Entropy as a measure of diffusion

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Abstract

The time variation of entropy, as an alternative to the variance, is proposed as a measure of the diffusion rate. It is shown that for linear and time-translationally invariant systems having a large-time limit for the density, at large times the entropy tends exponentially to a constant. For systems with no stationary density, at large times the entropy is logarithmic with a coefficient specifying the speed of the diffusion. As an example, the large time behaviors of the entropy and the variance are compared for various types of fractional-derivative diffusions.

PACS numbers: 05.40.-a, 02.50.-r
Keywords: Diffusion Equation, Anomalous Diffusion, Fractional Derivative

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1 Introduction

Diffusion-like processes could be roughly characterized as those processes in which some kind of density evolves so that its width increases with time. But to make this more rigorous, one needs to specify what exactly is meant by width. One choice is the variance, defined as

\[
\text{Var}(X) := \langle X^2 \rangle - \langle X \rangle^2.
\]  

(1)

It is well-known that in ordinary diffusion processes on vector spaces (which are of course unbounded) the variance varies linearly with time. One way to compare other diffusion-like processes is then to calculate the time dependence of the variance, to see whether its large time behavior grows faster or slower than linear time dependence. A group of diffusion-like processes are those called anomalous diffusion, which result in a power-law for the large time dependence of the variance. Investigations of such processes include, for example, [1–7]. There are, however, diffusion-like processes for which the variance is constant or blows up, an example of which is the diffusion-like process in which the time derivative in the ordinary diffusion is substituted with a Weyl fractional derivative. There are also systems for which ordinary variance is not defined. An example is diffusion on a compact space, like a circle or sphere. In a recent article it is shown that for linear diffusion equations which preserve both time-and space-translation invariance, all connected moments are at most linear functions of time [8].

An alternative for the variance as a means of quantifying the diffusion, is the entropy. Unlike the variance, entropy is defined for any density, and the way it grows could be a measure of how fast the diffusion occurs. Here by how fast, it is meant apart from a coefficient which could be absorbed in the definition of time. In [9], entropy has been used to detect scaling properties in the evolution of a one dimensional system.

The aim of this paper is to present the time variation of entropy as an alternative to the time derivative of moments of probability for investigations of diffusion, specially in cases when the moments are not well-defined, as it could happen in some forms of anomalous diffusion.

The scheme of the paper is the following. In section 2 the entropy corresponding to a density is defined. Section 3 is on the time variation of entropy for evolutions corresponding to which there is a stationary density. It is shown there that for linear and time-translationally invariant systems, for large times the entropy tends exponentially to a constant value. Section 4 is on the time variation of entropy for evolutions corresponding to which there is no stationary density. It is shown that for a group of such processes, at large times the entropy behaves like the logarithm of the time, with a coefficient specifying the speed of the diffusion. Some anomalous diffusion processes are investigated using the entropy instead of the variance. It is shown that different types of fractional derivatives with the same index, result in similar large time behaviors for the entropy, while they could result in completely different behavior for the variance. Finally, section 5 is devoted to the concluding remarks.
2 The entropy

Consider a state space the points of which are denoted by \( \mathbf{r} \). The entropy corresponding to the dimensionless density \( \rho \) is denoted by \( S \), and defined as

\[
S(\rho) := -\int dV \rho(\mathbf{r}) \ln[\rho(\mathbf{r})],
\]  
(2)

where integration is over the state space. The state space could be continuous or discrete, in the latter case integration is substituted with a summation. One has

\[
\int dV \rho(\mathbf{r}) = 1.
\]  
(3)

Corresponding to any density \( \rho_0 \) (including the stationary density, if such a thing exists), one defines \( S_{\rho_0} \) as

\[
S_{\rho_0}(\rho) := -\int dV \rho(\mathbf{r}) \ln \left[ \frac{\rho(\mathbf{r})}{\rho_0(\mathbf{r})} \right].
\]  
(4)

The motivation for such a definition is the following. The Shannon entropy for a system of discrete states is

\[
S_1 = -\sum_i p_i \ln p_i,
\]  
(5)

where \( p_i \) is the probability of the state \( i \). As \( p_i \)'s are all nonnegative and less than or equal to one, the above entropy is positive. To write something similar for a system of continuous states, one can divide the space into cells of volume \( \Delta V_i \), and define the entropy like

\[
S_2 = -\sum_i (\rho_i \Delta V_i) \ln(\rho_i \Delta V_i),
\]  
(6)

where \( \rho_i \) is the probability density in the \( i \)'th cell. One would expect to get an exact result, in the limit the cell sizes tend to zero. However, \( S_2 \) tends to (positive) infinity, as the cell sizes tend to zero. Moreover, it does depend on the way the space is divided into cells. One could say that the space can be divided into cells of equal volume \( v \), and a term \( -\ln v \) be subtracted from \( S_2 \), before tending \( v \) to 0, in order to get a finite result for the entropy. The entropy obtained this way, however, is not necessarily positive, as it is the Shannon entropy from which a positive infinite term is subtracted to make it regular. Another point is that the volume of cells does depend on the volume element (or the choice of coordinates). So the choice of cells of equal volume is not unambiguous. One way to define (remove) this unambiguity, is to use a reference density. Suppose the cells are selected so that the probability of each cell with the reference density \( \rho_0 \) is constant:

\[
(\rho_0)_i \Delta V_i = p.
\]  
(7)
One would then have

\[ S_2 = - \sum_i (\rho_i \Delta V_i) \ln \frac{p \rho_i}{(\rho_0)_i}. \]  

(8)

Sending the cell sizes to zero (but maintaining the condition that the probability of cells with regard to \(\rho_0\) be equal) is then equivalent to sending \(p\) to zero. To regularize \(S_2\), in the limit \(p\) tending to zero, one subtracts a constant term \((-\ln p)\) from it:

\[ S'_2 = \ln p - \sum_i (\rho_i \Delta V_i) \ln \frac{p \rho_i}{(\rho_0)_i}. \]  

(9)

The above, in the limit of cell sizes tending to zero, is (4). This entropy differs from \(S_2\) by a constant (infinite), and is no longer positive definite.

As the function \(S\) with \(S(\xi) := -\xi \ln \xi\)

(10)

is concave, \(S(\rho_0)(\rho)\) is negative, unless \(\rho\) is the same as \(\rho_0\). For \(\rho\) slightly different from \(\rho_0\), one has

\[ S_{\rho_0}(\rho) = - \int dV \left[ \rho_0 + (\rho - \rho_0) \right] \ln \left( 1 + \frac{\rho - \rho_0}{\rho_0} \right), \]

\[ = - \int dV \left[ \rho_0 + (\rho - \rho_0) \right] \left[ \frac{\rho - \rho_0}{\rho_0} - \frac{1}{2} \left( \frac{\rho - \rho_0}{\rho_0} \right)^2 \right] + \cdots, \]

\[ = - \int dV \left[ (\rho - \rho_0) + \frac{1}{2} \frac{(\rho - \rho_0)^2}{\rho_0} \right] + \cdots. \]  

(11)

The first order term is zero, as (3) holds for both \(\rho\) and \(\rho_0\). So,

\[ S_{\rho_0}(\rho) = - \frac{1}{2} \int dV \frac{[\rho(r) - \rho_0(r)]^2}{\rho_0(r)}. \]  

(12)

The evolution of entropy with time \((t)\) is, of course, obtained through the time evolution of the density. There are time evolutions for densities, which do have a stationary density; and there are time evolutions for densities, which do not have stationary densities. An example of the first is ordinary diffusion on a compact space. An example of the second is ordinary diffusion on a non-compact space. The large time behavior of the entropy corresponding to these two kinds of evolution is different.

### 3 Time variation if there is a stationary density

If there is a stationary density \(\rho_0\), then as mentioned above, \(S_{\rho_0}\) has a maximum which is attained if the density is the same as the stationary density. For large times, the density \(\rho\) approaches \(\rho_0\), so that one could use (12) for the entropy:

\[ S(t) = - \frac{1}{2} \int dV \frac{[\rho(t, r) - \rho_0(r)]^2}{\rho_0(r)}. \]  

(13)
If the evolution of the density is linear and time-translationally invariant, then
\[ \dot{\rho}(t, \mathbf{r}) = [H(t, \mathbf{r}, \mathbf{D})] \rho(t, \mathbf{r}), \] (14)
where \( \mathbf{D} \) is differentiation with respect to \( \mathbf{r} \), meaning that \([H(t, \mathbf{r}, \mathbf{D})]\) is a differential operator. An example is the simple diffusion, for which \( H \) is the Laplacian, or \((\mathbf{D} \cdot \mathbf{D})\).

For the stationary density \( \rho_0 \),
\[ [H(t, \mathbf{r}, \mathbf{D})] \rho_0(\mathbf{r}) = 0. \] (15)
If the evolution is so that the stationary density is the large-time density, that is, if all initial densities tend to \( \rho_0 \) at large times, and if all of the eigenvalues of \( H \), apart from zero, have real values smaller than a negative value, then
\[ \rho(t, \mathbf{r}) = \rho_0(\mathbf{r}) + \text{Re}[\rho_1(\mathbf{r}) \exp(E_1 t)] + \cdots, \] for large times, (16)
where \( E_1 \) is that eigenvalue of \( H \) which has the largest negative real part, and \( \rho_1 \) is the eigenfunction of \( H \) corresponding to \( E_1 \). One then arrives at
\[ S(t) = -\exp[2 \text{Re}(E_1) t] s_1(t), \] for large times, (17)
where \( s_1(t) \) is a positive constant if \( E_1 \) is real, and an oscillatory nonnegative non-decaying function if \( E_1 \) is not real.

### 3.1 Example: diffusion on compact spaces

The evolution corresponding to ordinary diffusion is
\[ \dot{\rho} = \mathbf{D} \cdot \mathbf{D} \rho. \] (18)
If the state space is compact and boundary-less, the Laplacian operator \( \mathbf{D} \cdot \mathbf{D} \) has a zero eigenvalue corresponding to the eigenfunction \( \rho_0 \), which is a constant function. One can also normalize this constant so that its integral is one. Moreover, the other eigenvalues of Laplacian are negative, so the density approaches \( \rho_0 \) at large times. The behavior of the entropy at large times is then determined by the largest negative eigenvalue of the Laplacian. Examples of such compact spaces are the circle and the (two-dimensional) sphere. One has
\[ E_1 = \begin{cases} -\frac{1}{a^2}, & \text{circle of radius } a \\ -\frac{2}{a^2}, & \text{sphere of radius } a \end{cases}. \] (19)

### 4 Time variation if there is no stationary density

Consider the equation
\[ \dot{\rho}(t, \mathbf{r}) = [H(t, \mathbf{r}, \mathbf{D})] \rho(t, \mathbf{r}). \] (20)
There are cases for which there is some function $f$ so that the solution to the above equation has the property that

$$\det \left[ \frac{\partial f(t, t_0, r)}{\partial r} \right] \rho[t, f(t, t_0, r)] = \rho(t_0, r). \quad (21)$$

This means the points around $r$ at the time $t_0$, go to the region around the point $f(t, t_0, r)$ at the time $t$. The determinant at the left-hand side takes into account the fact that the volume of the region is changing.

For such cases,

$$S(t) = - \int dV \rho(t, r) \ln[\rho(t, r)],$$

$$= - \int dV' \det \left[ \frac{\partial f(t, t_0, r')}{\partial r}(r') \right] \rho[t, f(t, t_0, r')] \ln[\rho[t, f(t, t_0, r')]],$$

$$= - \int dV' \rho(t_0, r') \ln[\rho(t_0, r')] + \int dV' \rho(t_0, r') \ln \left\{ \det \left[ \frac{\partial f(t, t_0, r')}{\partial r} \right] \right\},$$

$$= S(t_0) + \int dV \rho(0, r) \ln \left\{ \det \left[ \frac{\partial f(t, t_0, r)}{\partial r} \right] \right\}, \quad (22)$$

or

$$\dot{S} = \int dV \rho(t, r) D \cdot u(t, r), \quad (23)$$

where $f$ is the flux corresponding to the vector field $u$:

$$\left. \frac{\partial f(t, t_0, r)}{\partial t} \right|_{t=t_0} = u(t, r). \quad (24)$$

But (21) is equivalent to

$$\dot{\rho}(t, r) = -D \cdot [u(t, r) \rho(t, r)]. \quad (25)$$

This corresponds to a deterministic evolution of $r$, through the vector field $u$, and does not involve any diffusion. However, it could happen that for large times, when the density becomes slowly-varying with $r$, equation (21) holds approximately. Consider the following transformations:

$$t \to [\exp(\alpha)] t,$$

$$r \to [\exp(\alpha R)] r,$$

where $\alpha$ is a parameter and $R$ is a constant matrix. If (20) is invariant under this transformation (for large $\alpha$), then one could take $f$ to be

$$f \{ [\exp(\alpha)] t_0, t_0, r \} = \exp(\alpha R) r, \quad (27)$$

so that

$$\left. \frac{\partial f(t, t_0, r)}{\partial r} \right|_{t=t_0} = \exp \left( R \ln \frac{t}{t_0} \right), \quad (28)$$
resulting in
\[ S(t) = S(t_0) + [\text{tr}(R)] \ln \frac{t}{t_0}, \quad (29) \]
or
\[ \dot{S} = \frac{\text{tr}(R)}{t}. \quad (30) \]
Of course these hold for only large times.

4.1 Example: anomalous diffusion with no stationary state

Consider an evolution equation of the form
\[ D_{0(\beta_0)} \rho = [f(D)] \rho, \quad (31) \]
where \( D_{0(\beta_0)} \) is a fractional (time) derivative of order \( \beta_0 \), while \( D \) is the space derivative. \([f(D)]\) itself, could be fractional. Depending on what kind of fractional derivative is used, \( D_{0(\beta_0)} \) could depend on a time. That is, it could be that \( D_{0(\beta_0)} \) is not time invariant. But even if that is the case, for large times that special time is unimportant, and one has
\[ D_{0(\beta_0)} \rightarrow [\exp(-\alpha \beta_0)] D_{0(\beta_0)}, \quad \text{for } t \rightarrow [\exp(\alpha)] t. \quad (32) \]
One also has
\[ D \rightarrow D [\exp(-\alpha R)], \quad \text{for } r \rightarrow [\exp(\alpha R)] r. \quad (33) \]
So, if \( R \) can be chosen so that
\[ f[D \exp(-\alpha R)] = [\exp(-\alpha \beta_0)] f(D), \quad (34) \]
(for large values of \( \alpha \)), then (29) and (30) would hold. As an example, for
\[ D_{0(\beta_0)} \rho = \sum_j a_j D_j(\beta_j) \rho, \quad (35) \]
where \( D_j(\beta_j) \) is some (possibly fractional) differentiation of order \( \beta_j \) with respect to \( r^j \), is is easily seen that the transformation \( R \) satisfying (34) is the following.
\[ R \begin{pmatrix} r^1 \\ \vdots \\ r^n \end{pmatrix} = \begin{pmatrix} (\beta_0/\beta_1)r^1 \\ \vdots \\ (\beta_0/\beta_n)r^n \end{pmatrix}, \quad (36) \]
So that
\[ \dot{S} = \left( \sum_j \frac{1}{\beta_j} \right) \frac{\beta_0}{t}. \quad (37) \]
Normal diffusion corresponds to \( \beta_0 = 1 \) and \( \beta_j = 2 \), resulting in the following large time behavior.
\[ \dot{S} = \frac{d}{2t}, \quad (38) \]
where \( d \) is the dimension of space.

As special cases, consider the followings.
4.1.1 Anomalous diffusion with fractional time derivative

Consider an evolution of the form

$$D_{0(\beta_0)} \rho = D \cdot D \rho,$$

where $D_{0(\beta_0)}$ could be the Caputo or Weyl derivative of order $\beta_0$; see [10, 11], for example. For the Caputo derivative, the variance varies as $t^{\beta_0}$:

$$[\text{Var}^C(r)(t)] = [\text{Var}^C(r)](0) + \frac{2 d t^{\beta_0}}{\Gamma(1 + \beta_0)},$$

where $d$ is the dimension of the space. For the Weyl derivative, the variance is a finite constant for $\beta_0 < 1$; it is divergent at any positive time, for $\beta_0 > 1$; and it varies linearly with time for $\beta_0 = 1$ (ordinary diffusion). For both kinds of derivatives, however, it is seen from (37) that for large times

$$\dot{S} = \frac{\beta_0 d}{2 t},$$

4.1.2 Anomalous diffusion with fractional space derivative

Lévy flight is a stochastic, Markov process, which differ from regular Brownian motion by the occurrence of extremely long jumps the probability distribution of which is heavy-tailed. Lévy flight in continuum limit can be mapped onto the diffusion equation with fractional space derivative. One class of fractional space derivatives is defined as

$$[\mathcal{F}(D_{\beta} \rho)](k) := -|k|^{\beta} [\mathcal{F}(\rho)](k),$$

where $\mathcal{F}$ denotes the Fourier transform, (see [12], for example). If the evolution equation for $\rho$ (on a one-dimensional space) is

$$D_0 \rho = D_{(\beta)} \rho,$$

then the entropy satisfies at large times

$$\dot{S} = \frac{1}{\beta t}.$$

As a special case, consider

$$D_0 \rho = D_{(1)} \rho,$$

which corresponds to a special case of Lévy flights. This results in

$$\rho(t, x) = \int \! dy \frac{t \rho(0, y)}{\pi [t^2 + (y - x)^2]}.$$

For any positive $t$, the variance corresponding to the density $\rho$ diverges. The entropy, however, does not. As both $\beta_0$ and $\beta_1$ are equal to one, the large time behavior of the entropy is

$$\dot{S} = \frac{1}{t}.$$
4.2 Example: anomalous diffusion with fractional space derivative, and a drift

The evolution equation

$$D_0 \rho = D((DU) \rho) + D_\beta \rho,$$

(48)

corresponds to an anomalous diffusion with fractional space derivative, combined with a drift, (12, for example). The drift is the first term on the right hand side, so that the point $x$, apart from a random motion, is subject to a drift governed by

$$(D_0 x)(t) = -(DU)[x(t)].$$

(49)

To investigate the large time behavior of the entropy for such systems, the behavior of the potential $U$ for large values of its variable is needed. Let us assume a power law:

$$U(x) \sim -a |x|^c,$$

for large $|x|$. (50)

Applying the transformations (26) on (48), one arrives at

$$[\exp(-\alpha)] D_0 \rho = \{\exp[(c - 2) R \alpha]\} D[(DU) \rho] + [\exp(-\beta R \alpha)] D_\beta \rho.$$  

(51)

Of course this should hold only for large (positive) $\alpha$ (and with a positive $R$). So one obtains

$$[\min(2 - c, \beta)] R = 1,$$

(52)

where only a positive solution for $R$ is acceptable. If such a solution for $R$ exists, then the large time behavior of the entropy is

$$\dot{S} = \frac{R}{t}.$$  

(53)

It is assumed that $\beta$ is positive. The following cases occur.

i  $c < (2 - \beta)$

It is the diffusion which determines the large time behavior of the system. For large times,

$$\dot{S} = \frac{1}{\beta t}.$$  

(54)

ii  $(2 - \beta) < c < 2$, and $(a c) > 0$

It is the potential which determines the large time behavior of the system. The potential is repulsive, and for large times,

$$\dot{S} = \frac{1}{(2 - c) t}.$$  

(55)

iii  $2 < c$, and $(a c) > 0$

The potential is repulsive, and the evolution blows up at a finite time.
iv. $(2 - \beta) < c$, and $(a c) < 0$

It is the potential which determines the large time behavior of the system. The potential is attractive, and for large times the system tends to a nonzero density, so that the entropy does not grow indefinitely.

5 Concluding remarks

Entropy was introduced as a tool to study how fast the diffusion in a system occurs. It was shown that there are systems for which the evolution of variance is ill-defined, while the entropy and its evolution are well-defined. The long time behavior of the entropy was studied, and it was shown that there are cases where the density tends to a stationary state and the entropy tends exponentially towards its final value, and there are cases where the entropy behaves like the logarithm of time. Some anomalous diffusions were in particular studied, to compare the information obtained from the entropy to that obtained from the variance.

Acknowledgement: This work was supported by the Research Council of the Alzahra University.
References

[1] A. Blumen A, J. Klafter, & G. Zumofen, in “Optical Spectroscopy of Glasses” I. Zschokke (ed.) (Reidel, 1986)

[2] J. P. Bouchaud & A. Georges, Phys. Rep. 195 (1990) 127.

[3] M. F. Shlesinger, G. M. Zaslavsky, & J. Klafter, Nature 363 (1993) 31.

[4] B. D. Hughes, “Random Walks and Random Environments, Vol. 1: Random Walks” (Oxford University Press, 1995).

[5] R. Metzler & J. Kalfet, Phys. Rep. 339 (2000) 1.

[6] R. Metzler & J. Klafter, J. Phys. A37 (2004) 1505.

[7] L. Vlahos, H. Isliker, Y. Kominis, & K. Hizanidis, \[arXiv:0805.0419\].

[8] M. Khorrami, A. Shariati, A. Aghamohammadi, A. H. Fatollahi, Phys. Lett. A376 (2012) 687.

[9] N. Scafetta, & P. Grigolini, Phys. Rev. E66 (2002) 036130.

[10] A. A. Kilbas, H. M. Srivastava, & J. J. Trujillo, “Theory and applications of fractional differential equations”, (Elsevier 2006).

[11] I. Podlubny, “Fractional differential equations”, (Academic Press 1999).

[12] A. V. Chechkin, V. Yu. Gonchar, J. Klafter, R. Metzler, & L. V. Tanatarov, J. Stat. Phys. 115 (2004) 1505.