Deformed random walk: suppression of randomness and inhomogeneous diffusion

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STATISTICAL MECHANICS FOR COMPLEXITY
A CELEBRATION OF THE 80TH BIRTHDAY OF CONSTANTINO TSALLIS

Centro Brasileiro de Pesquisas Físicas (CBPF), Rio de Janeiro, 6th November, 2023

Universidade Estadual do Sudoeste da Bahia

Content

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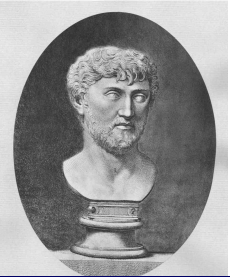
Random walk: some of historical review

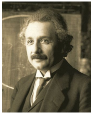
The poem *De rerum natura* (on the nature of the things), didactic work treating of the principles and the philosophy of the *epicurism* of the philospher and roman poet **Tito Lucrécio Caro** (94 a.C. - 50 a. C.) cites:

"The atoms moves in an infinite vacuum.
The universe is composed by atoms and vacuum, nothing else.
Because we are made up of a soup of atoms in constant motion.
Life forms in this world and in others are in constant movement, increasing the power of some forms and decreasing that of others.
Feelings perceive the macroscopic collisions and interactions of bodies"



Brownian motion

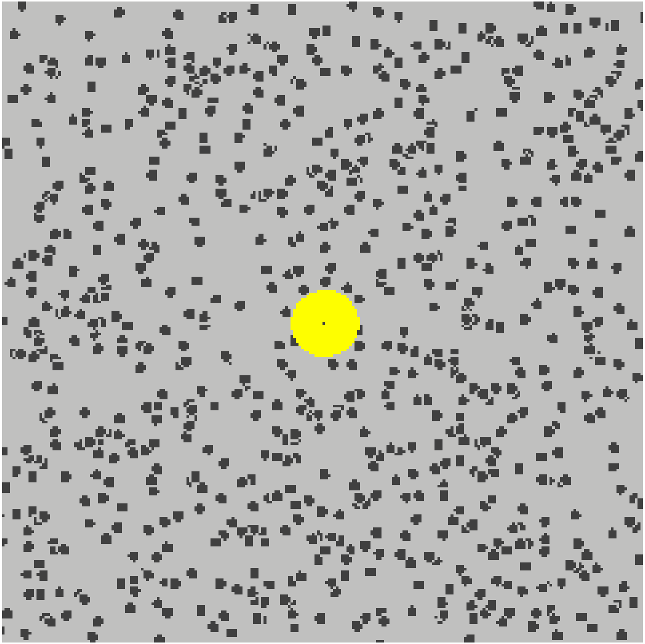
In 1827, Scottish biologist **Robert Brown** observed that particles found in grains of pollen in water moved through the water, with movements of “their own volition”.



In 1905, **Albert Einstein** in his doctoral thesis published the first theory of Brownian motion, obtaining, $\Gamma = RT/(6\pi a\eta N_A)$ for the diffusion coeficient

In 1908, French physicist **Paul Langevin** established the Langevin equation

$$\frac{dv}{dt} = \eta v + \xi(t) \quad , \quad \eta = \text{viscosity coefficient} \quad , \quad \xi(t) = \text{random force}$$



Deterministic and probabilistic descriptions

Let us assume the discrete dynamics of a system in one dimension, where $X_0, X_1, X_2, \ldots, X_n, \ldots$ represent the positions of a particle at times $t = 0, 1, 2, \ldots, n, \ldots$. This, for example, allows us to model Brownian motion in a discrete dynamics

$$\text{deterministic description (Hamilton)} \implies \text{probabilistic description (master equation)}$$

$$\text{particle mechanics} \Longrightarrow \text{statistical mechanics}$$

$$(x_1(t), \ldots, x_N(t), p_1(t), \ldots, p_N(t)) \implies P(x,t) \text{ distribution of the system}$$

with $P(x,t)dx$ the probability of the system being at $(dx - x, x + dx)$ at time t

Definition of classical random walk

Probability of taking an i-th step $X_i = 1$ or $X_i = -1$:

$$P(X_i = +1) = p \quad , \quad P(X_i = -1) = 1 - p$$

The mean value and variance in the i-th step are

$$E(X_i) = (+1)p + (-1)(1-p) = 2p - 1$$

$$V(X_i) = (1 - (2p-1))^2 p + (-1 - (2p-1))^2 (1-p) = 4p(1-p)$$

We see that for the particular case of a symmetric RW ($p = 1/2$) we have

$$P(X_i = \pm 1) = 1/2 \quad , \quad E(X_i) = 0 \quad , \quad V(X_i) = 1$$

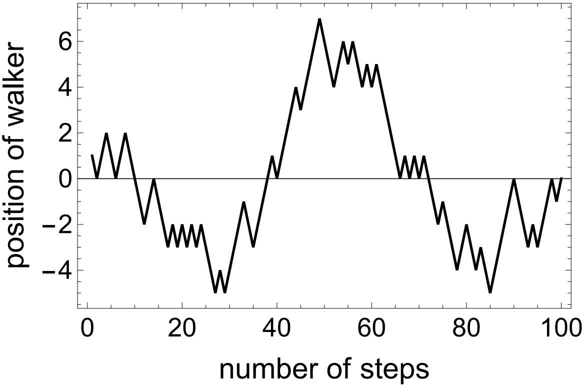
Pascal's triangle for $p = 1/2$ and $n = 5$

k	-5	-4	-3	-2	-1	0	1	2	3	4	5
$P(S_0 = k)$						0					
$2P(S_1 = k)$					1		1				
$2^2P(S_2 = k)$				1		2		1			
$2^3P(S_3 = k)$			1		3		3		1		
$2^4P(S_4 = k)$		1		4		6		4		1	
$2^5P(S_5 = k)$	1		5		10		10		5		1

Trajectories of RW - Homogeneity

$$S_n = X_1 + X_2 + \ldots + X_n = \sum_{i=1}^{n} X_i \quad \text{(position after } n \text{ steps)}$$

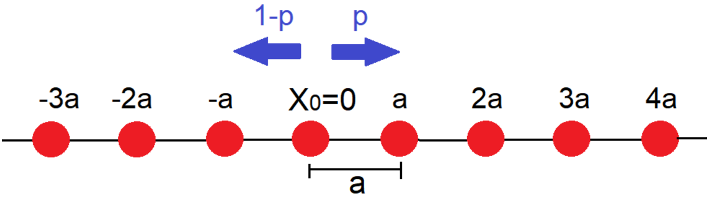
Mathematica code: ListLinePlot[Accumulate[RandomChoice[-1, 1, 100]], Frame → True, FrameLabel → Style["number of steps", FontSize → 18, Black], Style["position of walker", FontSize → 18, Black], LabelStyle → Directive[Black, FontSize → 16], PlotStyle → Black]



Connection of the RW with the diffusion equation

The master equation for $P(x,t)$ on a one-dimensional lattice of parameter a is

$$P(x,t+\Delta t) = pP(x+a,t) + (1-p)P(x-a,t)$$



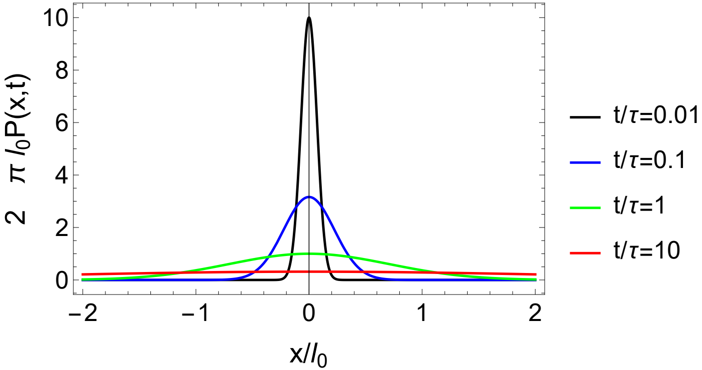
For $p = 1/2$ taking the limits $a \to 0$, $\Delta t \to 0$ and from the approximations

$$P(x \pm a, t) \approx P(x,t) \pm a\frac{\partial P}{\partial x} + \frac{a^2}{2}\frac{\partial^2 P}{\partial x^2} \quad , \quad P(x,t+\Delta t) \approx P(x,t) + \Delta t\frac{\partial P}{\partial t}$$

we obtain the **diffusion equation** (Fokker-Planck equation, FPE)

$$\frac{\partial P(x,t)}{\partial t} = \Gamma\frac{\partial^2 P(x,t)}{\partial x^2} \quad , \quad \Gamma = \frac{a^2}{2\Delta t}$$

Solution of the diffusion equation (free case)



$$P(x,t) = \frac{1}{\sqrt{2\pi\Gamma t}} e^{-\frac{x^2}{2\Gamma t}} \quad , \quad \langle x(t) \rangle = 0 \quad , \quad \langle x(t)^2 \rangle = \Gamma t \quad , \quad \tau = \frac{2\Gamma}{l_0^2}$$

Content

Nonextenstive statistics

Possible Generalization of Boltzmann–Gibbs Statistics

Constantino Tsallis[1]

Received November 12, 1987; revision received March 8, 1988

With the use of a quantity normally scaled in multifractals, a generalized form is postulated for entropy, namely $S_q \equiv k[1-\sum_{i=1}^{W} p_i^q]/(q-1)$, where $q \in \mathbb{R}$ characterizes the generalization and $\{p_i\}$ are the probabilities associated with W (microscopic) configurations ($W \in \mathbb{N}$). The main properties associated with this entropy are established, particularly those corresponding to the microcanonical and canonical ensembles. The Boltzmann–Gibbs statistics is recovered as the $q \to 1$ limit.

ADITIVITY: an entropy S is called **aditive** if for any two independent systems A, B we have

$$S(A+B) = S(A) + S(B)$$

The Tsallis entropy $S_q = \frac{\sum_{i=1}^{W} p_i^q - 1}{1-q}$ satisfies

$$S_q(A+B) = S_q(A) + S_q(B) + \left(\frac{1-q}{k_B}\right) S_q(A) S_q(B)$$

Nonextensive statistics and some associated structures

$$\textbf{Non-aditivity}: \quad S_q(A+B) = S_q(A) + S_q(B) + \left(\frac{1-q}{k_B}\right) S_q(A) S_q(B)$$

$$\text{q-sum:} \quad x \oplus_q y := x + y + (1-q)xy \longrightarrow x + y \quad \text{when} \quad q \to 0$$

$$\text{q-product:} \quad x \otimes_q y := [x^{1-q} + y^{1-q} - 1]^{1/(1-q)} \longrightarrow xy \quad \text{when} \quad q \to 0$$

L. Nivanen *et al.*, *RMP* **52**, 437-444 (2003) - E. P. Borges, *Phys. A* **340**, 95-101 (2004)

q-álgebra $(\oplus_q, \ominus_q, \otimes_q, \oslash_q)$ e **q-derivative** $D_q f(x) = (1 + (1-q)x) df/dx$

Mapping between the harmonic oscillator with deformed derivative and the Morse oscillator by means of the canonical transformation $\eta = \frac{\ln(1+\gamma x)}{\gamma}$ $\quad (\gamma = 1 - q)$

Raimundo N. Costa Filho et al 2013 EPL **101** 10009

$$\textbf{HO}: i\hbar \frac{\partial \psi(x,t)}{\partial t} = -(1+\gamma x)^2 \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) - \gamma(1+\gamma x) \frac{\hbar^2}{2m} \frac{\partial}{\partial x} \psi(x,t) + \frac{m\omega^2 x^2}{2} \psi(x,t)$$

$$\textbf{MO}: i\hbar \frac{\partial \phi(\eta,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \eta^2} \phi(\eta,t) + \frac{m\omega^2}{2\gamma^2} (e^{\gamma\eta} - 1)^2 \phi(\eta,t) \quad , \quad \phi(\eta,t) = \psi(x(\eta),t)$$

one-to-one correspondence between the position-dependent mass and the deformed derivative

$$T_g = \frac{g(x)}{2m_0}\frac{\partial^2}{\partial x^2} \Longleftrightarrow m(x) = \frac{m_0}{g(x)} \quad , \quad g(x) = (1+\gamma x)^2 \text{ (q-álgebra)}$$

PHYSICAL REVIEW E **102**, 062105 (2020)

Deformed Fokker-Planck equation: Inhomogeneous medium with a position-dependent mass

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We present the Fokker-Planck equation (FPE) for an inhomogeneous medium with a position-dependent mass particle by making use of the Langevin equation, in the context of a generalized deformed derivative for an arbitrary deformation space where the linear (nonlinear) character of the FPE is associated with the employed deformed linear (nonlinear) derivative. The FPE for an inhomogeneous medium with a position-dependent diffusion coefficient is equivalent to a deformed FPE within a deformed space, described by generalized derivatives, and constant diffusion coefficient. The deformed FPE is consistent with the diffusion equation for inhomogeneous media when the temperature and the mobility have the same position-dependent functional form as well as with the nonlinear Langevin approach. The deformed version of the H-theorem permits to express the Boltzmann-Gibbs entropic functional as a sum of two contributions, one from the particles and the other from the inhomogeneous medium. The formalism is illustrated with the infinite square well and the confining potential with linear drift coefficient. Connections between superstatistics and position-dependent Langevin equations are also discussed.

Deforming the RW (PRE, 2023)

PHYSICAL REVIEW E **107**, 034113 (2023)

Deformed random walk: Suppression of randomness and inhomogeneous diffusion

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We study a generalization of the random walk (RW) based on a deformed translation of the unitary step, inherited by the q algebra, a mathematical structure underlying nonextensive statistics. The RW with deformed step implies an associated deformed random walk (DRW) provided with a deformed Pascal triangle along with an inhomogeneous diffusion. The paths of the RW in deformed space are divergent, while those corresponding to the DRW converge to a fixed point. Standard random walk is recovered for $q \to 1$ and a suppression of randomness is manifested for the DRW with $-1 < \gamma_q < 1$ and $\gamma_q = 1 - q$. The passage to the continuum of the master equation associated to the DRW led to a van Kampen inhomogeneous diffusion equation when the mobility and the temperature are proportional to $1 + \gamma_q x$, and provided with an exponential hyperdiffusion that exhibits a localization of the particle at $x = -1/\gamma_q$ consistent with the fixed point of the DRW. Complementarily, a comparison with the Plastino-Plastino Fokker-Planck equation is discussed. The two-dimensional case is also studied, by obtaining a 2D deformed random walk and its associated deformed 2D Fokker-Planck equation, which give place to a convergence of the 2D paths for $-1 < \gamma_{q_1}, \gamma_{q_2} < 1$ and a diffusion with inhomogeneities controlled by two deformation parameters $\gamma_{q_1}, \gamma_{q_2}$ in the directions x and y. In both the one-dimensional and the two-dimensional cases, the transformation $\gamma_q \to -\gamma_q$ implies a change of sign of the corresponding limits of the random walk paths, as a property of the deformation employed.

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Random walk in deformed space

Probability of taking an i-th step $(X_i)_q = (+1)_q$ or ou $(X_i)_q = (-1)_q$ in deformed space x_q:

$$P((X_i)_q = (+1)_q) = p \quad , \quad P((X_i)_q = (-1)_q) = 1 - p$$

being

$$(\pm 1)_q = \frac{1}{\gamma_q} \ln(1 \pm \gamma_q) \quad , \quad x_q = \frac{1}{\gamma_q} \ln(1 + \gamma_q x)$$

the deformed position $(S_n)_q$ after n steps defined by

$$(S_n)_q = (X_1)_q + (X_2)_q + \ldots + (X_n)_q = \sum_{i=1}^{n} (X_i)_q$$

Hence the question arises: **What is the structure of the random walk X_i corresponding to the deformed random walk $(X_i)_q$?**

$$(X_i)_q \mapsto X_i \quad , \quad x_q = \frac{1}{\gamma_q} \ln(1 + \gamma_q x) \mapsto x$$

Structure of the deformed random walk in standard space x

Property: Given x, y real numbers, the q-sum $x \oplus_q y = x + y + \gamma_q xy$ satisfies

$$x_q + y_q = (x \oplus_q y)_q$$

so we have,

$$(S_n)_q = (X_1)_q + (X_2)_q + \ldots + (X_n)_q \implies S_n = X_1 \oplus_q X_2 \oplus_q \ldots \oplus_q X_n$$

being

$$S_n = X_1 \oplus_q X_2 \oplus_q \ldots \oplus_q X_n = \frac{e^{\gamma_q (\sum_{i=1}^{n} (X_i)_q)} - 1}{\gamma_q}$$

$$\begin{aligned} S_1 &= X_1 \\ S_2 &= X_1 + X_2 + \gamma_q X_1 X_2 \\ \ldots &= \ldots \\ S_n &= \sum_{i=1}^{n} X_i + \gamma_q \sum_{i<j}^{n} X_i X_j + \gamma_q^2 \sum_{i<j<k}^{n} X_i X_j X_k + \ldots \end{aligned}$$

The deformation parameter is manifested as perturbative corrections γ_q^i

Pascal's triangles of the RW and the DRW

Pascal's triangle of the RW with $p = 1/2$ and $n = 5$

k	-5	-4	-3	-2	-1	0	1	2	3	4	5
$P(S_0 = k)$						0					
$2P(S_1 = k)$					1		1				
$2^2 P(S_2 = k)$				1		2		1			
$2^3 P(S_3 = k)$			1		3		3		1		
$2^4 P(S_4 = k)$		1		4		6		4		1	
$2^5 P(S_5 = k)$	1		5		10		10		5		1

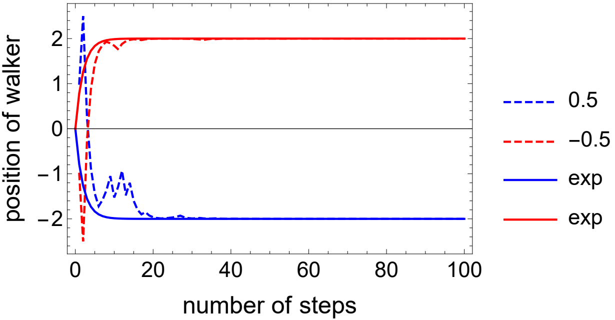
Pascal's triangle of the DRW with $p = 1/2$, $n = 5$ and $\gamma_q = 1/2$

			0			
		-1		1		
		-1.5 (1)	-0.5 (2)	2.5 (1)		
	-1.7 (1)	-1.2 (3)		0.2 (3)	5 (1)	
	-1.9 (1)	-1.6 (4)	-0.9 (6)	1.4 (4)	8.1 (1)	
-1.9 (1)	-1.8 (5)	-1.4 (10)		-0.3 (10)	3.1 (5)	13.2 (1)

Trajectories of the DRW - Inhomogeneity

$$S_n = X_1 \oplus_q X_2 \oplus_q \ldots \oplus_q X_n = \frac{e^{\gamma_q (\sum_{i=1}^{n} (X_i)_q)} - 1}{\gamma_q} \quad \text{(position after } n \text{ steps)}$$

Mathematica code: ListLinePlot[f[Accumulate[RandomChoice[g[-1], g[1], 100]]], k[Accumulate[RandomChoice[h[-1], h[1], 100]]], Table[k, 2*(Exp[-(0.5) k] - 1), k, 0, 100], Table[k, -2*(Exp[-(0.5) k] - 1), k, 0, 100], PlotStyle → Dashed, Blue, Dashed, Red, Blue, Red, Frame → True, FrameLabel → Style[“number of steps”, FontSize → 18, Black], Style[“position of walker”, FontSize → 18, Black], LabelStyle → Directive[Black, FontSize → 16], PlotLegends → “0.5”, “-0.5”, “exp”, “exp”]



Convergence theorem for DRW

We see that the trajectories of the deformed random walk asymptotically satisfy

$$\frac{dX}{dt} \approx 1 - |\gamma_q| X \quad , \quad X(0) = 0$$

whose solution $X(t) = (e^{-|\gamma_q| t} - 1)/\gamma_q$ is already observed after $n = 100$ steps

Theorem: (one-dimensional convergence of the DRW)
Let $f_+, f_- : \mathbb{R} \to \mathbb{R}$ be the functions $f_+(x) = x \oplus_q 1 = x(1 + \gamma_q) + 1$ and $f_-(x) = x \oplus_q (-1) = x(1 - \gamma_q) - 1$. Let X_n be the position of the walker at instant $t = n$. Then,

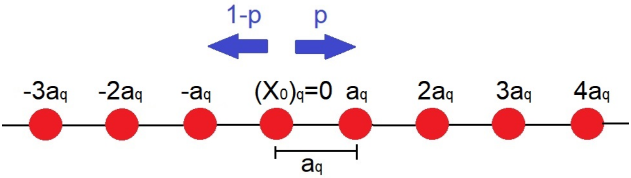
(i) $X_{n+1} = f_+(X_n)$ or $X_{n+1} = f_-(X_n)$ for all $n \in \mathbb{N}$.

(ii) If $|\gamma_q| < 1$ then $\lim_{n\to\infty} X_n = -\gamma_q^{-1}$.

Deformed random walk and deformed diffusion equation

The master equation for $\mathcal{P}_q(x_q, t)$ on a one-dimensional lattice of parameter a_q in deformed space x_q is

$$\mathcal{P}(x, t + \Delta t) = p\mathcal{P}(x + (+a)_q, t) + (1 - p)\mathcal{P}(x + (-a)_q, t)$$



For $p = 1/2$ taking the limits $a \to 0$, $\Delta t \to 0$, and using $(\pm a_q) \approx \pm a$ and the approximations

$$\mathcal{P}(x_q+(\pm a)_q, t) \approx \mathcal{P}(x_q, t)+(\pm a)_q D_q\mathcal{P}+\frac{(\pm a)_q^2}{2}D_q^2\mathcal{P} \ , \ \mathcal{P}(x_q, t+\Delta t) \approx \mathcal{P}(x_q, t)+\Delta t\frac{\partial \mathcal{P}}{\partial t}$$

we obtain the **deformed diffusion equation** (DFPE, PRE da Costa et al. (2020))

$$\frac{\partial \mathcal{P}(x_q, t)}{\partial t} = \Gamma D_q^2 \mathcal{P}(x_q, t) \quad , \quad \Gamma = \frac{a^2}{2\Delta t} \quad , \quad D_q f(x) = (1 + \gamma_q x)\frac{df}{dx}$$

Structure of the deformed diffusion equation

$$\frac{\partial \mathcal{P}(x_q,t)}{\partial t} = \Gamma D_q^2 \mathcal{P}(x_q,t) \quad , \quad \Gamma = \frac{a^2}{2\Delta t} \quad , \quad D_q f(x) = (1+\gamma_q x)\frac{df}{dx}$$

is equivalent to

$$\frac{\partial P}{\partial t} = \Gamma \frac{\partial}{\partial x}(1+\gamma_q x)\frac{\partial}{\partial x}(1+\gamma_q x)P(x,t) \quad \text{(van Kampen diffusion)}$$

with the relations

$$P(x,t) = \frac{\mathcal{P}(x_q,t)}{1+\gamma_q x} \quad , \quad 1 = \int P(x,t)dx = \int \mathcal{P}(x_q,t)dx_q$$

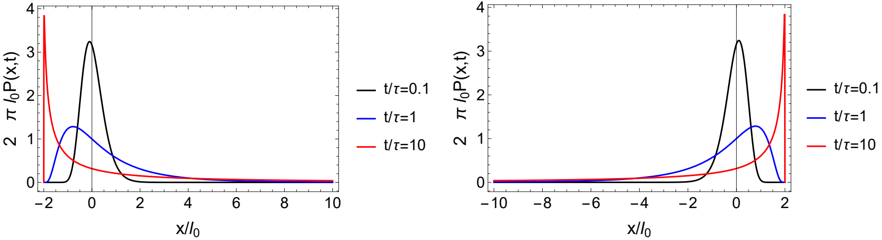
Hence, the solution of the **homogeneous free diffusion** in the deformed space x_q

$$\mathcal{P}(x_q,t) = \frac{1}{\sqrt{2\pi\Gamma t}} \exp\left(-\frac{x_q^2}{2\Gamma t}\right)$$

corresponds to the **inhomogeneous free diffusion** in standard space x given by

$$P(x,t) = \frac{1}{1+\gamma_q x}\frac{1}{\sqrt{2\pi\Gamma t}} \exp\left(-\frac{\ln^2(1+\gamma_q x)}{(2\Gamma t)\gamma_q^2}\right)$$

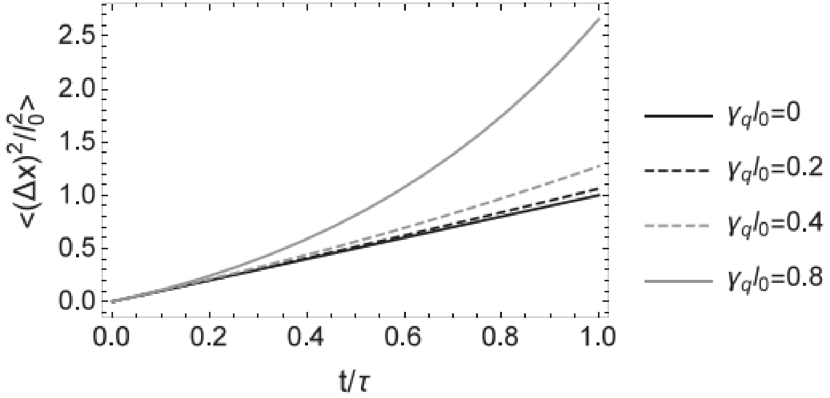
Stationary solution for long times ($t \to \infty$)



$$\tau = \frac{1}{\gamma_q^2 \Gamma} \qquad \text{(characteristic time)}$$

$$P_s(x) = \delta(x + 1/\gamma_q) \quad \text{with} \quad x > -1/\gamma_q \quad (\gamma_q > 0) \quad \text{or} \quad x < -1/\gamma_q \quad (\gamma_q < 0)$$

MSD (mean standard deviation)



$$\langle(\Delta x)^2(t)\rangle = \langle x^2(t)\rangle - \langle x(t)\rangle^2 = \frac{e^{2\Gamma t\gamma_q^2} - e^{\Gamma t\gamma_q^2}}{\gamma_q^2}$$

RW-DRW comparison

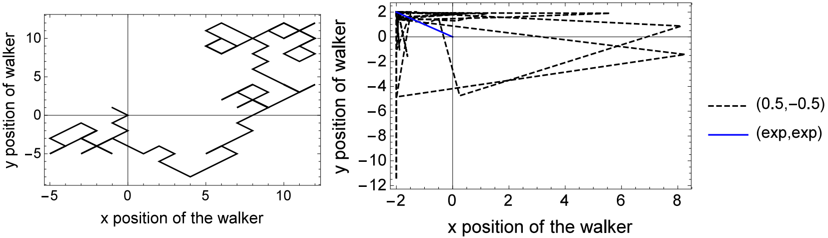
property	random walk	deformed random walk
Pascal's triangle	symmetry around $x = 0$	asymmetry
randomness	yes	not
asymptotic limit	not	$X_n \to -1/\gamma_q$
S_n	$X_1 + \ldots + X_n +$	$X_1 \oplus_q \ldots \oplus_q X_n$
memory effects	not	not
diffusion equation	$\partial_t P(x,t) = \Gamma \partial_{xx} P(x,t)$	$\partial_t \mathcal{P}(x_q,t) = \Gamma D_q^2 \mathcal{P}(x_q,t)$
stationary solution	constant ≈ 0	$P_s(x) = \delta(x + 1/\gamma_q)$
MSD $\langle(\Delta x)^2(t)\rangle$	Γt	$\frac{e^{2\Gamma t \gamma_q^2} - e^{\Gamma t \gamma_q^2}}{\gamma_q^2}$
type of diffusion	linear	exponential
characteristic time	∞	$\tau = 1/(\gamma_q^2 \Gamma)$
localization	not	$x = -1/\gamma_q$

Content

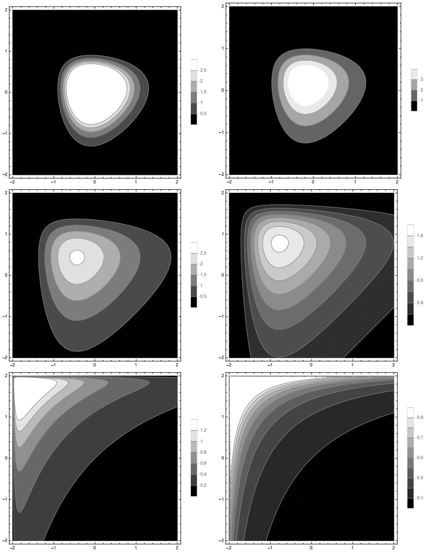
Final considerations

1. A suppression of randomness is observed for the DRW with $|\gamma_q| < 1$ reflected in the convergence of any trajectory starting at $X = 0$, with the asymptotic limit being $x = -1/\gamma_q$.
2. Exponential convergence of the DRW trajectories is a consequence of the q-deformation used.
3. The master equation of the DRW implies a deformed Fokker-Planck equation that results in a particular case of the inhomogeneous van Kampen diffusion equation.
4. A localization and a finite characteristic time are dependent on the deformation parameter γ_q, recovering the standard case for zero deformation.
5. Other deformations could be used to generate other DRW, such as the deformation of the Kaniadakis algebra inherited from Kaniadakis statistics.

DRW and DFPE: two dimensional case



Paths of the walker after $n = 100$ steps starting at $(x, y) = (0, 0)$ provided $p_1 = p_2 = p_3 = 1/4$. Left plot shows the two-dimensional RW Right plot below illustrates the two-dimensional DRW with a mixture of deformations $\gamma_{q_1} = 0.5$ and $\gamma_{q_2} = -0.5$, whose convergence to the fixed point $(-2, 2)$ is observed and the blue curve indicates the exponential asymptotic behavior $(X(t), Y(t)) \sim ((e^{-|\gamma_{q_1}|t} - 1)/\gamma_{q_1}, (e^{-|\gamma_{q_2}|t} - 1)/\gamma_{q_2})$.



Contours of the probability distribution $P(x, y, t)$ of the two-dimensional DFPE for times $t/\tau = 0.1, 0.2, 0.5, 1, 5, 10$ with $\gamma_{q_1} = 0.5$ and $\gamma_{q_2} = -0.5$ with the initial condition $P(x, y, t = 0) = \delta(x)\delta(y)$. In white and black are indicated the regions with low and high probability density.

References

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Happy Birthday Constantino
Thank you