and equal to  $\frac{1}{2}\sigma^2$ , ( $\sigma > 0$ ).

Using Itô's transform for (10), it is shown that the radial process  $R_t = \|(X_t, Y_t, Z_t)\|$  is a Markovian diffusion, solution of the stochastic differential equation, given by:

$$dR_t = \left( \frac{\frac{\sigma^2 R_t^{s-1}}{2} - K}{R_t^s} \right) dt + \sigma d\widetilde{W}_t, \quad t \in [0, T] \quad (11)$$

where  $2K > \sigma^2$  and  $\|\cdot\|$  is the Euclidean norm and  $\widetilde{W}_t$  is a determined Brownian motion.

We take interest in the random variable  $\tau_c^{(s)}$  first passage time (See Boukhetala 1998b,c) of the particle through a sphere of radius  $c$ , centered at the origin of  $\mathbb{R}^3$ -space. The random variable  $\tau_c^{(s)}$  is defined by :

$$\tau_c^{(s)} = \inf(t \geq 0 | R_t \leq c \quad \text{and} \quad R_0 = r) \quad (12)$$

This variable plays an important role in the prediction of the rate of particles reaching the attractive center. We denote by  $M_{s,\sigma}$  the family of models defined by (10) or (11).

### Code example

For example the simulation of the model  $M_{(s=1,\sigma)}$  can be made by discretization of equations (10) or (11) with  $s = 1$ , a simulate and estimate the density function of the random variable  $\widehat{\tau}_c^{(1)} = 1/\tau_c^{(1)}$  (12).

Simulation the models (10) by used the function RadialP3D\_1 with  $s = 1$ .

```
R> RadialP3D_1(N = 5000, t0 = 0, Dt = 0.001, X0 = 1, Y0 = 0.5, Z0 = 0.5, v = 0.2,
              K = 2, Sigma = 0.2)
```

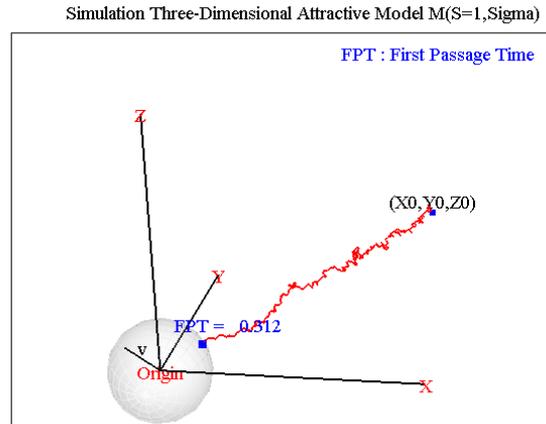


Figure 7: Simulation 3-dimensional attractive model  $M_{(s=1, \sigma=0.2)}$  for one diffusion process.

Simulation 100-sample for the first passage time "FPT" of the model  $M_{(s=1, \sigma)}$  used the function `tho_M1`, and estimate the density function of the  $\tilde{\tau}_c^{(1)}$  by the Gamma law.

```
R> tho_M1(N = 1000, M = 100, t0 = 0, T = 1, RO = 1, v = 0.2, K = 4, sigma = 0.9,
          Methods = "Euler")
R> FPT
```

```
[1] 0.071 0.124 0.046 0.117 0.165 0.126 0.178 0.059 0.218 0.118
[11] 0.305 0.064 0.135 0.188 0.271 0.161 0.099 0.123 0.086 0.137
[21] 0.135 0.101 0.135 0.265 0.204 0.084 0.139 0.186 0.133 0.099
[31] 0.340 0.099 0.133 0.073 0.160 0.217 0.091 0.181 0.139 0.097
[41] 0.118 0.235 0.133 0.371 0.096 0.301 0.106 0.206 0.137 0.233
[51] 0.082 0.156 0.135 0.154 0.060 0.113 0.077 0.132 0.230 0.135
[61] 0.212 0.169 0.238 0.236 0.211 0.098 0.176 0.117 0.205 0.176
[71] 0.220 0.116 0.167 0.073 0.220 0.160 0.099 0.169 0.102 0.197
[81] 0.128 0.172 0.080 0.196 0.120 0.219 0.161 0.283 0.254 0.113
[91] 0.392 0.050 0.138 0.111 0.074 0.216 0.202 0.098 0.091 0.056
```

```
R> Ajdgamma(X = 1/FPT, starts = list(shape = 1, rate = 1), leve = 0.95)
```

Profiling...

\$summary

Maximum likelihood estimation

Call:

```
mle(minuslogl = lik, start = starts)
```

Coefficients:

Estimate Std. Error

```
shape 5.0320084 0.69279984
rate 0.6426731 0.09304918
```

```
-2 log L: 514.6746
```

```
$coef
```

```
      shape      rate
5.0320084 0.6426731
```

```
$AIC
```

```
[1] 518.6746
```

```
$vcov
```

```
      shape      rate
shape 0.4799716 0.06130030
rate 0.0613003 0.00865815
```

```
$confint
```

```
      2.5 %      97.5 %
shape 3.7969651 6.5185981
rate 0.4768285 0.8423622
```

```
R> hist_general(Data = 1/FPT, Breaks = 'Sturges', Law = "Gamma")
R> Kern_general(Data = 1/FPT, bw = 'Ucv', k = "gaussian", Law = "Gamma")
```

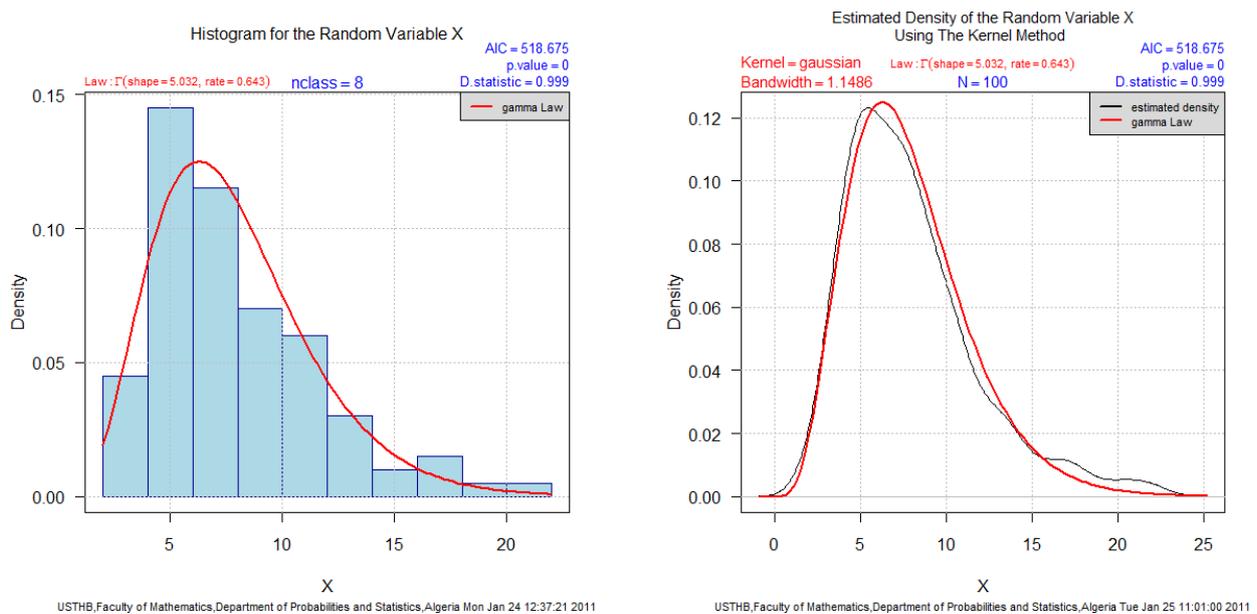


Figure 8: Estimation the density function of  $\tilde{\tau}_{c=0.2}^{(1)}$  by the Gamma law, used histograms and kernel methods.

### 3.2. Attractive model for two diffusions processes

In the following paragraph, we will propose a model of two diffusions in attraction  $M_{\mu(\cdot)}^\sigma(V_t^{(1)})$  and  $M_0^\sigma(V_t^{(2)})$ , can modeling the behavior of two insects, one attracts the other.

Considers  $V_t^{(1)} = (X_{t,1}, X_{t,2}, X_{t,3})$  and  $V_t^{(2)} = (Y_{t,1}, Y_{t,2}, Y_{t,3})$  two random processes of diffusion, which one supposes respectively representing the positions of a male insect and an insect female, and the male is attracted by the female. The behavior of the female is supposed to be a process of Brownian motion, defined by the following equation

$$dV_t^{(2)} = \sigma I_{3 \times 3} dW_t \quad (13)$$

Whereas the behavior of the male is supposed to be a process of diffusion, whose drift is directed, at every moment  $t$ , towards the position of the female, and who is given by Boukhetala (1998a)

$$dV_t^{(1)} = dV_t^{(2)} + \mu_{m+1}(\|D_t\|)D_t dt + \sigma I_{3 \times 3} d\widetilde{W}_t, \quad (14)$$

where  $W_t$  and  $\widetilde{W}_t$  are two Brownian motion independent, and

$$\begin{cases} D_t = V_t^{(1)} - V_t^{(2)} \\ \mu_m(\|d\|) = -\frac{K}{\|d\|^m} \end{cases} \quad (15)$$

$K$  and  $m$  are positive constants.

The model suggested is following form

$$dV_t^{(1)} \Leftrightarrow \begin{cases} dX_{t,1} = dY_{t,1} - \frac{K(X_{t,1}-Y_{t,1})}{(\sqrt{(X_{t,1}-Y_{t,1})^2+(X_{t,2}-Y_{t,2})^2+(X_{t,3}-Y_{t,3})^2})^{m+1}} dt + \sigma d\widetilde{W}_t^1 \\ dX_{t,2} = dY_{t,2} - \frac{K(X_{t,2}-Y_{t,2})}{(\sqrt{(X_{t,1}-Y_{t,1})^2+(X_{t,2}-Y_{t,2})^2+(X_{t,3}-Y_{t,3})^2})^{m+1}} dt + \sigma d\widetilde{W}_t^2 \\ dX_{t,3} = dY_{t,3} - \frac{K(X_{t,3}-Y_{t,3})}{(\sqrt{(X_{t,1}-Y_{t,1})^2+(X_{t,2}-Y_{t,2})^2+(X_{t,3}-Y_{t,3})^2})^{m+1}} dt + \sigma d\widetilde{W}_t^3 \end{cases} \quad (16)$$

$$dV_t^{(2)} \Leftrightarrow \begin{cases} dY_{t,1} = \sigma dW_t^1 \\ dY_{t,2} = \sigma dW_t^2 \\ dY_{t,3} = \sigma dW_t^3 \end{cases} \quad (17)$$

Using Itô's transform for (16) and (17), it is shown that the process  $X_t = \|(V_t^{(1)}, V_t^{(2)})\|$  is a Markovian diffusion, solution of the stochastic differential equation, given by:

$$dX_t = \frac{\sigma^2 X_t^{m-1} - K}{X_t^m} dt + \sigma d\overline{W}_t, \quad t \in [0, T] \quad (18)$$

where  $K > \sigma^2$  and  $\|\cdot\|$  is the Euclidean norm and  $\overline{W}_t$  is a determined Brownian motion.

This model makes it possible to carry out a dynamic simulation of the real phenomenon. Using these simulations, one can also estimate the density of probability of the moment of the first meeting  $\tau(V_t^{(1)}, V_t^{(2)})$  between the two insects, defined by

$$\tau(V_t^{(1)}, V_t^{(2)}) = \liminf_{c \rightarrow 0} \{t \geq 0 \mid \|D_t\| \leq c\}$$

### Code example

For example the simulation two dimensional of the phenomenon  $M_{\mu(\cdot)}^\sigma(V_t^{(1)}) \leftrightarrow M_0^\sigma(V_t^{(2)})$ , can be made by discretization of equations (16) and (17), by used the function `TwoDiffAtra2D`

```
R> TwoDiffAtra2D(N = 5000, t0 = 0, Dt = 0.001, T = 1, X1_0 = 2, X2_0 = 2,
  Y1_0 = -0.5, Y2_0 = -1, v = 0.05, K = 3, m = 0.1, Sigma = 0.3)
```

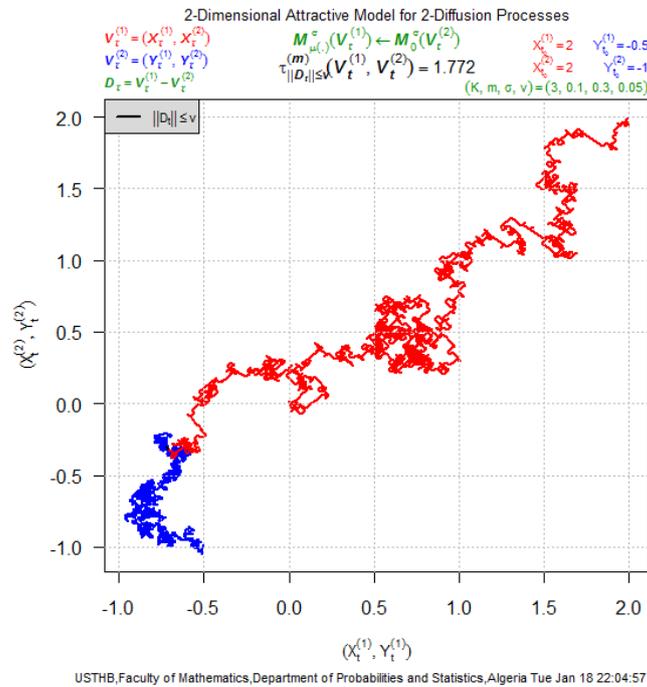


Figure 9: Illustration of simulation two dimensional of a trajectory of the interaction between two insects.

Simulation three dimensional of the phenomenon by used the function `TwoDiffAtra3D`, and simulation 100-sample for the moment of the first meeting  $\tau(V_t^{(1)}, V_t^{(2)})$  between the two insects used the function `tho_02diff`

```
R> TwoDiffAtra3D(N = 5000, t0 = 0, Dt = 0.001, T = 1, X1_0 = 1, X2_0 = 0.5,
  X3_0 = 0, Y1_0 = -0.5, Y2_0 = 0.5, Y3_0 = -1, v = 0.05,
  K = 3, m = 0.1, Sigma = 0.15)
```

## 3-Dimensional Attractive Model for 2-Diffusion Processes

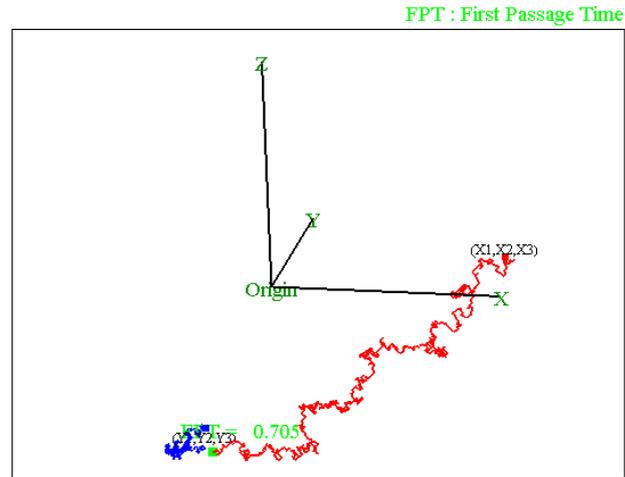


Figure 10: Illustration of simulation three dimensional of a trajectory of the interaction between two insects.

```
R> tho_02diff(N = 1000, M = 100, t0 = 0, Dt = 0.001, T = 1, X1_0 = 1, X2_0 = 1,
  Y1_0 = 0.5, Y2_0 = 0.5, v = 0.05, K = 4, m = 0.2, Sigma = 0.2)
```

```
R> FPT
```

```
[1] 0.143 0.109 0.123 0.106 0.133 0.123 0.189 0.120 0.270 0.140 0.198 0.131
[13] 0.144 0.107 0.092 0.165 0.178 0.124 0.146 0.113 0.136 0.158 0.169 0.203
[25] 0.108 0.160 0.143 0.201 0.122 0.091 0.154 0.096 0.189 0.198 0.147 0.123
[37] 0.147 0.128 0.105 0.192 0.106 0.139 0.174 0.134 0.105 0.090 0.165 0.128
[49] 0.284 0.098 0.136 0.092 0.093 0.077 0.149 0.171 0.125 0.151 0.122 0.132
[61] 0.221 0.199 0.154 0.140 0.145 0.217 0.106 0.097 0.121 0.131 0.153 0.158
[73] 0.152 0.168 0.127 0.100 0.120 0.130 0.181 0.175 0.166 0.102 0.136 0.126
[85] 0.127 0.136 0.137 0.081 0.112 0.204 0.113 0.109 0.185 0.130 0.186 0.126
[97] 0.193 0.140 0.106 0.191
```

```
R> Ajdgamma(X = 1/FPT, starts = list(shape = 1, rate = 1), leve = 0.95)
```

```
Profiling...
```

```
$summary
```

```
Maximum likelihood estimation
```

```
Call:
```

```
mle(minuslogl = lik, start = starts)
```

```
Coefficients:
```

```
Estimate Std. Error
```

```
shape 15.525968 2.1834585
rate 2.077233 0.2968927
```

```
-2 log L: 403.2067
```

```
$coef
```

```
shape rate
15.525968 2.077233
```

```
$AIC
```

```
[1] 407.2067
```

```
$vcov
```

```
shape rate
shape 4.7674910 0.63784671
rate 0.6378467 0.08814528
```

```
$confint
```

```
2.5 % 97.5 %
shape 11.657589 20.252660
rate 1.551179 2.719831
```

```
R> hist_general(Data = 1/FPT, Breaks = 'Sturges', Law = "GAMMA")
R> Kern_general(Data = 1/FPT, bw = 'Ucv', k = "gaussian", Law = "GAMMA")
```

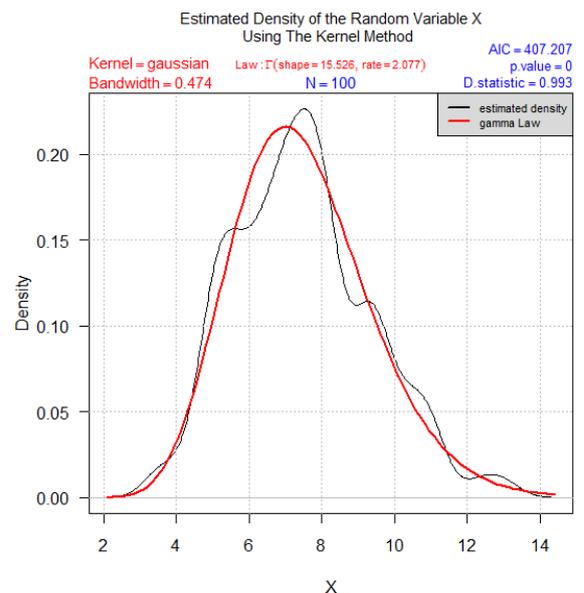
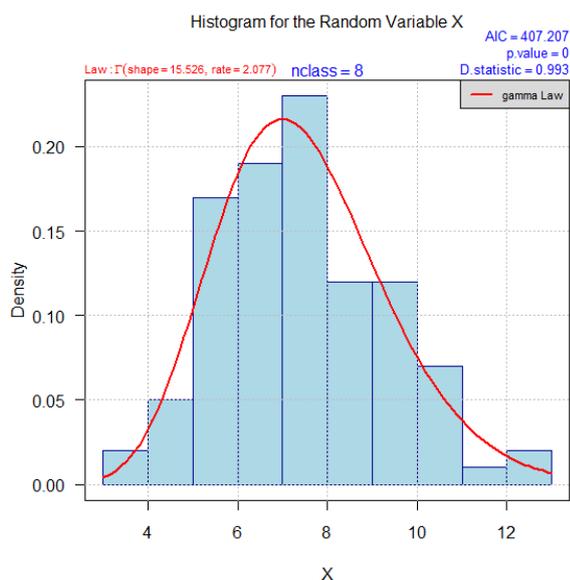


Figure 11: Estimation the density of probability of the moment of the first meeting between the two insects, used histograms and kernel methods.

## 4. Graphical User Interface for **Sim.DiffProc**

Unlike S-PLUS, R<sup>2</sup> does not incorporate a statistical graphical user interface (GUI), but it does include tools for building GUIs.<sup>3</sup> Based on the **tcltk** package (which furnishes an interface to the Tcl/Tk GUI toolkit), the **Sim.DiffProcGUI** package (Boukhetala and Guidoum 2011b) provides a graphical user interface for some functions in the **Sim.DiffProc** package, the design objectives of the **Sim.DiffProcGUI** were as follows: to support **Sim.DiffProc**, through an easy-to-use, extensible, crossplatform GUI, keep things relatively simple, and to render visible, in a reusable form. The **Sim.DiffProcGUI** package uses a simple and familiar menu/dialog-box interface. Top-level menus include *File*, *Edit*, *Brownian Motion*, *Stochastic Integral*, *Stochastic Models*, *Parametric Estimation*, *Numerical Solution of SDE*, *Statistical Analysis*, and *Help*.

Each dialog box includes a Help button, which leads to a relevant help page, the R-Sim.DiffProc console also provides the ability to edit, enter, and re-execute commands. Data sets in this GUI are simply R data frames, and can be read from attached packages or imported from files, although several data frames may reside in memory.

Once R is running, simply loading the **Sim.DiffProcGUI** package by typing the command `library("Sim.DiffProcGUI")` into the R Console starts the GUI. After loading the package, the GUI window should appear more or less as in the following figure 12

```
R> library(Sim.DiffProcGUI)
```

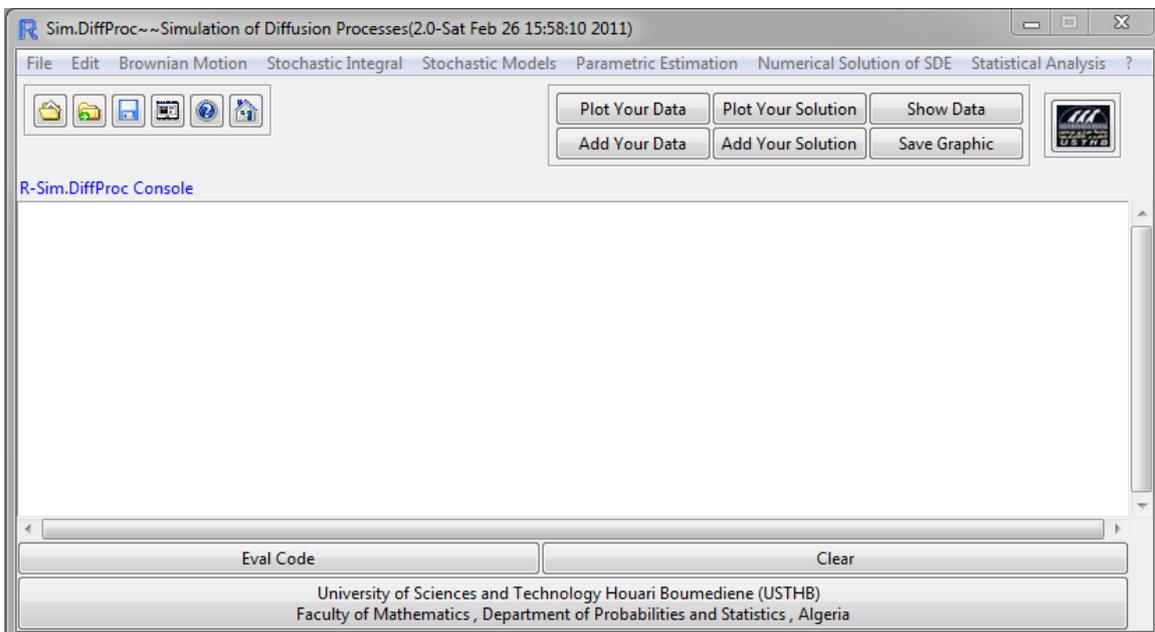


Figure 12: Graphical User Interface for **Sim.DiffProc** package at start-up.

<sup>2</sup>R is a programming language and software environment for statistical computing and graphics, are available for download from CRAN at URL: <http://www.r-project.org/>.

<sup>3</sup>The **Sim.DiffProcGUI** package, described in this paper, is based on the **tcltk** package (Dalgaard 2001, 2002), which provides an interface to Tcl/Tk (Welch 2000).

This and other screen images were created under Windows seven, if you use another version of Windows (or, of course, another computing platform), then the appearance of the screen may differ.<sup>4</sup>

The **Sim.DiffProcGUI** package and R Console windows float freely on the desktop. You will normally use the menus and dialog boxes of the **Sim.DiffProcGUI** to read, manipulate, and simulated or analyze data.

## 5. Conclusion

This paper introduces new package **Sim.DiffProc** for a simulation of diffusion processes in R language, and graphical user interface (GUI) for this package, the actual development of computing tools (software and hardware) has motivated us to analyze by simulation. Many theoretical problems on the stochastic differential equations have become the object of practical research, as statistical analysis and the simulation the solution of SDE, enabled many searchers in different domains to use these equations to modeling and to analyse practical problems. The dispersion problem that we have treated in this paper is a good example which shows the important use of the SDE in the practice, this problem is very hard, hence the SDE approach seems to be a good approximation to treat such problem, the difficulty to obtain the exact solution of the SDE, the simulation gives information on the density function of the random variable first passage time  $\tau_c$  and enables to estimate a density function, this estimation is based, on either, the histograms and the kernel methods. These results can be applied, as a first approximation, of the dispersal phenomenon, in presence of an attractive source. The density function of  $\tau_c$  can be used to determine the rate of the pollutant particles in a neighborhood of the attractive centre, it has been shown by graphical and numerical simulations. The simulation studies implemented in R language seems very preferment and efficient, because it is a statistical environment, which permits to realize and to validate the simulations.

## Acknowledgments

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<sup>4</sup>The examples in this document use the Windows version of R, R, however, is available on other computing platforms as well (Macintosh computers and Unix/Linux systems), and the use of R and the **Sim.DiffProcGUI** package on these other systems is very similar to their use under Windows.

- ogy Houari Boumediene, BP 32 El-Alia, U.S.T.H.B, Algeria. URL [http://www.math.sciences.univ-nantes.fr/CRDM/biblio/opac/index.php?lvl=author\\_see&id=5529/](http://www.math.sciences.univ-nantes.fr/CRDM/biblio/opac/index.php?lvl=author_see&id=5529/).
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