Estimating the nonextensivity of systems from experimental data: a nonlinear diffusion equation approach

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Abstract

We consider nonextensive systems that are related to the nonextensive entropy proposed by *Tsallis* and can be described by means of the nonlinear porous medium equation and the nonlinear Fokker-Planck equation proposed by *Plastino* and *Plastino*. We show how to determine the degree of nonextensivity of these systems from experimental data. Both transient and stationary cases are addressed.

Key words: nonextensivity, data analysis, nonlinear diffusion equations
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1 Introduction

Thermostatistics and information theory based on the Boltzmann-Gibbs-Shannon measure has found wide applicability in various disciplines ranging from solid state physics to the physics of open nonequilibrium systems [1–4]. However,

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as pointed out time and again in the literature, this approach is subjected to various limitations (e.g., [5,6]). Recently, *Tsallis* suggested a generalization of thermostatistics involving the nonextensive entropy measure S_q that depends on a parameter q, which measures the degree of nonextensivity of systems [7–9]. While for $q = 1$ we deal with extensive systems (and S_q recovers the Boltzmann-Gibbs-Shannon measure), for $q \neq 1$ we deal with nonextensive systems. The hope is that such a nonextensive extention of the Boltzmann-Gibbs-Shannon thermostatistics and information theory applies to systems for which the extensive theory fails. Indeed, nonextensive thermostatistics has been successfully applied to describe, for example, the statistics of systems with long range interactions [10,11], chaotic systems involving fractal phase spaces [12,13], systems for which temperature fluctuations might become relevant [14–16], and systems exhibiting power law distributions [17–19]. In this context, a crucial issue is to determine the parameter q. For particular systems with long range interactions a q-value of about 7 has been found [10,11]. In economics, q-values of about 1.5 have been reported [20,21]. For chaotic systems q-values have been related to system parameters [12,13]. Furthermore, for systems subjected to temperature fluctuations q-values have been related to the spatial scales on which key properties of these systems are typically studied [14,22,23].

In the present manuscript the focus is on systems that exhibit power law distributions and can be treated within the framework of the nonextensive thermostatistics suggested by *Tsallis*. In particular, we assume that we deal with systems that can be described by means of the nonlinear Fokker-Planck equation proposed by *Plastino* and *Plastino*, whose stationary solutions are power law distributions that make the entropy S_q maximal under appropriate energy constraints [24]. This nonlinear Fokker-Planck equation is of particular interest because if we interpret the probability density as a particle density function $\rho(x, t)$ then the Fokker-Planck equation corresponds to the porous medium equation

$$\frac{\partial}{\partial t}\rho = Q\frac{\partial^2}{\partial x^2}\rho^q \tag{1}$$

used in hydrodynamics [25–27]. Using a data analysis technique developed for Markov diffusion processes [28–31] and the concept of strongly nonlinear Fokker-Planck equations [32], we will show in this manuscript how to determine the parameter q from experimental data.

2 Estimating the degree of nonextensivity

2.1 General considerations

Let us describe a stochastic process by means of a random variable $X(t)$ that is defined on a phase space Ω and distributed like $u(x)$ at time $t = t_0$. Let $P(x, t; u) = \langle\delta(x - X(t))\rangle$ denote the probability density of X. Here and in what follows, $\langle\cdot\rangle$ describes ensemble averages. We assume that the evolution of P is given by a nonlinear Fokker-Planck equation of the form

$$\frac{\partial}{\partial t}P(x,t;u) = -\frac{\partial}{\partial x}D_1(x,P)P(x,t;u) + \frac{\partial^2}{\partial x^2}D_2(x,P)P(x,t;u)\ . \tag{2}$$

We further assume that correlations of the process under consideration can appropriately be described by correlation functions of Markov diffusion processes. More precisely, we assume that the process can be written in terms of a Markov diffusion process given by

$$\frac{\partial}{\partial t}P(x,t;u) = -\frac{\partial}{\partial x}D_1'(x,t,u)P(x,t;u) + \frac{\partial^2}{\partial x^2}D_2'(x,t,u)P(x,t;u) \tag{3}$$

with drift and diffusion coefficients

$$D_1'(x,t,u) = D_1(x,P)\ ,\ D_2'(x,t,u) = D_2(x,P)\ , \tag{4}$$

where $P(x,t;u)$ corresponds to the solution of Eq. (2). In this case, we deal with a strongly nonlinear Fokker-Planck equation and the transition probability density of the process under consideration satisfies

$$\begin{aligned}\frac{\partial}{\partial t}P(x,t|x',t';u) = & -\frac{\partial}{\partial x}D_1(x,P(x,t;u))P(x,t|x',t';u) \\ & +\frac{\partial^2}{\partial x^2}D_2(x,P(x,t;u))P(x,t|x',t';u) \ . \end{aligned} \tag{5}$$

For details see [32]. Accordingly, for every initial distribution $u(x)$ the stochastic process is completely defined by a hierarchy of joint probability densities, which reads

$$\begin{aligned} P(x,t;x',t';u) &= P(x,t|x',t';u)P(x',t';u) \ , \\ P(x,t;x',t';x'',t'';u) &= P(x,t|x',t';u)P(x',t'|x'',t'';u)P(x'',t'';u) \\ \cdots & \end{aligned} \tag{6}$$

Alternatively, the process can be described by means of the Ito-Langevin equation

$$\frac{\mathrm{d}}{\mathrm{d}t}X(t) = D_1(x,P)|_{x=X(t)} + \sqrt{D_2(x,P)}\Big|_{x=X(t)} \Gamma(t) \tag{7}$$

involving a Langevin force $\langle \Gamma(t)\Gamma(t')\rangle = 2\delta(t-t')$ [33]. The drift and diffusion coefficients of the Markov diffusion process given by Eqs. (3), (4), and (5) can be determined from experimental data by means of

$$D_1'(x,t,u) = \lim_{\Delta t\to 0} \frac{1}{\Delta t} \left\langle X(t+\Delta t) - X(t)\right\rangle\Big|_{X(t)=x} \tag{8}$$

and

$$D_2'(x,t,u) = \lim_{\Delta t\to 0} \frac{1}{2\Delta t} \left\langle [X(t+\Delta t) - X(t)]^2\right\rangle\Big|_{X(t)=x} \ , \tag{9}$$

see [28–31]. In view of this result, from Eq. (4) it follows that D_1 and D_2 can formally be computed from

$$D_1(x,P) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left\langle X(t+\Delta t) - X(t) \right\rangle \Big|_{X(t)=x} \tag{10}$$

and

$$D_2(x,P) = \lim_{\Delta t \to 0} \frac{1}{2\Delta t} \left\langle [X(t+\Delta t) - X(t)]^2 \right\rangle \Big|_{X(t)=x} \ . \tag{11}$$

Note that Eqs. (10) and (11) can also be explicitly derived from Eq. (5) (see Appendix A).

We consider now the Fokker-Planck equation

$$\frac{\partial}{\partial t} P(x,t;u) = \frac{\partial}{\partial x} P \frac{\partial}{\partial x} \frac{\delta F}{\delta P} \tag{12}$$

involving a free energy functional F [34–39]. We assume that the free energy functional reads

$$F[P] = U_{\mathrm{L}}[P] - Q S_q[P] \ , \tag{13}$$

where U_{L} denotes a linear internal energy functional

$$U_{\mathrm{L}}[P] = \int_{\Omega} U_0(x) P(x) \, \mathrm{d}x \tag{14}$$

and S_q is given by the entropy measure

$$S_q[P] = \begin{cases} \frac{1}{1-q} \int_{\Omega} [P^q - P] \, \mathrm{d}x & : q \neq 1 \\ - \int P \ln P \, \mathrm{d}x & : q = 1 \end{cases} \tag{15}$$

proposed by *Tsallis* [7–9]. For this choice, Eq. (12) becomes

$$\frac{\partial}{\partial t} P(x,t;u) = \frac{\partial}{\partial x} \left[\frac{\mathrm{d}U_0}{\mathrm{d}x} P \right] + Q \frac{\partial^2}{\partial x^2} P^q \ , \tag{16}$$

which is the nonlinear Fokker-Planck equation studied by *Plastino* and *Plastino* [24]. Note that if we put $U_0 = 0$ and $P \propto \rho$, then Eq. (16) recovers the porous medium equation (1). It is clear from Eq. (16) that we have $D_1(x) = -\mathrm{d}U_0/\mathrm{d}x$ and

$$D_2(P) = QP^{q-1} \ , \tag{17}$$

which implies that the Ito-Langevin (7) reads

$$\frac{\mathrm{d}}{\mathrm{d}t}X(t) = -\left.\frac{\mathrm{d}U_0}{\mathrm{d}x}\right|_{x=X(t)} + \left.\sqrt{QP^{q-1}(x,t;u)}\right|_{x=X(t)} \Gamma(t) \tag{18}$$

(see also [40,41]). Recall that for two statistically independent systems the entropy measure (15) satisfies [7]

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B) \ . \tag{19}$$

From Eqs. (16), (18), and (19) we read off that for $q = 1$ we deal with a linear Fokker-Planck equation, a conventional Ito-Langevin equation and an extensive entropy measure. In contrast, for $q \neq 1$ the Fokker-Planck equation is nonlinear with respect to P, we have a self-consistent Ito-Langevin equation, and S_q is nonextensive. Finally, from Eq. (17) it follows that

$$\ln D_2 = \ln Q + (q-1)\ln P \ . \tag{20}$$

Consequently, if we present D_2 and P in a log-log plot, we will obtain a straight line with a slope $\lambda = q - 1$. In other words, the idea is to determine in a first step for several states x_i with $i = 1, \ldots, L$ both the diffusion coefficient $D_2(P)$ (using Eq. (11)) and the probability density P. In a second step, we plot the pairs $(\ln D_2, \ln P)$ for $i = 1, \ldots, L$ as points in the XY-plane and fit a straight line. The slope λ of this line gives us q in terms of $q = 1 + \lambda$.

2.2 Numerics

In line with similar studies on nonlinear Fokker-Planck equations [42–44], we use an Euler forward method to solve Eq. (18) numerically. More precisely, we consider time in steps of Δt like $t = t_0 + n\Delta t$ and compute $X_n = X(t_0 + n\Delta t)$ from

$$\frac{\mathrm{d}}{\mathrm{d}t} X_n = -\Delta t \left.\frac{\mathrm{d}U_0}{\mathrm{d}x}\right|_{x=X_n} + \left.\sqrt{\Delta t Q P^{q-1}(x,t;u)}\right|_{x=X_n} w_n \ , \tag{21}$$

where w_n is a Gaussian distributed random variable with $\langle w_n w_{n'} \rangle = 2\delta_{nn'}$ [33]. At every time step n we compute $l = 1, \ldots, N$ realizations X_n^l and w_n^l of X_n and w_n, respectively. Then, P is obtained from the ensemble average $P(x) = \langle \delta(x - X_n) \rangle$ using a representation $\delta_\epsilon(x)$ of the delta function: $\lim_{\epsilon \to 0} \delta_\epsilon(x) = \delta(x)$. Consequently, we have

$$P(x,t;u) = \frac{1}{N} \sum_{l=1}^{N} \delta_\epsilon(x - X_n^l) \ . \tag{22}$$

in the limit $\epsilon \to 0$ and $N \to \infty$. For example, in previous studies a Gaussian distribution for δ_ϵ has been used [42–44]. Here, we will use a box measure defined by $\delta_\epsilon(x) = 1/(2\epsilon)$ for $|x| \leq \epsilon$ and $\delta_\epsilon(x) = 0$ for $|x| > \epsilon$ (because our programs run much faster with the box measure by comparison to the Gaussian measure). In sum, Eqs. (21) and (22) reduce to the self-consistent Langevin equation (18) in the limit $\Delta t \to 0, \epsilon \to 0, N \to \infty$ (where first the limit $N \to \infty$, then the limit $\epsilon \to 0$, and finally the limit $\Delta t \to 0$ has to be carried out). Therefore, Eqs. (21) and (22) provide us with a good approximation of Eq. (18) if we choose N large and Δt and ϵ small.

2.3 Examples

Generalized Wiener process

We consider a Wiener process in the context of the entropy S_q. That is, we put $U_0 = 0$. At the initial time $t = 0$ the Brownian particle is assumed to be at the origin leading to the initial distribution $u(x) = \delta(x)$. In this case, Eq. (16) admits for exact time-dependent solutions [24,45]. The first moment vanishes. The second moment $M_2(t)$ evolves like [46]

$$M_2(t) = \frac{1}{3q-1}\left[2qQ[z_q]^{(1-q)}\ (1+q)t)\right]^{2/(1+q)} \tag{23}$$

for $q \in (1/3, 1)$ with z_q defined by $z_q = \sqrt{\pi/(1-q)}\Gamma((1+q)/[2(1-q)])/\Gamma(1/[1-q])$ (here Γ denotes the Gamma function and not the Langevin force!). Fig. 1 shows M_2 computed from Eq. (23) and as obtained by solving numerically the Langevin equation (21). Fig. 2 shows D_2 and QP^{q-1} as obtained from the data set produced by Eq. (21). Finally, Fig. 3 shows a log-log plot of the pairs $(\ln D_2, \ln P)$ and a straight line obtained from a least square fit to the data points. The slope $\lambda = q-1$ thus obtained is $\lambda \approx -0.21$ and corresponds nicely to the value $q = 0.80$ that has been used in the simulation.

Insert Figs. 1, 2, and 3 about here.

Generalized Ornstein-Uhlenbeck process

Let us study now an Ornstein-Uhlenbeck process in the context of nonextensive systems described by S_q. In this case, we have a parabolic potential $U_0(x) = \gamma x^2/2$ with $\gamma > 0$. Again, we consider an initial distribution $u(x) = \delta(x)$ and simulate the nonlinear Fokker-Planck equation (16) by means of the Langevin equation (21) for times $t \in [0, t_f]$. Now, the second moment evolves like [46]

$$M_2(t) = \frac{1}{3q-1}\left[\frac{2qQ[z_q]^{(1-q)}}{\gamma}\ (1-\exp\{-(1+q)\gamma t\})\right]^{2/(1+q)} . \tag{24}$$

Fig. 4 shows the evolution of $M_2(t)$ as obtained from Eq. (24) and from the simulation. From the graph $M_2(t)$ it is clear that at $t = t_f$ the stochastic process can be regarded as a stationary process. Figures 5 and 6 show D_2 and QP^{q-1} as well as the graph $\ln P \to \ln D_2$ and the corresponding interpolation line for this stationary case. Here, $\lambda = q - 1$ is found as $\lambda = -0.21$ and is in good agreement with the exact value of $q = 0.80$ used to generate the data. Finally, Fig. 7 depicts the analytical expression of $P_{\rm st}(x)$ versus $P_{\rm st}(x)$ computed from the computer simulation for the stationary case related to Figs. 5 and 6. Note that since we deal with a power-law function, we have depicted $P_{\rm st}$ in a log-normal plot.

Insert Figs. 4,. . . , 7 about here.

3 Conclusion

We have demonstrated how to estimate the nonextensivity parameter q from experimental data. In doing so, we have added a new method to the methods that have been developed so far in order to assess the value of q, see Table 1. In particular, we have shown that the proposed method applies both to the nonstationary and the stationary case.

Insert Table 1 about here.

The method proposed here can also be used to distinguish between linear Fokker-Planck equations exhibiting maximum entropy solutions of S_q [47–49] and the nonlinear Fokker-Planck equation (16). In the former case, the drift and diffusion coefficients do not depend on P. Therefore, in the case of linear Fokker-Planck equations our data analysis method will reveal that the drift and diffusion coefficients are not correlated to the probability density. In contrast, as shown explicitly in our examples, in the case of the nonlinear Plastino-Plastino Fokker-Planck equation there is a simple power-law relationship between the diffusion coefficient and the probability density.

A Direct derivation of Eqs. (10) and (11)

We multiply Eq. (5) with x, integrate with respect to x, and use integration by parts in order to obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left.\langle X(t)\rangle\right|_{X(t')=x'} &= \int_{\Omega} D_1(x,P(x,t;u))P(x,t|x',t';u)\,\mathrm{d}x \\ &= \left.\langle D_1\rangle\right|_{X(t')=x'} \ . \end{aligned} \tag{A.1}$$

Next, we consider the limit $t \to t'$ for which we have $P(x,t|x',t';u) = \delta(x-x')$. Then, we get

$$\frac{\mathrm{d}}{\mathrm{d}t'}\left.\langle X(t')\rangle\right|_{X(t')=x'} = D_1(x',P(x',t';u)) \ . \tag{A.2}$$

From

$$\frac{\mathrm{d}}{\mathrm{d}t'}\left.\langle X(t')\rangle\right|_{X(t')=x'} = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\left.\langle X(t'+\Delta t)-X(t')\rangle\right|_{X(t')=x'} \tag{A.3}$$

and Eq. (A.2) it follows that

$$D_1(x',P) = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\left.\langle X(t'+\Delta t)-X(t')\rangle\right|_{X(t')=x'} \ . \tag{A.4}$$

If we replace t' by t and x' by x, we obtain Eq. (10). Now, let us multiply Eq. (5) with x^2, integrate the result with respect to x, and use integration by parts. Thus, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\left.\left\langle X^2(t)\right\rangle\right|_{X(t')=x'} = 2\left.\langle X(t)D_1\rangle\right|_{X(t')=x'} + 2\left.\langle D_2\rangle\right|_{X(t')=x'} \tag{A.5}$$

and in the limiting case $t \to t'$ we have

$$\frac{\mathrm{d}}{\mathrm{d}t'}\left.\left\langle X^2(t')\right\rangle\right|_{X(t')=x'} = 2x'D_1(x',P(x',t';u)) + 2D_2(x',P(x',t';u)) \ . \tag{A.6}$$

We use Eq. (A.4) to eliminate D_1:

$$\underbrace{\left[\frac{\mathrm{d}}{\mathrm{d}t'}\left\langle X^2(t')\right\rangle - 2x'\frac{\mathrm{d}}{\mathrm{d}t'}\left\langle X(t')\right\rangle\right]_{X(t')=x'}}_{Y} = 2D_2(x', P(x',t';u)) \ . \qquad \text{(A.7)}$$

The squared bracket can be transformed into

$$\begin{aligned} Y &= \lim_{\Delta t\to 0}\frac{1}{\Delta t}\left\langle X^2(t'+\Delta t) - (x')^2 - 2x'[X(t'+\Delta t) - x']\right\rangle\Big|_{X(t')=x'} \\ &= \lim_{\Delta t\to 0}\frac{1}{\Delta t}\left\langle [X(t'+\Delta t) - x']^2\right\rangle\Big|_{X(t')=x'} \\ &= \lim_{\Delta t\to 0}\frac{1}{\Delta t}\left\langle [X(t'+\Delta t) - X(t')]^2\right\rangle\Big|_{X(t')=x'} \ . \end{aligned} \qquad \text{(A.8)}$$

From Eqs. (A.7) and (A.8) we obtain Eq. (11) if we replace t' and x' by t and x.

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Tables:

Table 1

Systems for which methods to determine q have been proposed (FPE=Fokker-Planck equation).

Systems	Ref.
Systems with long range interactions	[10,11]
Chaotic systems on fractal phase spaces	[12,13]
Systems subjected to temperature fluctuations	[14,22,23]
Porous medium equation & Plastino-Plastino FPE	present study

Figure captions:

Fig. 1: Second moment M_2 of a q-generalized Wiener process as a function of time t. Solid line: analytical result given by Eq. (23). Diamonds: M_2 computed from the Langevin equation given by Eqs. (21) and (22) for $U_0 = 0$, $Q = 1$, $q = 0.8$, $\Delta t = 0.1$, and $N = 80000$.

Fig. 2: Comparison of QP^{q-1} (solid line) and D_2 (diamonds) as obtained from a simulation of the Langevin equation given by Eqs. (21) and (22) for the q-generalized Wiener process at $t = 4$. Parameters as in Fig. 1.

Fig. 3: Data points of Fig. 2 plotted as pairs $(x, y) = (\ln P, \ln D_2)$. Least square fit yields a straight line with $y = -0.02 - 0.21x$.

Fig. 4: Second moment M_2 of a q-generalized Ornstein-Uhlenbeck process as a function of time t. Solid line: analytical result given by Eq. (24). Diamonds: M_2 computed from the Langevin equation given by Eqs. (21) and (22) for $U_0 = \gamma x^2/2$, $\gamma = 0.1$, $Q = 1$, $q = 0.8$, $\Delta t = 0.1$, and $N = 80000$.

Fig. 5: Comparison of QP^{q-1} (solid line) and D_2 (diamonds) as obtained from a simulation of the Langevin equation given by Eqs. (21) and (22) for the q-generalized Ornstein-Uhlenbeck process at $t = t_f = 15$. Parameters as in Fig. 4.

Fig. 6: Data points of Fig. 5 plotted as pairs $(x, y) = (\ln P, \ln D_2)$. Least square fit yields a straight line with $y = -0.03 - 0.21x$.

Fig. 7: Distribution $P(x)$ obtained from the data points depicted in Fig. 4) (diamonds) and stationary distribution $P_{\rm st}(x)$ (solid line) computed from Eq. (26) in [46]. Distributions are shown in a log-normal plot.

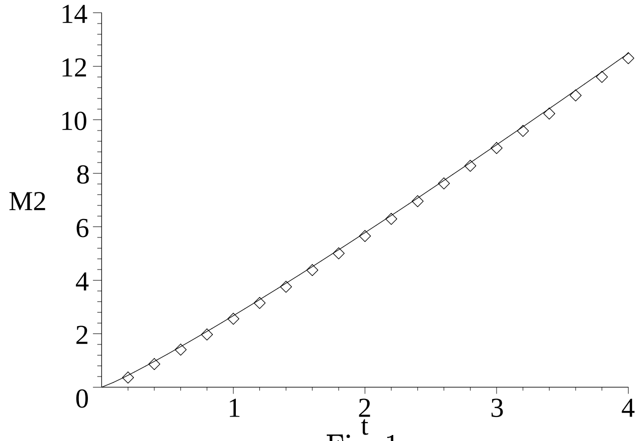

Fig. 1.

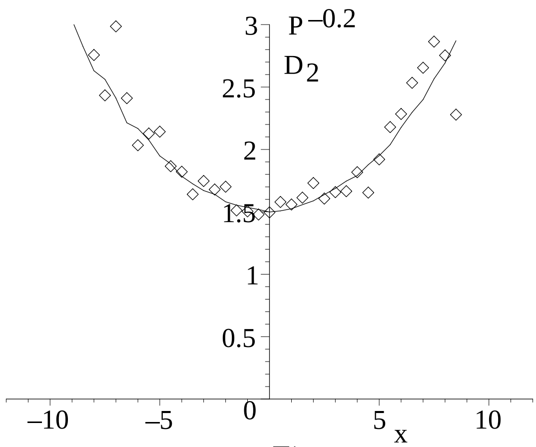

Fig. 2.

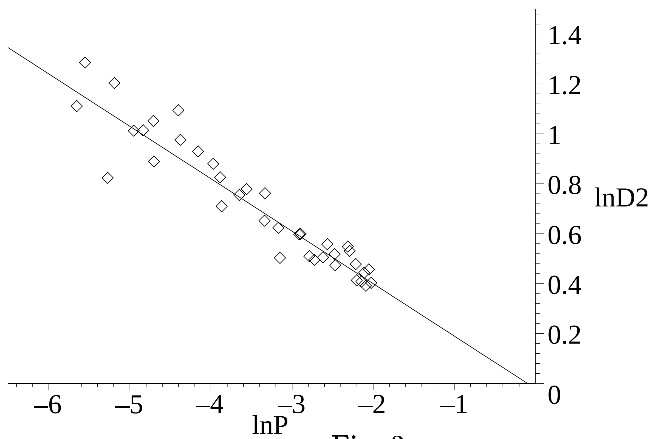

Fig. 3.

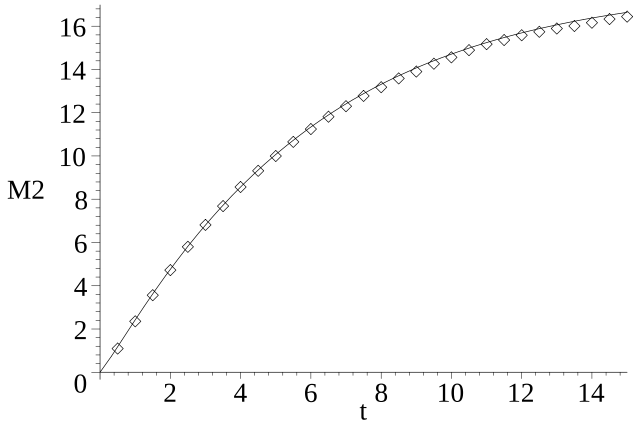

Fig. 4.

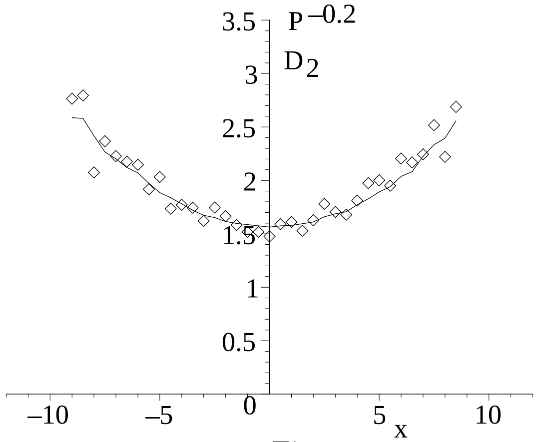

Fig. 5.

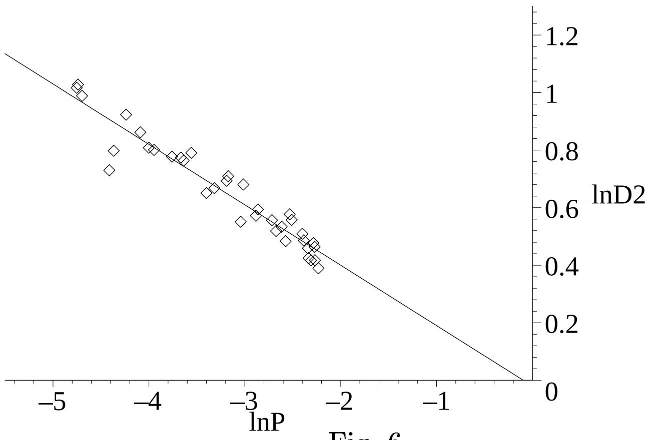

Fig. 6.

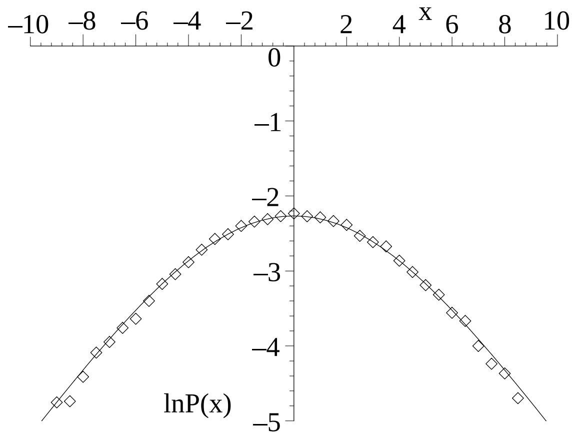

Fig. 7.