The maximum relative entropy principle

Jayanth R. Banavar\textsuperscript{1} and Amos Maritan\textsuperscript{2}
\textsuperscript{1}Department of Physics, The Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802
\textsuperscript{2}Dipartimento di Fisica “G. Galilei,” Università di Padova, CNISM, via Marzolo 8, 35131 Padova, Italy

We show that the naive application of the maximum entropy principle can yield answers which depend on the level of description, i.e. the result is not invariant under coarse-graining. We demonstrate that the correct approach, even for discrete systems, requires maximization of the relative entropy with a suitable reference probability, which in some instances can be deduced from the symmetry properties of the dynamics. We present simple illustrations of this crucial yet surprising feature in examples of classical and quantum statistical mechanics, as well as in the field of ecology.

PACS numbers: 02.50.Cw,05.90.+m,87.23.Cc

There are numerous situations in the natural and social sciences, medicine, and business which can be described at different levels of detail in terms of probability distributions. Such descriptions arise either intrinsically as in quantum mechanics, or because of the vast amount of details necessary for a complete description as, for example, in Brownian motion and in many body systems. Variational methods can be used for constructing an estimate both complex equilibrium and non-equilibrium systems.

The maximum entropy principle: Consider the maximization of the entropy \[ H(P) = -\sum_c P(C) \ln P(C), \] where \( P(C) \) is the probability that a certain event \( C \) occurs subject to the constraints:

\[ \langle Q_r \rangle = \sum_c P(C)Q_r(C) = \bar{Q}_r \quad r = 0, 1, 2, ..., \] where the \( r \)-th constraint requires that the mean value of a quantity \( Q_r \) is equal to \( \bar{Q}_r \). The entropy is reduced as a result of the partial knowledge encoded in \( Q_r \). The entropy maximization principle arises from the observation that the entropy must be the highest possible that includes the available information, because a lower entropy would imply that more information has been incorporated than is available. Using Lagrange multipliers, \( \lambda_r \), to impose the constraints, one seeks to maximize

\[ -\sum_c P(C) \ln P(C) - \sum_r \lambda_r Q_r(C). \] The general solution is found to be

\[ P(C) = e^{-\sum_r \lambda_r Q_r(C)}, \]

where the \( \lambda \)'s have to be determined in order to satisfy the constraints [2]. In order to illustrate the potential problems associated with a naive application of the maximum entropy principle, we begin with a simple classical example.

Application of the maximum entropy principle to classical statistical mechanics – derivation of Boltzmann statistics: Consider a canonical ensemble of \( N \) non-interacting particles that can occupy discrete, non-degenerate energy levels (the extension to the degenerate case is straightforward but results in more cumbersome equations) having an energy \( \epsilon_j \), with \( j = 1, 2, 3, ... \). We impose an energy constraint: \( Q_1 = \sum_j n_j \epsilon_j = E \), where \( n_j \) is the number of particles in level \( j \) and \( \langle \cdot \rangle \) denotes the average value. The temperature is a measure of the average total energy. The goal is to determine the probability, \( P \), of observing a given distribution of particles among the levels subject to a constraint on the average total energy. For the classical case, the particles are distinguishable, the identities of the particles are known and the energy level occupied by the \( \alpha \)-th particle can be indicated by \( i_\alpha \), \( \alpha = 1, N \). A straightforward application of the maximum entropy principle yields the well-known Boltzmann result: the probability of observing the particle configuration \( i \)

\[ P_B(1) \propto e^{-\beta \sum_{\alpha=1,N} \sum_j \delta_{j,i_\alpha} \epsilon_j}, \]

where \( i \) denotes the event in which particle 1 is in level \( i_1 \), particle 2 is in level \( i_2 \), and so on, the Lagrange parame-
ter \( \beta \) is proportional to the inverse temperature and the subscript \( B \) stands for Boltzmann. In a coarse-grained description \cite{22}, in which one keeps track of just the number of particles in each level (the occupation number representation), the relevant event is \( n \), where \( n_j \) is the number of particles in level 1, \( n_2 \) is the number of particles in level 2, and so on, without regard to their identity. Within the \( n \) description and starting from Eq. \cite{5}, one obtains for the probability, \( P'_B(n) \), of the event \( n \)

\[
P'_B(n) \propto \frac{1}{\prod_j n_j!} e^{-\beta \sum_i n_i \epsilon_i},
\]

where the prime superscript denotes that the result has been obtained on coarse-graining.

**Quantum statistics and a puzzle:** The surprising feature of the maximum entropy principle is that its direct application to the quantity \( P(n) \) yields a result different from applying the maximum entropy principle to \( P(1) \) and then coarse-graining the result to obtain \( P(n) \). One obtains instead the celebrated Bose-Einstein distribution:

\[
P_{BE}(n) \propto e^{-\beta \sum_i n_i \epsilon_i}, \quad n_j = 0, 1, 2, \ldots
\]

On constraining \( n_j = 0, 1 \) for all \( j \) one gets the Fermi-Dirac statistics. This result is pleasing because the \( n \) representation is in fact the appropriate one for deriving quantum statistics. The particles are indistinguishable and all the information that one has is encapsulated by \( P(n) \). The conundrum is that the results obtained by applying the maximum entropy principle to \( P(1) \) and then coarse-graining the result to obtain \( P(n) \) is different from applying the maximum entropy principle directly to \( P(n) \). In other words, the operations of maximizing the entropy and of coarse-graining do not commute.

**Relative entropy and resolution of the puzzle:** We suggest that the correct and consistent application of the maximum entropy principle entails the maximization of the relative entropy \cite{24} instead of the Shannon entropy in Eq. \cite{4} subject again to the constraints obtained from partial knowledge that one has about the system. The relative entropy of \( P \) with respect to \( P_0 \) is defined as

\[
\mathcal{H}(P|P_0) = -\sum_C P(C) \ln \frac{P(C)}{P_0(C)},
\]

where the new term in the denominator \( P_0(C) \) is a reference term. Such a reference term has been discussed in the literature in the different context of going from a discrete to a continuous system and is “proportional to the limiting density of discrete points” \cite{2}, where it is needed for dimensional reasons. The reference term is, however, not commonly invoked as an essential ingredient in the discrete case. It has been shown by Shore and Johnson \cite{3} that “given a continuous prior density and new constraints, there is only one posterior density satisfying these constraints that can be chosen by a procedure that satisfies the axioms”. The unique posterior can be obtained by maximizing the relative entropy and the axioms pertain to uniqueness, invariance, system independence and subset independence. If \( P_0(C) \) can be chosen to be a constant or simply equal to 1, Eq. \cite{8} becomes equivalent to Eq. \cite{11}. Due to the convexity of the function \( x \ln x \), the relative entropy is never positive and it reaches its maximum value of zero when \( P = P_0 \).

In the absence of any constraint, the maximization of the relative entropy leads to the result \( P(C) = P_0(C) \).

If the space of events is coarse grained, i.e. it is partitioned into subsets \( C' \), which are pair disjoined, representing collections of events in \( C \), then the relative entropy is given by

\[
\mathcal{H}(P'|P'_0) = -\sum_{C'} P'(C') \ln \frac{P'(C')}{P'_0(C')}
\]

where the reference term \( P'_0(C') \) is obtained straightforwardly by coarse-graining \( P_0(C) \) as

\[
P'_0(C') = \sum_{C \subset C'} P_0(C).
\]

If the constraints Eq. \cite{2} are functions only of \( C' \) then the relative entropy maximization commutes with the operation of coarse graining and one obtains

\[
P'(C') = P'_0(C') e^{-\sum_r \lambda_r Q_r(C')},
\]

In the derivation of Eq. \cite{5}, it was implicitly assumed that \( P_{0,B}(i) = 1 \). On coarse-graining to a description involving the variable \( n \), Eq. \cite{10} leads to \( P'_{0,B}(n) = N! / \prod_j n_j! \) yielding once again the standard Boltzmann distribution, Eq. \cite{9}. If, instead, one assumes that \( P'_{0,BE}(n) = 1 \) then one derives the Bose Einstein distribution, Eq. \cite{7}.

**Role of system dynamics:** The success of the principle of maximum entropy hinges on the choice of the reference probability, \( P_0 \), and the identification of the correct constraints not encapsulated in \( P_0 \). In the statistical mechanics examples studied above, the constraint is imposed by fixing the average energy while the choice of \( P_0 \) is guided by the postulate that all states are \( a \) priori equally probable when one works at the finest level of description for the system being studied. Of course, this follows from the dynamics of the system.

Consider the dynamics, in terms of a Markov process, in the occupation number representation. If the transition rate, \( W^{quantum}(n_j \rightarrow n_j + 1) \)
(\(W^{\text{quantum}}(n_j \rightarrow n_j - 1)\)) is proportional to \(n_j + 1\) \((n_j)\) then, in the stationary state, \(P_{0, BB}(n) = \text{constant}\) in agreement with the implicit choice made for the Bose-Einstein case, Eq. (7). These transition rates follows from the symmetry of the quantum wave function describing indistinguishable particles [25]. For classical (distinguishable) particles, the transition rate \(W^{\text{classical}}(n_j \rightarrow n_j + 1)\) is simply constant whereas the transition rate \(W^{\text{classical}}(n_j \rightarrow n_j - 1)\) is proportional to \(n_j\). In the stationary state, \(P_{0, B}(n)\) is proportional to \(1/\prod_j n_j!\), which, when used as the reference probability, correctly leads to Eq. (8). At the description level \(i\), this is equivalent to \(P_{0, B}(i) = \text{constant}\).

**An ecology application:** A fundamental quantity in ecology is the probability distribution of the species abundance, i.e. the probability, \(P_{\text{ECO}}(n)\), that the first species has a population \(n_1\), the second species, \(n_2\) and so on. As an illustration, consider the simple symmetric case in which all species are demographically equivalent [20] and are governed by similar death and birth rates. The direct application of the maximum entropy principle without the appropriate non-trivial reference term and with the constraint that the average population, \(\langle \sum n_j \rangle\), is fixed yields a simple exponential form for the species abundance

\[
P_{\text{ECO}}(n) \propto e^{-\beta \sum n_j}
\]

(12)

The relative species abundance (RSA), \(P^{(k)}_{\text{RSA}}(n) \equiv \langle \delta_{n,n_k} \rangle\), the probability that the \(k\)-th species has population \(n\), is thus proportional to \(e^{-\beta n}\).

In order to choose the reference entropy, we turn to the dynamics as a guide. Consider a Markov process with transition rates \(W^{\text{eco}}(n_j \rightarrow n_j \pm 1) = n_j + c\) where \(c\) is a constant term that, for simplicity, is species independent. When \(c = 0\), one has a simple birth-death process, whose rate is proportional to the number of individuals of a given species. A non-zero value of \(c\) introduces density dependence in the birth and death rates with a positive value of \(c\) corresponding to a rare-species advantage [27]. The stationary state corresponding to these dynamics provides a measure of the reference probability \(P_{0, \text{ECO}}(n) \propto \prod_j 1/(n_j + c)\). On applying the principle of maximum relative entropy with this reference probability, we find

\[
P_{\text{ECO}}(n) \propto \prod_j e^{-\beta n_j} n_j + c
\]

(13)

instead of Eq. (12). This leads to a \(P^{(k)}_{\text{RSA}}(n) \propto \exp(-\beta n)/\langle n \rangle\). When \(c = 0\) we obtain the celebrated Fisher log series [28]. This result can also be obtained from the standard application of the principle of maximum entropy by imposing a constraint on the average value of \(\ln n\), a constraint with no ecological basis. When \(c\) is positive, one obtains the result derived using a density dependent neutral approach [27] which fits the RSA data of several tropical forests fairly well. The Fisher log-series has a simple physical interpretation: the \(e^{-\beta n}\) term results from the constraint on the average population whereas the \(1/n\) factor follows from the dynamics. The characteristic time scale of a birth or death event is inversely proportional to \(n\), the number of individuals in a given species – each individual is a candidate for dying or for giving birth. The \(c\) correction arises straightforwardly from density dependence in the birth and/or death rates.

**Summary:** The maximum entropy principle is an inference technique for constructing an estimate of a probability distribution using available information. We suggest that, in order to guarantee that the results do not depend on the description level, one ought to maximize the relative entropy subject to the known constraints. This provides a natural interpretation of the relative entropy [24] in the context of statistical mechanics. In order to be successful, the method requires knowledge of the reference probability, which, in turn, depends on the system dynamics. Alternatively [6], one could maximize the ordinary entropy \(H(P)\), Eq. (1), and continue to add additional constraints until one obtains the correct \(P\). In order to obtain the correct answer, in the absence of the reference entropy, one requires the knowledge of which optimal constraints to use (e. g. the constraint on the average value of \(\ln n\) in the ecology illustration) or the use of a large enough number of constraints [6] to ensure convergence. Unfortunately, in general, there is no a priori guarantee that either of these approaches will be successful.

**Acknowledgements** We are indebted to Sandro Azaele, Roderick Dewar, John Harte, Flavio Seno, Antonio Trovato, and Igor Volkov for insightful discussions. This work was supported by COFIN 2005 and NSF grant DEB-0346488.

[1] Boltzmann L., Lectures on Gas Theory Cambridge University Press, London (1964).
[2] Shannon C. E., Bell Syst. Tech. J. 27, 379-423 (1948).
[3] Jaynes E. T., Phys. Rev. 106, 620-630 (1957).
[4] Jaynes E. T., Phys. Rev. 108, 171-190 (1957).
[5] Shore J. E., Johnson R. W., IEEE Trans. on Inform. Theory IT-26, 26-37 (1980).
[6] Mead L. R., Papanicolaou N., J. Math. Phys. 25, 2408 (1984).
[7] Jaynes E. T., Probability theory, Cambridge University Press, London (2003); P. 375.
[8] Dewar R. C., J. Phys. A 36, 631-641 (2003).
[9] Dewar R. C., J. Phys. A 38, L371-L381 (2005).
[10] Whitfield J., Nature **436**, 905-907 (2005).

[11] Skilling J., Bryan R. K., *Monthly notices of the Royal Astronom. Soc.* **211**, 111-114 (1984).

[12] Delaglio F., Grzesiek S., Vuister G. W., Zhu G., Pfeifer, J. and Bax A., *Jour. of Biomolecular NMR* **6**, 277-293 (1995).

[13] Ulrych T. J. and Bishop T. N., *Rev. Geophys.* **13**, 183-200 (1975).

[14] Shipley B., Vile D., Garnier E., *Science* **314**, 812-814 (2006).

[15] Werner J. H., Joggerst R., Dyer R. B., Goodwin P. M., *Proc. Natl. Acad. Sci. USA* **103**, 11130-11135 (2006).

[16] Sibisi S., Skilling J., Bereton R. G., Laue E. D., Staunton J., *Nature* **311**, 446-447 (1984).

[17] Kitaura R., Kitagawa S., Kubota Y. et al., *Science* **298**, 2358-2361 (2002).

[18] Kiessling M. K. H., Neukirch T., *Proc. Natl. Acad. Sci. USA* **100**, 1510-1514 (2003).

[19] Rabani E., Reichman D. R., Krilov G., Berne B. J., *Proc. Natl. Acad. Sci. USA* **99**, 1129-1133 (2002).

[20] Turkington B., Majda A., Haven K., DiBattista M., *Proc. Natl. Acad. Sci. USA* **98**, 12346-12350 (2001).

[21] Dong W., Baird T., Fryer J. R. et al., *Nature* **355**, 605-609 (1992).

[22] Schneidman E., Berry M. J., Segev R, Bialek W. *Nature* **440**, 1007-1012 (2006).

[23] Tseng C. -Y., Caticha A., in *Bayesian Inference and Maximum Entropy Methods in Science and Engineering* ed. by Fry R. L., A.I.P. Conf. Proc. Vol. 617, p. 331 (2002).

[24] Kullback S., *Information Theory and Statistics*, Wiley, New York (1959).

[25] Ashby N., Miller, S. C., *Principles of Modern Physics*, Holden-Day Inc., San Francisco (1970).

[26] Hubbell S. P., *The unified neutral theory of biodiversity and biogeography*, Princeton University Press, Princeton (2001).

[27] Volkov I., Banavar J. R., He F., Hubbell S. P., Maritan A., *Nature* **438**, 658-661 (2005).

[28] Fisher R. A., Corbet A. S., Williams C. B., *J. Anim. Ecol.* **12**, 42-58 (1943).