Vol. 40 (2009) ACTA PHYSICA POLONICA B No 5

STOCHASTIC DIFFUSION: FROM MARKOV TO NON-MARKOV MODELING*

E. Gudowska-Nowak, B. Dybiec, P.F. Góra, R. Zygadło

M. Smoluchowski Institute of Physics, Department of Statistical Physics
and
Mark Kac Complex Systems Research Center, Jagellonian University,
Reymonta 4, 30-059 Kraków, Poland

(Received May 7, 2009)

We briefly discuss omnipresence of stochastic modeling in physical science by recalling definitions of Markovian diffusion and generally, non-Markovian continuous time random walks (CTRW). If the motion of an idealized system can be described by a sum of independent displacements whose statistic over short time intervals has a well defined variance, the resulting random walk converges to a normal diffusion process. In turn, if formulation of such motion assumes the idea of distribution of waiting times between subsequent steps, the CTRW scenario emerges, which typically violates the Markovian property.

PACS numbers: 05.20.Dd, 05.40.Jc, 05.45.–a, 05.40.Fb

1. Markov and non-Markov processes

A *stochastic process* [1–3] $\{x(t)\}$ is composed by a family of random variables which are indexed by time, *i.e.* for each time t, the random variable $x(t)$ takes on the value x with some probability. The most popular example of a stochastic process is a Brownian movement, discovered by a botanist R. Brown in 1827 [4]. Brown has observed under the microscope a strong irregular motion of pollen particles on a surface of water. The trajectories of particles in a "Brownian process" are irregular and a displacement of a Brownian particle at time t is a probabilistic, random variable.

2. Markov property

Stochastic processes and *Markov processes*, in particular, serve as a powerfull tool to describe and understand various phenomena at different levels of complexity — from the molecular to the population level. Modeling

* Presented at the XXI Marian Smoluchowski Symposium on Statistical Physics Zakopane, Poland, September 13–18, 2008.

diverse complex systems via stochastic processes allows to incorporate the effects of secondary factors for which the detailed knowledge is missing. The technique has been widely used to model not only physical and chemical systems [1] but also population growth and extinction [5, 6], population genetics [7, 8], chemical kinetics [1, 9], firing of neurons [10, 11], opening and closing of biological channels [12] or cell survival after irradiation [13, 14]. In what follows we first recall briefly a definition of Markovianity which simplifies mathematical tools employed in stochastic modeling. We shall emphasize however, that the assumption of Markovianity relates mostly to natural systems perturbed by (equilibrium or non-equilibrium) fluctuations which are uncorrelated in time. Such an idealization seems to be insufficient in many physical realms where some degree of memory on the "past behavior" influences future evolution of the system and driving fluctuations are usually correlated.

A real stochastic process is fully statistically determined if its *n-th order or n-point* distribution function [1] is given

$$P(x_1, t_1; x_2, t_2; x_3, t_3; \ldots x_{n-1}, t_{n-1}; x_n, t_n)\,, \tag{1}$$

for any n and t, where $P(x_1, t_1; x_2, t_2; x_3, t_3; \ldots, x_{n-1}, t_{n-1}; x_n, t_n)$ stands for the probability that the process $\{x(t)\}$ is in the state x_n (takes the value x_n) at time t_n and in the state x_{n-1} at time t_{n-1} ... and in the state x_1 at time t_1. These functions are not arbitrary but they must satisfy certain conditions. A distribution of a given order is determined from a distribution of lower order by use of the Bayes rule for conditional probabilities:

$$\begin{aligned} & P(x_1, t_1; x_2, t_2; x_3, t_3; \ldots x_{n-1}, t_{n-1}; x_n, t_n) \\ &= P(x_n, t_n | x_{n-1}, t_{n-1}; \ldots x_1, t_1) \ldots P(x_2, t_2 | x_1, t_1) P(x_1, t_1)\,, \end{aligned} \tag{2}$$

where

$$P(x_n, t_n | x_{n-1}, t_{n-1}; \ldots x_1, t_1) = \frac{P(x_1, t_1; x_2, t_2; x_3, t_3; \ldots x_{n-1}, t_{n-1}; x_n, t_n)}{P(x_1, t_1; x_2, t_2; x_3, t_3; \ldots x_{n-1}, t_{n-1})} \tag{3}$$

defines the *conditioned probability* that the process takes on value x_n at time t_n provided the sequence of events $\{x_{n-1}, t_{n-1}; \ldots x_2, t_2; x_1, t_1\}$ took place at earlier times. A *Markov process* is a stochastic process $\{x(t)\}$ which can be fully characterized by a conditioned probability and a one-point probability functions [1].

The basic definition of Markovianity of the process can be expressed as

$$P(x_n, t_n | x_{n-1}, t_{n-1}; \ldots x_1, t_1) = P(x_n, t_n | x_{n-1}, t_{n-1})\,. \tag{4}$$

This criterion is to be complemented by the so-called Smoluchowski–Chapman –Kolmogorov (SCK) equation ($t_n > t_m > t_k$):

$$P(x_n, t_n|x_k, t_k) = \int_{-\infty}^{\infty} P(x_n, t_n|x_m, t_m) P(x_m, t_m|x_k, t_k) dx_m \,, \tag{5}$$

which follows directly from the definitions Eqs. (3) and (4). Therefore, a process which does not satisfy either the basic definition Eq. (4) or the SCK equation (5) is not Markovian. A non-Markovian process may satisfy one of these relations but both are necessary conditions of Markovianity (*i.e.* neither is a sufficient one).

3. Itô transformation formula

A continuous time parameter Markovian process, for which sample paths $\{x(t)\}$ are continuous functions of time, is called a diffusion process [1, 2]. The stochastic diffusion process is fully determined by two moments:

$$\lim_{h\to 0} \frac{1}{h} \langle \varDelta_h X(t)|X(t) = x\rangle \;=\; \mu(x,t)\,, \tag{6}$$

$$\lim_{h\to 0} \frac{1}{h} \langle \{\varDelta_h X(t)\rangle\}^2|X(t) = x\rangle \;=\; \sigma^2(x,t)\,, \tag{7}$$

where $x \in \varOmega, \varDelta_h = X(t+h) - X(t)$. The functions $\mu(x,t)$ and $\sigma^2(x,t)$ are called expected infinitesimal displacement (drift coefficient) and infinitesimal variance, respectively. In addition to infinitesimal relations (6), (7), higher order infinitesimal moments are zero. Based on (6) and (7), it can be shown [2] that the probability density function for the process follows the evolution equation:

$$-\frac{\partial P(x,t'|y,t)}{\partial t} = \mu(y,t')\,\frac{\partial P(x,t'|y,t)}{\partial y} + \frac{1}{2}\,\sigma^2(y,t')\,\frac{\partial^2 P(x,t'|y,t)}{\partial y^2}\,. \tag{8}$$

An alternative approach to deriving evolution equation for the transition probability densities of a Markov diffusion process was presented by Itô [15]. Itô's version of stochastic calculus starts with the stochastic differential equation of the form

$$dx(t) = \mu(x,t)dt + \sigma(x,t)dW(t)\,, \tag{9}$$

where $W(t)$ is an unit Wiener process describing Brownian motion (*i.e.* a normal Gaussian process with stationary independent increments fulfilling the relations $E[W(t)] = 0$ and $E[(W(t) - W(s))^2] = |t-s|$). Accordingly, given that $X(t) = x$, the increment $\Delta x(t)$ in a small time interval Δt has the mean value $\mu(x,t)\Delta t$, the variance $\sigma^2(x,t)\Delta t$ and is independent of all previous increments. In this scheme, the Smoluchowski–Fokker–Planck equation (being the adjoint equation to the Kolmogorov backward equation)

$$\frac{\partial P(x,t'|y,t)}{\partial t'} = -\frac{\partial[\mu(x,t')P(x,t'|y,t)]}{\partial x} + \frac{1}{2}\frac{\partial^2[\sigma^2(x,t')P(x,t'|y,t)]}{\partial x^2} \tag{10}$$

can be derived by introducing the time-derivative for the moment generating function $\Phi(s,t)$ of the process $X(t)$

$$\Phi(s,t) = E[e^{-sX(t)}] = \int\limits_{-\infty}^{\infty} e^{-sx}p(x,t)dx \tag{11}$$

and truncating the Taylor series expansion at the second order.

According to the theorem proved by Itô, a continuous, strictly monotonic function g with continuous derivatives g' and g'' may be used to transform an arbitrary stochastic diffusion process $\{X(t)\}$ into another diffusion process $\{Y(t)\}$, $y = g(x)$ by use of so called Itô transformation formula [2]. Infinitesimal parameters of the transformed process are:

$$\mu_Y(y) = \frac{1}{2}\sigma^2(x)g''(x) + \mu(x)g'(x) \tag{12}$$

and

$$\sigma_Y^2 = \sigma^2(x)[g'(x)]^2\,. \tag{13}$$

4. Random sums and Lévy random walks

With the results summarized above, the stochastic diffusion process may be viewed as "locally" Gaussian. Further generalizations of Itô's approach are possible by *e.g.* introducing increments $dW(t)$ as following the stable law (self-similar but non-Gaussian) or, by analyzing properties of $\Delta W(t)$ incorporated in Eq. (9) as of a random sum of random elements

$$\Delta\tilde{W}(t) = \Delta x(t) = \sum_{i=1}^{N(t)} X_i\,, \tag{14}$$

where the number of summands $N(t)$ is statistically independent from X_i and governed by a renewal process $\sum s_{i=1}^{N(t)} T_i \leqslant t < \sum_{i=1}^{N(t)+1} T_i$ with $t > 0$. Let us assume further that T_i, X_i belong to the domain of attraction of stable distributions, $T_i \sim S_{\lambda,1}$ and $X_i \sim S_{\alpha,\beta}$, whose corresponding characteristic functions $\phi(k) = \langle \exp(ikS_{\alpha,\beta})\rangle = \int_{-\infty}^{\infty} e^{ikx} l_{\alpha,\beta}(x;\sigma,\mu=0)dx$, with the density $l_{\alpha,\beta}(x;\sigma,\mu=0)$, are given by

$$\phi(k) = \exp\left[-\sigma^\alpha |k|^\alpha \left(1 - i\beta \text{sign} k \tan\frac{\pi\alpha}{2}\right)\right] , \tag{15}$$

for $\alpha \neq 1$ and

$$\phi(k) = \exp\left[-\sigma|k| \left(1 + i\beta\frac{2}{\pi}\text{sign} k \log|k|\right)\right] \tag{16}$$

for $\alpha = 1$. Here the parameter $\alpha \in (0,2]$ denotes the stability index, yielding the asymptotic long tail power law for the x-distribution, which for $\alpha < 2$ is of the $|x|^{-(1+\alpha)}$ type. The parameter σ ($\sigma \in (0,\infty)$) characterizes the scale whereas β ($\beta \in [-1,1]$) defines an asymmetry (skewness) of the distribution and μ represents the shift, which for the strictly stable distributions [17] is set to 0. For $0 < \nu < 1$, $\beta = 1$, the stable variable $S_{\nu,1}$ is defined on positive semi-axis. Within the above formulation, the counting process $N(t)$ satisfies

$$\begin{aligned}
\lim_{t\to\infty} \text{Prob}\left\{\frac{N(t)}{(t/c)^\nu} < x\right\} &= \lim_{t\to\infty} \text{Prob}\left\{\sum_{i=1}^{[(t/c)^\nu x]} T_i > t\right\} \\
&= \lim_{n\to\infty} \text{Prob}\left\{\sum_{i=1}^{[n]} T_i > \frac{cn^{1/\nu}}{x^{1/\nu}}\right\} \\
&= \lim_{n\to\infty} \text{Prob}\left\{\frac{1}{cn^{1/\nu}}\sum_{i=1}^{[n]} T_i > \frac{1}{x^{1/\nu}}\right\} \\
&= 1 - L_{\nu,1}\left(x^{-1/\nu}\right) ,
\end{aligned} \tag{17}$$

where $[(t/c)^\nu x]$ denotes the integer part of the number $(t/c)^\nu x$ and $L_{\nu,1}(x^{-1/\nu})$ represents the cumulative distribution function of the stable density.

Moreover, since $\lim_{n\to\infty} \text{Prob}\left\{(1/c_1 n^{1/\alpha})\sum_{i=1}^n X_i < x\right\} \to L_{\alpha,\beta}(x)$ and $p(x,t) = \sum_n p(x|n)p_n(n(t))$, asymptotically one gets $(dL_{\alpha,\beta}(x)/dx = l_{\alpha,\beta}(x))$

$$p(x,t) \sim (c_2 t)^{-\nu/\alpha} \int_0^\infty l_{\alpha,\beta}((c_2 t)^{-\nu/\alpha} x \tau^{\nu/\alpha}) l_{\nu,1}(\tau)\tau^{\nu/\alpha} d\tau , \tag{18}$$

where c_1 and c_2 are constants. The resulting (non-Markov) process becomes ν/α self-similar Lévy random walk [18–20], *i.e.* $p(x,t) = t^{-\nu/\alpha} p(xt^{-\nu/\alpha}, 1)$.

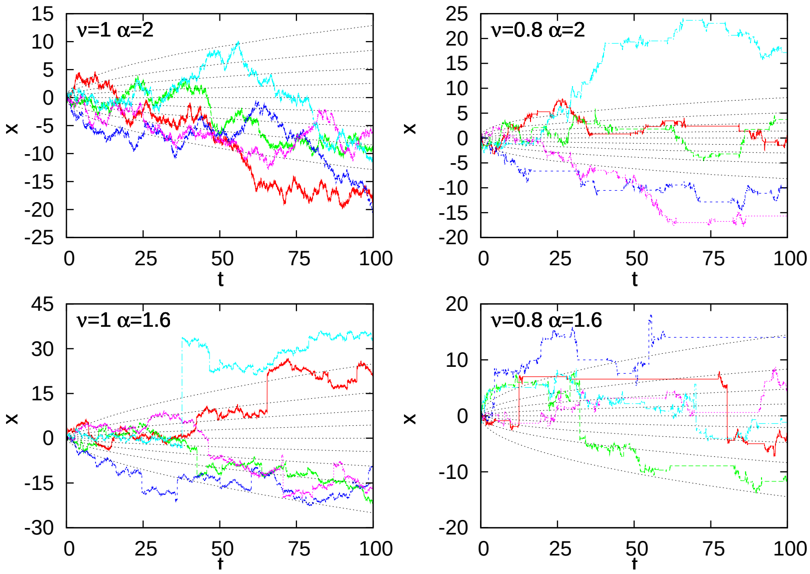

Fig. 1. (Color online) Examples of sample trajectories of ν/α self-similar random walk. The spread of trajectories is visualized by quantile lines $(0.1, 0.2, \ldots, 0.9$ — from bottom to the top). The p-quantile line for the process is a function $q_p(t)$ defined via relation $\mathrm{Prob}\,\{X(t) \leqslant q_p(t)\} = p$.

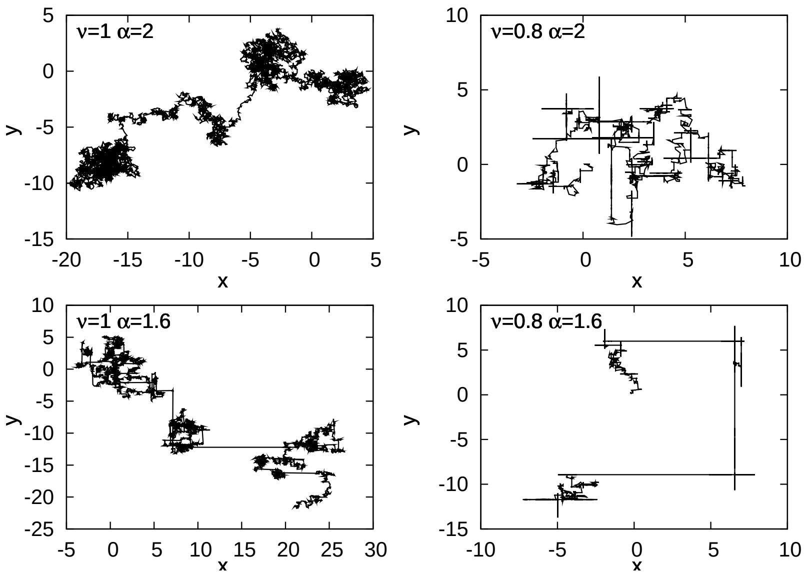

Fig. 2. Exemplary ν/α self-similar motion in 2D. The trajectories have been simulated independently in x and y direction. The values for time and space fractional parameters are displayed.

In general, Lévy random walks are neither Gaussian nor Markov [21–23]. An interesting class of these processes can be built up by allowing coupling between $N(t)$ and X_i and introducing the hierarchical clustering transformation [24]. In consequence, the asymptotic distribution of the resulting diffusion front $\tilde{W}(t)$ depends on the way the jumps are correlated within the clusters. Time relaxation patterns of such fronts are interesting models of transport and relaxation phenomena in complex, inhomogeneous systems.

The 2008 Marian Smoluchowski Symposium on Statistical Physics has been entitled "Questioning Appearance of Stable Noises in Statistical Physics" and has been devoted to contemporary trends exploring and making use of the theory of stochastic processes and anomalous diffusion in a number of branches: chemical kinetics and biological devices, nonlinear flows, quantum processes and information theory. We had a privilege of hosting groups of mathematicians and physicists whose works in the field have profoundly progressed the theory and influenced applications of anomalous diffusion in various domains of natural science. We hope that their contributions, presented in this volume of *Acta Physica Polonica B* will be an inspiring step towards exciting problems of stochastic complexity, process subordinations, fractional diffusion and coupled CTRW.

On behalf of the Organizers we thank all institutions which have sponsored the conference with much hope for possibility of next meetings to come and illuminating discussions within the scope of future Smoluchowski symposia.

E. Gudowska-Nowak, B. Dybiec, P.F. Góra, R. Zygadło.

REFERENCES

[1] N.G. Van Kampen, *Stochastic Processes in Physics and Chemistry*, North Holland, Amsterdam 1981.

[2] S. Karlin, H. Taylor, *First Course in Stochastic Processes*, Academic Press, New York 1976.

[3] A. Papoulis, *Probability, Random Variables and Stochastic Processes*, McGraw-Hill, Tokyo 1981.

[4] R. Brown, *Philos. Mag.* **4**, 161 (1828).

[5] N. Goel, N. Richter-Dyn, *Stochastic Processes in Biology*, Academic Press, New York 1974.

[6] D.R. Nelson, N.M. Shnerb, *Phys. Rev.* **E58**, 1384 (1998).

[7] T. Maruyama, *Mathematical Modeling in Genetics*, Springer Verlag, Berlin 1981.

[8] W. Horsthemke, R. Lefever, *Noise-Induced Transitions. Theory and Applications in Physics, Chemistry and Biology*, Springer Verlag, Berlin 1984.

[9] S. Larsson, *Bioch. Biophys. Acta* **1365**, 294 (1998).

[10] J.J. Hopfield, *Proc. Natl. Acad. Sci. USA* **79**, 2554 (1982).

[11] A. Crisanti, H. Sompolinsky, *Phys. Rev.* **A36**, 4922 (1987).

[12] B. Hille, *Ionic Channels of Excitable Membranes*, Sinauer Inc., Sunderland, MA 1992.

[13] C.A. Tobias, E. Goodwin, E. Blakely, in *Quantitative Mathematical Models in Radiation Biology*, J. Kiefer, Ed., Springer Verlag, Berlin 1988, p. 135.

[14] N. Albright, *Radiat. Res.* **118**, 1 (1989).

[15] K. Itô, *Memoir Am Math Soc* **4**, 1 (1951).

[16] J. Neyman, *Am. Math. Stat.* **10**, 35 (1939).

[17] A. Janicki, A. Weron, *Simulation and Chaotic Behavior of α-Stable Stochastic Processes,* Marcel Dekker, New York 1994.

[18] A.I. Saichev, G.M. Zaslavsky, *Chaos* **7**, 753 (1997).

[19] *Lévy Flights and Related Topics in Physics*, Ed. M.F. Shlesinger, G.M. Zaslavsky, J. Frisch, Springer Verlag, Berlin 1995.

[20] *Lévy Processes: Theory and Applications*, Ed. O.E. Barndorff-Nielsen, T. Mikosch, S.I. Resnick, Birkhäuser, Boston 2001.

[21] M. Magdziarz, A. Weron, *Phys. Rev.* **E75**, 056702 (2007).

[22] M. Magdziarz, A. Weron, J. Klafter, *Phys. Rev. Lett.* **101**, 210601 (2008).

[23] M. Magdziarz, A. Weron, K. Weron, *Phys. Rev.* **E75**, 016708 (2007).

[24] A. Jurlewicz, K. Weron, M. Teuerle, *Phys. Rev.* **E78**, 011103 (2008).

[25] R. Graham,*Stochastic Models*, in *Springer Tracts in Modern Physics*, Vol. **66**, Springer, Berlin 1973; *Models of Stochastic Behaviour*, in S.B. Chen, B. Chu, R. Nossal (Eds.); *Scattering Technique*, Plenum Press, New York 1978.

[26] I. Eliazar, J. Klafter, *Proc. Natl. Acad. Sci. USA* **27**, 13779 (2005).

[27] R. Zygadlo, *Phys. Rev.* **E47**, 4067 (1993).