When do generalized entropies apply? How phase space volume determines entropy

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Abstract – We show how the dependence of phase space volume $\Omega(N)$ on system size $N$ uniquely determines the extensive entropy of a classical system. We give a concise criterion when this entropy is not of Boltzmann-Gibbs type but has to assume a generalized (non-additive) form. We show that generalized entropies can only exist when the dynamically (statistically) relevant fraction of degrees of freedom in the system vanishes in the thermodynamic limit. These are systems where the bulk of the degrees of freedom is frozen and statistically inactive. Systems governed by generalized entropies are therefore systems whose phase space volume effectively collapses to a lower-dimensional “surface”. We illustrate these results in three concrete examples: accelerating random walks, a microcanonical spin system on networks and constrained binomial processes. These examples suggest that a wide class of systems with “surface-dominant” statistics might in fact require generalized entropies, including self-organized critical systems such as sandpiles, anomalous diffusion, and systems with topological defects such as vortices, domains, or instantons.

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Entropy relates the number of states of a system to an extensive quantity, which plays a fundamental role in its thermodynamical description. Extensive means that when two initially isolated systems $A$ and $B$ —with $\Omega_A$ and $\Omega_B$ the respective numbers of states— are brought into contact, the entropy of the combined system $A + B$ is $S(\Omega_{A+B}) = S(\Omega_A) + S(\Omega_B)$. Extensivity is not to be confused with additivity which is the property that $S(\Omega_A\Omega_B) = S(\Omega_A) + S(\Omega_B)$. Both, extensivity and additivity coincide if the number of states in the combined system is $\Omega_{A+B} = \Omega_A\Omega_B$. Clearly, for a non-interacting system Boltzmann-Gibbs (BG) entropy, $S_{BG}[p] = \sum_{i=1}^{\Omega} g_{BG}(p_i)$, with $g_{BG}(x) = -x \ln x$, is simultaneously extensive and additive. By “non-interacting” systems (short-range, ergodic, mixing, Markovian, ...) we mean $\Omega_{A+B} = \Omega_A\Omega_B$. For interacting statistical systems this is in general not true. If phase space is only partly visited this means $\Omega_{A+B} < \Omega_A\Omega_B$. In this case, it may happen that an additive entropy (such as BG) no longer is extensive and vice versa. With the hope to understand interacting statistical systems within a thermodynamical formalism and to ensure extensivity of entropy, the so-called generalized entropies have been introduced which usually assume trace form

$S_{gen}[p] = \sum_{i=1}^{\Omega} g(p_i), \quad (\Omega \text{ is the number of states}), \quad (1)$

where $g(p)$ is some function of $p$. It has been shown that $g$ can not assume any functional form, but generalized entropies of trace form are restricted to the family of functions

$S_{c,d}[p] \propto \sum_{i=1}^{\Omega} \Gamma(d+1, 1-c \log p_i), \quad (2)$

$\Gamma(.,.)$ being the incomplete gamma function, whenever a minimum set of requirements on $g$ holds [1]. These requirements are the first three of the four Shannon-Khinchin (SK) axioms [2,3], SK1: Entropy $S$ depends continuously on $p$ (it is concave; in physical systems this represents the equi-partition principle in microcanonical ensembles), SK2: entropy is maximal for the equi-distribution $p_i = 1/\Omega$ ($g$ is concave; physical systems this represents the equi-partition principle in microcanonical ensembles), SK3: adding a

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zero-probability state to a system, $\Omega + 1$ with $p_{\Omega+1} = 0$, does not change the entropy ($g(0) = 0$), and SK4: the entropy of a system composed of sub-systems $A$ and $B$ equals the entropy of $A$ plus the expectation value of the entropy of $B$, conditional on $A$. If SK1–SK4 hold, the only possible entropy is BG [2,3]. If only SK1–SK3 hold (additivy axiom violated) eq. (2) is the generalized entropy with the constants $(c, d)$ characterizing the universality class of entropy. $(c, d) = (1, 1)$ is the class of BG entropy, $(c, d) = (0, 0)$ is the class of Tsallis entropies. A universality class $(c, d)$ not only characterizes the entropy of the system completely in the thermodynamic limit, it also specifies its distribution functions. Many recently introduced generalized entropic forms appear to be special cases of eq. (2) [1].

The associated distribution functions are

$$E_{c,d}(x) = e^{-\frac{1}{c}W_k(B(\frac{x}{1-x})) - W_k(B)},$$

with $B \equiv \frac{(1-c)r}{1-(1-c)r} \exp\left\{\frac{(1-c)r}{1-(1-c)r}\right\}$, and as one possible choice, $r = (1-c+cd)^{-1}$, [1]. The function $W_k$ is the $k$-th branch of the Lambert-$W$ function, which is a solution of the equation $x = W(x)$ (exp($W(x)$)). Only branch $k = 0$ and branch $k = -1$ have real solutions $W_k$. Branch $k = 0$ is necessary for all classes with $d \geq 0$, branch $k = -1$ for $d < 0$. The generalized logarithm for the entropy, eq. (2), is the inverse of $E = \Lambda^{-1}$. Further properties of systems where SK1–SK3 hold are reported in [4].

It has often been argued that for statistical systems with strong and long-range correlations, Boltzmann-Gibbs statistical mechanics loses its applicability, and that under these circumstances generalized entropies become necessary. This is certainly not true in general. While correlations can be the reason for non-Boltzmann distribution functions, BG entropy often remains the correct extensive entropy of the system [5].

In this paper we clarify the conditions under which BG entropy breaks down as the extensive entropy of a system. For ergodic systems, covering phase space, BG is always valid, regardless of what the correlations in the system might be. This was explicitly shown for binary systems in [5]. It is obvious that the structure of phase space, i.e. Gibbs $\Gamma$-space, is responsible for the Boltzmann-Gibbs framework to collapse and for generalized entropies to become necessary. Here we show that mere non-ergodicity is not enough: for generalized entropies to become necessary, $\Gamma$-space has to collapse in a specific way.

In the following we derive all results in terms of growth of phase space volume as a function of system size. We illustrate our results for binary systems where a graphical representation is possible in terms of decision trees. Binary systems with correlations [6,7] have been studied in the light of generalized entropies in [5,8–11]. On the basis of growth of $\Gamma$-space as a function of the number of states we present a set of concise criteria when generalized entropies are unavoidable and specify them by their universality classes.

What does extensivity mean? Consider a system with $N$ elements. The number of system configurations (microstates) are denoted by $\Omega(N)$, which depends on $N$ in a system-specific way. Extensivity means that entropy is proportional to $N$, i.e. $S_g(\Omega(N)) = \varphi N$. Starting with eq. (1) for equi-distribution, $p_i = 1/\Omega$ (for all $i$), we have $S_g = \sum p_i g(p_i) = \Omega g(1/\Omega)$, the extensivity condition implies

$$\frac{d}{dN} S_g = \Omega' \left( \frac{g(1/\Omega)}{\Omega} \right) = \varphi.$$  \hspace{1cm} (4)

Given the phase space volume as a function of system size we can now directly compute the generalized entropy, i.e. its universality class characterized by $(c, d)$. The primary scaling relation, which applies to all generalized entropies satisfying the first three SK axioms (see [1]),

$$\lim_{x \to 0} g'\left(\frac{\lambda x}{g(x)}\right) = \lambda^c,$$

yields $g'(1/\Omega) = c \Omega g(1/\Omega)$, for large $N$. Using this in eq. (4) gives $\Omega'(1-c)g(1/\Omega) = \varphi$, and the extensivity condition, $\Omega g(1/\Omega) = \varphi N$, leads us to the first component, $c$, of the universality class,

$$\frac{1}{1-c} = \lim_{N \to \infty} N \frac{\Omega'}{\Omega}.$$ \hspace{1cm} (5)

For $d$ we use the secondary scaling relation —which also was proven to be valid for all generalized entropies satisfying the first three SK axioms (see [1]),

$$\lim_{x \to 0} g'\left(\frac{\lambda x}{g(x)}\right) = \lambda^d,$$

Taking the derivative with respect to $a$ on both sides, setting $a \to 0$ and using the extensivity condition we get the second component, $d$, of the university class

$$d = \lim_{N \to \infty} \log \Omega \left( \frac{\Omega}{\Omega'} + c - 1 \right).$$ \hspace{1cm} (6)

By knowing $(c, d)$ we have now uniquely specified the entropy in eq. (2), needed for an extensive system with known phase space volume dependence on system size, $\Omega(N)$.

To see how the number of microstates $\Omega$ is related to the distribution function in an extensive system we take the derivative of $g(1/\Omega) = \Omega^{1/\Omega}$ with respect to $N$, use eq. (5) and use the fact that the derivative of $g$ is the generalized logarithm, $g'(x) = -\Lambda(x)$, to get the asymptotic result $\varphi(N - \Omega'/\Omega') = \Lambda(1/\Omega)$. In terms of the generalized exponential function eq. (3), this is

$$\Omega(N) = \frac{1}{\varphi c N} \exp \left[ \frac{d}{1-c} W_k \left( \frac{(1-c)e^{\frac{1}{cN}}}{cd} \left( \frac{\varphi c N}{r} \right)^{\frac{1}{r}} \right) \right].$$ \hspace{1cm} (7)

Note that for most non-BG systems, i.e. $(c, d) \neq (1, 1)$, the number of states $\Omega(N)$ grows sub-exponentially with $N$. The only super-exponential growth is found at $c = 1$ and $0 < d < 1$.

We now discuss these results in 3 concrete examples.
Example 1, super-diffusion. Consider a one-dimensional accelerating random walk of the following kind: each up-down decision of the random walker is followed by \([N^β]_+\) consecutive steps in the same direction (\(N\) being the total number of steps the walker has taken so far). \([N^β]_+\) means rounded to the next higher integer and \(1 > \beta > 0\). In other words, if after \(N\) timesteps a decision “up or down” is made, the decision will be kept for the next \([N^β]_+ - 1\) steps. At timestep \(N + [N^β]_+\), the next free up-down decision is possible. For example, fix \(\beta = 0.5\). At step \(N = 1\) the random walker decides to go up, \(\omega(1) = 1\). He has to go up for \([N^{0.5}]_+ = 1\) steps. At \(N = 2\) he freely decides to go down \(\omega(2) = -1\). He now has to continue to go down for \([N^{0.5}]_+ = 2\) steps, i.e. \(\omega(3) = \omega(2) = -1\). At \(N = 4\) he can decide again, and so on. After \(N\) steps the walker is at position \(x_β(N) = \sum_{n=1}^{N} \omega(n)\), see fig. 1(a). Let us denote by \(k(N)\) the number of random decisions within the walk up to step \(N\). Clearly, \(k\) grows like \(N^{1-\beta}\), and the number of possible sequences \(\Omega(N) \sim 2^{N^{1-\beta}}\). Consequently the associated extensive entropy (production) is of class \((c,d) = (1, \frac{1}{1-\beta})\). Interestingly the continuum limit of such processes is well defined. By defining the measure \(dW(t) = \lim_{\Delta t \to 0} dt^\alpha \omega((t/df)_)\) with \(\alpha = (1 + \beta)/2\) it is possible to show that for \(W(t) = \int_0^t dW(\tau)\) one gets \((W(t)^2) = t^{2\alpha}\). Since \(2\alpha > 1\) these processes are super-diffusive. Some realizations are shown in fig. 1(b).

Example 2, spin system. Consider an Ising-type spin model (spins up or down) on a growing undirected random network of \(N\) nodes (carrying the spin), connected by \(L\) links (allowing for a spin-spin interaction). Two (anti) parallel spins contribute \(J^+ (J^-)\) to the total system energy \(E\). Let \(\epsilon = E/N\) denote the energy density per node, and \(\mu = -J^+\) the energy cost for a link. \(n^+(-)\) is the number of up (down) spins. Assume the network connectivity \(k = L/N\), to be large enough for reasonable mean-field approximations, then the total energy \(E\) can be estimated by

\[
E = \frac{L}{N(N-1)} \left\{ \begin{array}{ll}
\beta \left( n^+ (n^+ - 1) + n^- (n^- - 1) \right) J^+ + 2 n^+ n^- J^- \right. & + \mu L \nonumber \\
\left. \phi n^+ (N - n^+) \Delta J \right. & 
\end{array} \right.
\]

where \(\Delta J = J^+ - J^-\), and \(\phi = L/N(N - 1)\) is the connectancy of the network. \(2\phi\) is the limit probability in the network. Consequently one finds

\[
n^+ = \frac{N}{2} \left( \sqrt{1 - \frac{2\epsilon}{k\Delta J}} - 1 \right) \sim \frac{\epsilon}{2\phi\Delta J}. \quad (9)
\]

The right-hand side is an approximate solution for \(n^+\) for \(2\epsilon/k\Delta J\) small. Of the two solutions for \(n^+\) of eq. (8) we consider eq. (9) (the other is obtained by exchanging \(n^+\) with \(n^-\)). Fixing the energy \(E\) determines \(n^+\). The number of accessible states \(\Omega\) (microcanonical partition function of the spin system) is the number of ways \(n^+\) up-spins can be distributed over \(N\) nodes, so that \(\Omega = \left(\begin{array}{c} N \\ n^+ \end{array}\right)\). For increasing the size of the network \(N\) extensively one has to keep \(\epsilon\) fixed such that the total energy \(E = Ne\) of the spin-system is extensive. However, networks can grow in various ways. Let us consider the two limiting cases of keeping either the connectivity \(k\) or the connectancy \(\phi\) constant.

i) For \(k = \text{const.}\) eq. (9) gives \(n^+ = \alpha N\) with \(0 < \alpha < 1\) constant. Sterling’s approximation yields \(\Omega = \left(\begin{array}{c} N \\ n^+ \end{array}\right) \sim b^N\) with \(b = a^{-\alpha}(1-a)^{\alpha - 1} > 1\). From eq. (5) we find \(c = 1\) and from eq. (6) \(d = 1\). The extensive entropy of the system is BG, as expected.

ii) For growing constant connectancy networks, i.e. \(\phi = \text{const.}\) during the growth process, we have \(k = \phi N\)
The number of which does not depend on the order of events, but only on the number of events in state \(\varphi_i = 1\) and \(N - n\) events in state \(\varphi_j = 0\). Leibnitz rule (scale invariance) [8] holds if \(\lim_{N \to \infty} \frac{K(N)}{N} = \xi\), where \(\xi \in (0, 1)\), then asymptotically the number of states grows exponentially \((Ω(N) = b^N)\) for some \(b > 0\), and the extensive entropy is BG.

The proof is to show that both, lower and upper bounds for \(Ω(N)\), yield BG. The theorem states that for generalized entropies to exist it is necessary that the sequences are constrained to the situation where either \(\lim_{N \to \infty} \frac{K(N)}{N} = 0\), or \(\lim_{N \to \infty} \frac{K(N)}{N} = 1\). In other words the sequences are asymptotically confined to a region of measure zero around the flanks of the decision triangle, i.e. the boundary of phase space. The theorem has two further implications:

1) In case of probability distributions \(p_N\) which are not totally symmetric in their arguments, generalized entropies can exist even though phase space need not be limited to the boundary of the decision triangle (as in the theorem). If the number of sequences \(\varphi \in \Gamma(N)\) (i.e. the number of free decisions) up to level \(N\) grows sufficiently sub-linearly with \(N\), then the limit-points of sequences may be found along the entire base of the decision triangle (compare Example 1). This means that the multiplicity of sequences with \(k\) out of \(N\) “ones” in the large \(N\) limit grows sufficiently more slowly than the binomial multiplicity for totally symmetric \(p_N\).

2) The theorem can trivially be generalized from binary processes to \(m\)-state systems. This is done by passing from the binomial to a multinomial description.

We now show how different restrictions on phase space lead to various specific generalized entropies. We assume the existence of a critical sequence \(\varphi^{\text{crit}}\) which follows the path \(k^{\text{crit}}(N)\), see fig. 3(a). This means that after \(N\) steps the sequence has produced a maximum of \(k^{\text{crit}}(N)\) “ones”. To the right of this sequence all sequences are
Fig. 3: (Colour on-line) Binary decision trees: (a) Schematic view of allowed sequence regions. If sequences are confined to the shaded regions (left of critical sequence line $k^{\text{crit}}$) the extensive entropy of the system is not BG but a generalized entropy. (b) Maximum line $k^{\text{crit}}$ at which BG entropy starts. Any system containing this line or sequences to the right of it, will be BG. (c) If the region is confined to a strip of size $b$, the extensive entropy is Tsallis entropy, $S_{q,0}$, with $q = 1 - \frac{1}{b}$.

Forbidden. The phase space volume of such systems grows like:

$$\Omega(R)(N) = \sum_{i=1}^{k^{\text{crit}}(N)} \binom{N}{i}.$$  \hspace{1cm} (11)

For any $k$, $\lim_{N \to \infty} \frac{\sum_{i=1}^{k} \binom{N}{i}}{\binom{N}{k}} = 1$, which allows to asymptotically approximate eq. (11)

$$\Omega(R)(N) \approx \binom{N}{k^{\text{crit}}(N)}.$$ \hspace{1cm} (12)

Using Stirling’s formula, taking logs on both sides and keeping terms to leading order we arrive at

$$k^{\text{crit}}(N) \approx N \exp\left[ -W_{-1}\left( \frac{1}{N} \log \Omega(N) \right) \right].$$ \hspace{1cm} (13)

This means that for any system whose sequences are confined to regions left to the critical sequence $k^{\text{crit}}(N)$, generalized entropies as specified in eq. (7) are necessary.

We now discuss specific examples.

**Maximum restricted phase space.** Consider $(c, d) = (1, 1)$, i.e. $\Omega(N) = 2^N$. From eq. (13) we get $k^{\text{crit}}(N) \approx N$. This means that for systems with generalized entropies $k^{\text{crit}}(N)$ grows in a sufficiently sub-linear way with $N$, e.g. $k^{\text{crit}}(N) \propto N^\alpha$ with $0 < \alpha < 1$. If $\alpha = 1$ and $k^{\text{crit}}(N) = \varepsilon N$, no matter how small $\varepsilon > 0$, the system belongs to BG.

**Power-law growth.** For a power-like growth of phase space, $\Omega(N) = N^b$, we have $k^{\text{crit}}(N) \approx N \exp\left[ W_{-1}\left( \frac{b}{b} \log \frac{b}{2} - \frac{b}{b} \log b \right) \right]$. Expanding the Lambert-W function we get $k^{\text{crit}}(N) \approx b \exp\left( -e^\frac{b}{b} \log \frac{b}{2} \right)$, in the large-$N$ limit. The phase space collapse is seen in the decision triangle as a restriction to a strip of width $b$, fig. 3(c). In this case $(c, d) = (1 - \frac{1}{b}, 0)$, i.e. Tsallis entropy applies exactly. This is a well-known result \[8,12\].

**Stretched exponential growth.** For stretched exponential growth $\Omega(N) = \exp(\lambda N^d)$, eq. (13) can be rewritten to $k^{\text{crit}}(N) \approx \log \Omega / W_{-1}[-\log \Omega / N]$ and the Lambert-W term is reasonably approximated by $\log (N / \log \Omega) + \log (\log (N / \log \Omega))$. With this $k^{\text{crit}}(N) \approx \frac{\lambda}{1 - \gamma} N^{\gamma}$, and the entropy is $(c, d) = (1, 1/\gamma)$.

Note that systems with confined areas in their “decision space” as in the above examples are examples for strong memory. The system has to remember how many “ones” have occurred in its trajectories, see examples in [9,10].

**Conclusion.** – Given the knowledge of phase space volume $\Omega$ as a function of system size, we showed how to determine the associated extensive (generalized) entropy by computing the exponents $(c, d)$. We demonstrated that different generalized (non-additive) entropies —i.e. $(c, d) \neq (1, 1)$— correspond to different ways of sub-exponential growth of $\Gamma$-space. We related the growth of phase space volume to the increase of the number of statistically relevant (dynamical) microstates in the system. We found that whenever the fraction of dynamical variables $\frac{N}{\Gamma}$ vanishes for large $N$, $\lim_{N \to \infty} \frac{N}{\Gamma} = 0$, generalized entropies become unavoidable. This extreme confinement of relevant variables to a set of measure zero means that almost all states in the system are the same, or equivalently, the bulk of the degrees of freedom is frozen. In other words, statistically relevant activity happens within a tiny fraction, $\frac{N}{\Gamma}$, of the system. This corresponds to a collapse of phase space volume to some low-dimensional “surface”. While correlations can basically be ruled out as the origin for generalized entropies [5], this is not the case for strong long-range interactions which may cause a collapse of dimensionality of phase space.

We demonstrated in three concrete examples how statistical systems require generalized entropies as their extensive entropy. All three examples are simplifications of more general real-world situations. The constraint binomial process example is a toy model for much more general situations where decisions (binary or multinomial) are path dependent and the space for decisions becomes more constrained over time. The case of the accelerated random walk corresponds to a situation where the density of decisions decreases with time. This is again a model for a system that becomes more and more constrained as it evolves. It is possible to show that in the continuum limit this process is statistically equivalent to ordinary diffusion with a diffusion constant changing over time. Finally, the example of the spin system can be conceptualized in a social setting: imagine that there is a club where you become a new member. It is expected that you become familiar with a certain percentage of the members of the club, you become part of the club’s friendship network. People in the club (the nodes in the network) are opinionated and have a binary opinion on a theme, yes or no. The opinion of your new friends influences your own opinion in an Ising-like fashion. By adding new members to the club more and more constraints on the individuals’ opinion formation are created, and the dynamics (with a given “energy”) within the two forming opinion clusters is freezing out. The only opinion flips occurring happen on the
“surface” defined by those members who have the same number of “yes” and “no” friends.

Considering the relevance of “surface-dominant” statistics in systems of the above kind, one might be tempted to hypothesize that generalized entropies should be relevant for physical systems exhibiting such “surface effects”, including the following:

Self-organized critical systems. In a sandpile consider discrete sites where sand grains can be. The (binary) state of a site is being occupied by a grain or not. In a sandpile the bulk of the system is occupied and just the surface of the pile contains its statistically relevant degrees of freedom. The trajectory of a sand grain in a classical sandpile model follows sequences much alike those in the decision tree, fig. 3(c).

Spin systems with dense topological defects. such as spin-domains, vortices, instantons, caging, etc. If these meta-structures bind a vast majority of spins into (metastable) mesoscopic “objects”, the remaining spins—not belonging to these structures— can move freely only in surface-like regions between these objects.

Anomalous diffusion. The presented results could also apply whenever states of a statistical system are excluded by the presence of other materials restricting mobility in Euclidean space. Think, e.g., of diffusion in porous media where statistically relevant action takes place on restricted surface-like areas, and not in full 3D.

For non-commutative variables alternative routes to generalized entropies may exist [13,14].

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