MaxEnt and dynamical information

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Abstract. The MaxEnt solutions are shown to display a variety of behaviors (beyond the traditional and customary exponential one) if adequate dynamical information is inserted into the concomitant entropic-variational principle. In particular, we show both theoretically and numerically that power laws and power laws with exponential cut-offs emerge as equilibrium densities in proportional and other dynamics.

1 Introduction

The principle of maximum entropy is a fundamental idea of contemporary science. It states that, subject to known constraints, the probability distribution which best represents the current state of knowledge is the one with largest entropy [1–4]. In other words, let some testable information about a probability distribution function be given and consider the set of all trial probability distributions that encode this information. The probability distribution that maximizes the information entropy should be regarded as the optimal probability distribution with respect to the a priori available information. In most practical cases, the testable information is given by a set of conserved quantities (average values of some moment functions), associated with the probability distribution in question. This is the way the maximum entropy principle is most often used in statistical thermodynamics. Another possibility is to prescribe some symmetries of the probability distribution. An equivalence between the conserved quantities and corresponding symmetry groups implies the same level of equivalence for both these two ways of specifying the testable information in the maximum entropy method. The maximum entropy principle is also needed to guarantee the uniqueness and consistency of probability assignments obtained by different methods, statistical mechanics and logical inference in particular. The maximum entropy principle makes explicit our freedom in using different forms of prior information. As a special case, a uniform prior probability density (Laplace’s principle of indifference) may be adopted. Thus, the maximum entropy principle is not just an alternative to the methods of inference of classical statistics, but it is an important conceptual generalization of those methods [4].

In this communication we reveal how to accommodate dynamical information into the principle via a special treatment of the equations of motion that considers proportional and larger-than-proportional dynamics due to their importance in the study of complex systems. Some rather surprising results ensue (power-laws and power-laws with exponential cut-offs [5]) that illustrate the power of the approach.

We demonstrate that taking into account dynamical information within MaxEnt involves adding to the pertinent Hamiltonian new terms and that these resemble the so-called “information cost” lucidly introduced by the authors of reference [6]. In this way we explicitly reconcile two apparent different viewpoints, i.e., that of the growth models of Simon [7] and the information-treatment of Mandelbrot [8], showing that the equilibrium density of a growth process is the one that maximizes the entropy associated to the enlarged Hamiltonian introduced here.

Our presentation is organized as follows: in Section 2 we present the basics of the problem; in Section 3 we describe the theoretical approach finding the equilibrium densities by means of MaxEnt according to the dynamical equation that governs the system at hand; in Section 4 we confirm our findings by means of numerical experiments with random walkers, and we close drawing some conclusions in Section 5.

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2 Preliminary matters

Our system consists of \( n \) abstract “elements” characterized by a given “size”. Let us define

(i) \( n \) as the total number of “elements” one is dealing with;
(ii) \( x_i \) as a positive-definite “size” assigned to the \( i \)th element;
(iii) \( x_0 \) and \( x_M \) as the minimum and maximum possible sizes;
(iv) \( p(x) \) as the relative number of elements with a size given by \( x \);
(v) \( \overline{x} \) as the average-size.

Considering the continuous limit of the distribution \( p(x) \), the conservation of both \( \overline{x} \) and \( n \) guarantees

\[
\int_{x_0}^{x_M} dx p(x) = 1 \quad \text{and} \quad \int_{x_0}^{x_M} dx p(x)x = \overline{x}.
\]

(1)

Our goal here is to find out, via MaxEnt, the explicit form of \( p(x)dx \) from either some simple expectation-values’ constraints or, and this is the novelty, from dynamical information not of that kind.

3 Theoretical approach

3.1 Brownian motion and statistical analogues

We first consider, as a control case, the dynamics behind the evolution of elements of sizes \( x \) via the linear equation:

\[
\dot{x} = k
\]

(2)

where the dot denotes a time derivative, and \( k \) involves the derivative of a Wiener process i.e., \( k_i(t)k_j(t') = K\delta_{ij}\delta(t - t') \), with \( K \) the variance of \( k \). We are in the presence of the well-know Brownian motion, which obeys the diffusion equation

\[
\partial_t p(x, t) = D\partial_x^2 p(x, t),
\]

(3)

with \( D \) the diffusion coefficient and \( p(x, t) \) the non-equilibrium density at instant \( t \). Starting at \( t = 0 \) with a Dirac-delta distribution \( p(x, 0) = \delta(x - x') \), the solution to this equation is a gaussian distribution of the form

\[
p(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x - x')^2}{4Dt}}.
\]

(4)

Without constraints, the system evolves according to this distribution. At this point we introduce our main hypothesis, that will be amply validated below via numerical simulation of the equation of motion’s workings.

**Central hypothesis:** consider an ensemble of elements that evolve with a specified dynamics. If a coordinate can be defined that follows a dynamical equation, like that of (2), for example, the possible equilibrium situations towards which the system may evolve can be obtained via MaxEnt by (i) expressing the entropy in terms of this dynamical coordinate; and (ii) employing appropriate constraints.

The Shannon entropy measure in terms of \( x \) is defined (up to a constant) as

\[
S = -\int_\Omega dx p(x) \log p(x),
\]

(5)

where \( \Omega \) is a “volume” in \( x \)-space defined by the lower and upper limits for the allowed sizes (\( x_0 \) and \( x_M \), respectively: \( x_0 \leq x \leq x_M \)). Accordingly, \( \Omega = x_M - x_0 \).

The simplest scenario. We attempt first to use MaxEnt in the simplest possible instance, with just the normalization constraint. The ensuing variational problem becomes

\[
\delta \left[ S - \mu \int_\Omega dx p(x) \right] = 0,
\]

(6)

where \( \mu \) is the associated Lagrange multiplier. The density that extremizes this quantity is the constant one \( p(x)dx = Z^{-1}dx \) with \( Z = \Omega \) the normalization constant (and also by definition the partition function [4]). Remark on the similarities of this scenario with that of a 1D classical ideal gas, with \( x \) representing the absolute value of a position. Our example also describes an ensemble of non-interacting particles of constant density represented by a gaussian distribution of velocities. We speak here of statistical analogies between our original problem and physical ones.

Adding one additional constraint. In a second scenario we add a constraint on the first moment (the mean value of the sizes) \( \langle x \rangle = \overline{x} \), being thus led to the variational problem

\[
\delta \left[ S - \mu \int_\Omega dx p(x) - \lambda \int_\Omega dx p(x)x \right] = 0,
\]

(7)

where \( \lambda \) is the new associated Lagrange multiplier. The concomitant distribution is the well-know exponential density

\[
p(x)dx = \frac{\exp(-\lambda x)}{Z}.
\]

(8)

Note that \( x_M \) could diverge here, but \( x_0 \) has a lower bound. The constants \( Z \) and \( \Lambda = x_0\lambda \) (defined for convenience) can be obtained according to

\[
Z = x_0 e^{-\Lambda}, \quad \Lambda^{-1} + 1 = \frac{\overline{x}}{x_0}.
\]

(9)

We depict in Figure 1 an arbitrary case for \( x_0 = 1 \), \( n = 100000 \) and \( \overline{x} = 2.5 \) (\( \Lambda = 1/24 \)). Let us assume...
that our constraint is a mean-energy-one. Then, the distribution \( \Omega \) can be associated to a “Hamiltonian” [4]

\[
H = \Lambda x/x_0. \tag{10}
\]

Pursuing our analogy with the physical 1D ideal gas we note that working with a constraint on the mean size is equivalent to dealing with the Hamiltonian of a constant force (the gravitational field comes to mind, with \( x \) representing the height of the particles). Our example is again statistically analogous to a physical one, and thus the equilibrium density (the exponential-one) is the same as that obtained for the air density in a gravitational field. Note in addition that, having a Hamiltonian, it is straightforward to introduce a temperature here by multiplying it by \( \beta = 1/T \). The partition function defined as 

\[
Z = \int dx \exp(-\beta H) \quad \text{(Eq. (9))}
\]

seemingly remains invariant but with a redefined \( \Lambda \) that changes in the fashion \( \Lambda \to \beta \Lambda \).

We have seen that changing constraints we obtain, via MaxEnt, different equilibrium solutions with remarkable statistical analogues.

### 3.2 Geometric Brownian motion: the scale-free ideal gas

It is well-known that some social, physical, and economic systems display a scale-free behavior (see, for instance [9–11], and references therein). Usually, the dynamics related to these systems are described by the geometric Brownian motion (GBM) (also known as exponential Brownian motion). It is used in mathematical finance to model stock prices in the BlackScholes model [12] or in the growth models of Simon [7]. Thus, we attempt now introducing a proportional growth into the orthodox Jaynes-MaxEnt treatment. We start by considering the equation,

\[
\dot{x} = kx \tag{11}
\]

where \( k \) is again indicative of the derivative of a Wiener process. We now proceed to linearize the dynamic equation via the new variable \( u = \log(x/x_0) \) obtaining thereby

\[
\dot{u} = k. \tag{12}
\]

In analogy with the precedent case, we have the usual Brownian motion for this variable \( u \), that obeys a diffusion equation of type (3) with \( u \) instead of \( x \). As for the \( x \) observable one has

\[
\partial_t p(x, t) = D \partial_x (x \partial_x (xp(x, t))) \tag{13}
\]

solved (with an initial Dirac-delta \( p(x, 0) = \delta(x - x' \)) via the log-normal distribution

\[
p(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(\log(x/x')^2)}{4Dt}}. \tag{14}
\]

As in the precedent case, this distribution describes the evolution of the system without constraints.

By recourse to the central hypothesis we assume now that the equilibrium density is that obtained from the MaxEnt approach in terms of the linearized variable \( u \). The Shannon entropy in this variable is written as

\[
S = -\int \Omega du p(u) \log p(u). \tag{15}
\]

The first constraint (normalization) is expressed, as usual, in the fashion

\[
\delta \left[ S - \mu \int \Omega du p(u) \right] = 0, \tag{16}
\]

that yields a constant density for \( u \) as \( p(u)du = Z^{-1}du \), with \( Z = \Omega = \log(x_M/x_0) \). Changing back to the observable \( x = x_0 e^u \) we find

\[
p(x)dx = \frac{1}{Z} \frac{dx}{x} \tag{17}
\]

which follows the density-behavior of the scale-free ideal gas (SFIG), as found before by means of Fisher’s information in references [10,11].

We remind the reader here of Benford’s law (BL) or first-digit law [13,14], which states that, in lists of numbers from many sources of data, the leading digit is distributed in a specific discrete way. It was shown by means of a heuristic derivation in reference [14] that, if a list of numbers follows the rule \( p(x) \sim 1/x \) (and thus Eq. (17)) the first-digit discrete distribution for those numbers mimics BL. Its occurrence is typical of low self-correlated data with no characteristic size, and thus agrees with the SFIG-definition of a non-interacting system with scale invariance. Therefore, the kind of scale-free systems described here obey BL.
We introduce now a second constraint, expressed in terms of $u$ via $(x) = x_0(e^u) = \bar{x}$, so that the Jaynes-MaxEnt extremization problem becomes
\begin{equation}
\delta \left[ S - \mu \int_{\Omega} p(u) du - A \int_{\Omega} p(u)e^u \right] = 0,
\end{equation}
where we have used the definition $A = x_0 \lambda$. We obtain the density $p(u)du = Z^{-1} \exp(-Ae^u)du$. Changing back to the observable $x$ we arrive at
\begin{equation}
p(x)dx = \frac{1}{Z} \exp(-Ax/x_0) dx.
\end{equation}
The pertinent constants are obtained from the constraints in the fashion
\begin{equation}
Z = \Gamma(0, A)
\end{equation}
and
\begin{equation}
\frac{\Gamma(0, A)}{\Gamma(0, \lambda)} = \frac{\bar{x}}{x_0},
\end{equation}
where $\Gamma(a, z)$ is the so-called incomplete Gamma function. This is then the expected equilibrium distribution for a scale-free system, as those encountered in “opinion cluster dynamics” in networks with fixed number of nodes [11]. We display in Figure 2 the present scenario for the same values of $x_0, \bar{x}$ and $\lambda$ as in the preceding section (now with $A = 0.360743$).

Assume again that our constrain is a mean-energy-one. We can associate then to the distribution (19) the effective proportional-growth Hamiltonian [4]
\begin{equation}
H = \lambda x/x_0 + \ln(x/x_0),
\end{equation}
where the new term $\ln(x/x_0)$ is the dynamical counterpart of the information-cost of reference [6].

3.3 q-metric Brownian motion: the generalization to hyper-exponential growth

We now relax the condition of proportional growth and appeal to the more general expression
\begin{equation}
\dot{x} = kx^q,
\end{equation}
where $q$ is a dimension-less parameter. It is easy to see that the two former examples are particular cases corresponding to $q = 0$ (Brownian motion) and $q = 1$ (geometric Brownian motion). We call this new generalization of the dynamics the q-metric Brownian motion. As new tools we need here the concepts of $q$-logarithm and $q$-exponential [15–17]
\begin{equation}
\log_q(x) = \frac{x^{1-q} - 1}{1-q}, \text{ if } x > 0
\end{equation}
\begin{equation}
\exp_q(x) = [1 + (1 - q)x]^{1/(1-q)}, \text{ if } 1 + (1 - q)x > 0,
\end{equation}
so as to proceed to a linearization of the dynamic equation by introduction of the variable
\begin{equation}
u = \log_q(x/x_0).
\end{equation}
One finds in this fashion
\begin{equation}
\dot{u} = k.
\end{equation}
As before, this equation describes a Brownian motion and thus a diffusion equation of type (3) in $u$. The equivalent for $x$ is of the form
\begin{equation}
\partial_t p(x, t) = D \partial_x^2 \left( \exp_q(x) \partial_x (x^q p(x, t)) \right),
\end{equation}
whose solution for an initial Dirac-delta $p(x, 0) = \delta(x - x_0)$ is the $q$-log-normal distribution
\begin{equation}
p(x, t) = \frac{1}{\sqrt{4\pi Dt x_0^q}} \exp\left(-\frac{\left[\log_q(x/x_0) - \log_q(x_0/x_0)\right]^2}{4Dt}\right).
\end{equation}
We keep referring to our central hypothesis and using Shannon’s entropy in terms of $u$ in the MaxEnt approach for finding equilibrium density:
\begin{equation}
S = -\int_{\Omega} p(u) \log p(u).
\end{equation}
The first constraint (normalization) is expressed, as usual, via
\begin{equation}
\delta \left[ S - \mu \int_{\Omega} p(u) \right] = 0,
\end{equation}
which yields a constant density for $u$ as $p(u)du = Z^{-1}du$, with $Z = \int_{\Omega} \log_q(x_0/m) - \log_q(x_0)$. Now, changing to the observable $x = x_0 \exp_q(u)$ we obtain
\begin{equation}
p(x)dx = \frac{1}{Z} dx, \quad x^q,
\end{equation}
i.e., a power law.

We express now the second constraint as $(x) = x_0(\exp_q(u)) = \bar{x}$, writing
\begin{equation}
\delta \left[ S - \mu \int_{\Omega} p(u) - A \int_{\Omega} p(u) \exp_q(u) \right] = 0,
\end{equation}
whose variational solution is the density
\begin{equation}
p(u)du = Z^{-1} \exp(-A \exp_q(u))du.
\end{equation}
Comparing with equation (35) the partition function $Z$ remains invariant save for a redefinition $q \to \beta q$ and $\Lambda \to \beta \Lambda$. Note also that comparing with equation (20) we recover the proportional growth partition function at that special temperature for which $\beta = 1/q$. Thus, by increasing $T$ from zero to $q$ we can cancel out a dynamical behavior via "heating". Interestingly enough, in the limit $\beta \to \infty$ ($T \to 0$) the equilibrium density distribution is $p(x)dx = \delta(x-x_0)dx$, i.e., all elements become placed at the same $x_0$. The absolute entropy vanishes, as it should (third law of thermodynamics).

4 Numerical experiments and results

4.1 Brownian motion

We have proceeded to confirm our theoretical findings by means of numerical experiments, simulating the dynamics of a set of random walkers who move according to the dynamical equations proposed here. As a control case, we start with the linear $q=0$ instance, much employed in molecular dynamics, statistical mechanics, and so on. Our algorithm works as follows:

(i) first we fix the minimum $x_0$, the number of walkers $n$, and the mean value $\bar{x}$. The one generates a vector $x$ with $n$ elements as $x_i = \bar{x}$, $\forall i$, which represents the walkers;

(ii) we randomly select the $i$th walker and generate a new position by discretizing the dynamical equation via $x_i = x_i + k\Delta t$, where $k$ is a gaussian random number with variance $K$ and zero mean, and $\Delta t$ is an arbitrary small time-interval;

(iii) we correct the mean value in a way compatible with the dynamical equation, i.e., linearly. As a general approach one effects the change $\Delta x = x + \Delta$, where $\Delta = \bar{x} - \langle x \rangle$. It is worth mentioning that the computational time is reduced by randomly choosing a second $j$th walker and making it evolve with $x_j = x_j - k\Delta t$, using the same value of $k$ indicated above. We finally accept the changes if, and only if, $\min(x) \geq x_0$;

(iv) we repeat (ii) and (iii) iteratively until achieving convergence in the distribution of $x$.

We display in Figure 4 the diffusion of $n = 100000$ walkers initially peaked at $x = \bar{x} = 2.5$, for different simulation times, at 0.2, 1.5, and 4 Monte-Carlo steps, defining each MC step as $n$ iterations using $K = 1$ and $\Delta t = 10$. We have checked that at first stages of the evolution, when the diffusion is not yet affected by the constraints, the density follows equation (3) as expected. We compare the evolution with the asymptotic equilibrium distribution (also shown in Fig. 1) and depict the convergence of the relative difference of the standard deviation to what is predicted by our MaxEnt treatment, $\epsilon(\sigma) = |\sigma_{\text{MaxEnt}} - \sigma(\tau)|$. As expected, after some steps we finally reproduce the theoretical MaxEnt distribution. We remark on the importance of correcting the positions of the walkers in linear fashion, i.e., respecting the dynamical equation and...
guaranteeing maintenance of the operative constraint at the mean value $\langle x \rangle$.

4.2 Geometric brownian motion

We have proceeded for $q = 1$ in a similar manner as above, with the difference that now there are two equivalent descriptions for the dynamics involved. The algorithm for the first of them is as follows:

(i) we fix the values of $x_0$, $n$, and $\mathcal{X}$. We again generate the walkers as a vector $\mathbf{x}$ with $n$ elements as $x_i = \mathcal{X}$, $\forall i$;

(ii) we randomly select the $i$th walker and generate a new position as $x_i = x_i + k x_i d\tau$;

(iii) we now correct the mean value in a way compatible with the dynamical equation, i.e., proportionally. We change $\mathbf{x}' = \mathbf{x} \Delta$, where now $\Delta = \sqrt[3]{(x_i/\langle x_i \rangle)}$. We accept the changes if, and only if $\min(x) \geq x_0$;

(iv) we repeat (ii) and (iii) iteratively until encountering convergence in the distribution of $\mathbf{x}$.

This algorithm solves explicitly the equation of motion in $x$, which requires a specially small time interval $d\tau$ in order to reduce the error in the discretization of the time derivative. The convergence is achieved after a somewhat large computational effort since $d\tau \ll (\sqrt{\mathcal{X} M})^{-1}$. We highly recommend working with the variable $u = \log(x/x_0)$ to linearize the equations, and apply afterwards the forthcoming algorithm:

(i) we fix the values of $x_0$, $n$, and $\mathcal{X}$ to generate the walkers as a vector $\mathbf{u}$ with $u_i = \log(\mathcal{X}/x_0)$, $\forall i$;

(ii) we randomly select the $i$th walker and generate a new position as $u_i = u_i + k d\tau$;

(iii) we now correct the mean value as $\mathbf{u}' = \mathbf{u} + \Delta$, where now $\Delta = \log[(x_0 \exp(u))]$ — note that we use now the mean value of the exponential. We accept the changes if, and only if $\min(u) \geq 0$;

(iv) we repeat (ii) and (iii) iteratively until reaching convergence in the distribution of $\mathbf{u}$.

It is easy to see that both algorithms are equivalents since $x_i(1+k d\tau) \simeq x_i e^{k d\tau} = e^{u_i+k d\tau}$. We depict in Figure 5 the diffusion of the initial delta distribution at 0.2, 0.8 and 2.5 MC steps using $K = 1$ and $d\tau = 1$ until getting convergence, with the same values for the parameters as in the previous instance. As expected, the diffusion in $u$ at first stages follows equation (3), whereas for $x$ follows equation (14). The final equilibrium distribution follows that predicted by MaxEnt, thus demonstrating the validity of our central hypothesis.

4.3 q-metric brownian motion

We finally describe the algorithm used for the general case, by recourse to the variable $x$:

(i) we fix the values of $x_0$, $n$, and $\mathcal{X}$ to generate the vector $\mathbf{x}$ with $x_i = \mathcal{X}$, $\forall i$;
(ii) we randomly select the ith walker and generate a new position as \( x_i = x_i + k x_i^q d\tau \);

(iii) we now correct the mean value as \( x' = x + x^q \Delta \), where now \( \Delta = (r - \langle r \rangle)/\langle x^q \rangle \), which guarantees obeying the dynamical equation – note that we explicitly recover the previous cases when \( q = 0 \) and \( q = 1 \). We accept the changes if, and only if \( \min(x) \geq x_0 \);

(iv) we repeat (ii) and (iii) iteratively until convergence in the distribution of \( x \).

We again recommend the use of the linearized variable \( u = \log_q(x/x_0) \) via

(i) we fix the values of \( x_0 \), \( n \), and \( r \) to generate the vector \( u \) with \( u_i = \log_q(r/x_0) \), \( \forall i \);

(ii) we randomly select the ith walker and generate a new position as \( u_i = u_i + k d\tau \);

(iii) we now correct the mean value as \( u' = u + \Delta \). Here \( \Delta \) has no analytical expression, and is obtained from the equation \( \langle x_0 \exp_q(u + \Delta) \rangle = r \) using an iterative Newton algorithm, reaching convergence in few steps. We accept the changes if, and only if \( \min(u) \geq 0 \) and \( \max(u) \leq 1/(q-1) \);

(iv) we repeat (ii) and (iii) iteratively until obtaining convergence in the distribution of \( u \).

Using the same parameters as in the previous case, we depict if Figure 6 the diffusion process at 0.1, 0.5, and 2 MC steps for the cases \( q = 1.5 \) and \( q = 2 \) respectively, also showing the convergence of the standard deviation. In a similar fashion to the precedent case at first stages, the diffusion in \( u \) follows equation (3), and for \( x \) follows equation (28). Systematically, the equilibrium densities do follow the predicted distributions found via the MaxEnt in terms of our central hypothesis.

5 Conclusions

It is commonly believed that Jaynes’ MaxEnt (JM), used in conjunction with Shannon’s logarithmic information measure yields, after the concomitant variational process, only exponential probability distribution functions (PDF). This fact was largely responsible for motivating statistical mechanics’ practitioners to look for other information measures [15–17]. We have shown here that great versatility is gained by MaxEnt if some further, appropriate a priori “dynamical” knowledge is added to the JM-technique, a way of proceeding that entirely agrees with Jaynes’ philosophy [1–4]. Indeed, we see that effective Hamiltonians for the process at hand are also a result of the MaxEnt technique.

The JM-procedure can in this fashion still keep Shannon’s measure while at the same yielding almost any functional form for the ensuing variational PDF, power laws in particular.

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Fig. 6. (Color online) Top panels: same as Figure 4 for the \( q = 1.5 \) case at \( \tau = 0.1 \) (blue), 0.5 (green) and 2 (red) MC steps. Bottom panels: \( q = 2 \) case.
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