Parameter estimation in nonextensive thermostatistics

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Equilibrium statistical physics is considered from the point of view of statistical estimation theory. This involves the notions of statistical model, of estimators, and of exponential family. A useful property of the latter is the existence of identities, obtained by taking derivatives of the logarithm of the partition sum. It is shown that these identities still exist for models belonging to generalised exponential families, in which case they involve escort probability distributions. The percolation model serves as an example. A previously known identity is derived. It relates the average number of sites belonging to the finite cluster at the origin, the average number of perimeter sites, and the derivative of the order parameter.

I. INTRODUCTION

Central to this paper is the notion of escort probability distribution. It was introduced in non-extensive thermostatistics [1] on heuristic grounds. The notion has been generalised in [2], where it was shown that the definition of exponential family can be generalised by considering pairs of probability distributions, one of which is called the escort of the other. The probability distributions of nonextensive thermostatistics then belong to generalised exponential families.

The example used in the present paper is that of the site percolation problem. Percolation theory is a well-established domain of statistical physics [3]. The number of publications in this domain is vast. It is not the intention of the present work to make progress in understanding percolation but rather to show that the notions of escort probabilities and of generalised exponential family in a natural way fit in and lead to an interesting result.

The next two sections relate equilibrium statistical physics to estimation theory and recall well-known material such as the definition of the exponential family. In Section 4, the definition of escort probability distribution is given. It is used in subsequent sections to recall the generalised lower bound of Cramer and Rao and the definition of generalised exponential families. Section 7 shows that for any generalised exponential family one can derive identities, as many as there are model parameters. Sections 8 and 9 treat the example of percolation. The final Section 10 contains a short discussion.

II. PARAMETER ESTIMATION IN STATISTICAL PHYSICS

In first instance, statistical physics studies statistical properties of model systems. Hence, the mathematical theory of parameter estimation can be applied. In this theory, the average value of one or more quantities, called estimators, is used to estimate parameters of the model. Here, these quantities are called Hamiltonians because, quite often in statistical physics, one of the parameters of the model is inverse temperature $\beta$ and because energy, which is the average value of the Hamiltonian, is used to estimate temperature.

More formally, a model consists of a probability distribution $p_\theta$, which depends on some parameters $\theta_1, \theta_2, \ldots, \theta_n$, and a set of Hamiltonians $H_1, H_2, \ldots, H_n$, which can be used to estimate the value of the parameters. In statistical physics all these Hamiltonians are added up to form a single Hamiltonian $H$. This is not done here for simplicity of notations. Let us illustrate this point. The Hamiltonian of the $d = 1$-Ising model is

$$H = -J \sum_{m=1}^{n-1} \sigma_m \sigma_{m+1} - h \sum_{m=1}^{n} \sigma_m. \quad (1)$$

The variables $\sigma_m$ can take on the values $\pm 1$. The probability distribution of the model is

$$p(\sigma) = \frac{1}{Z} \exp(-\beta H) \quad \text{with} \quad Z = \sum_{\sigma} \exp(-\beta H). \quad (2)$$

The parameters of the model are inverse temperature $\beta > 0$ and external field $h$. However, it is convenient to introduce
new parameters $\theta_1 = \beta$ and $\theta_2 = \beta h$, and corresponding Hamiltonians

$$
H_1(\sigma) = -J \sum_{m=1}^{n-1} \sigma_m \sigma_{m+1} \quad \text{and} \quad H_2(\sigma) = -\sum_{m=1}^{n} \sigma_m.
$$

(3)

Then, using Einstein’s summation convention, the probability distribution can be written as

$$
p(\sigma) = \frac{1}{Z} \exp(-\theta^k H_k(\sigma)).
$$

(4)

### III. EXPONENTIAL FAMILY

A parametrised probability distribution $p_\theta(i)$ belongs to the exponential family if it can be written into the form

$$
p_\theta(i) = c(i) e^{G(\theta) - \theta^k H_k(i)}.
$$

(5)

The function $G(\theta)$ is determined by the normalisation condition and is given by

$$
G(\theta) = -\ln \sum_i c(i) e^{-\theta^k H_k(i)}.
$$

(6)

In the present paper, the variables $H_k$ are called Hamiltonians. At first sight one might think that every non-vanishing probability can be written in exponential form. However, the variables $c$ and $H_k$ in (5) must not depend on the parameters $\theta^k$. This poses a rather strong condition, which is not always satisfied. An example of a distribution not belonging to the exponential family is

$$
p_\alpha(i) = \frac{1}{Z(\alpha)} \frac{1}{\alpha^2 + i^2} \quad \text{with} \quad Z(\alpha) = \sum_{i=0}^{\infty} \frac{1}{\alpha^2 + i^2}.
$$

(7)

Of course, the Ising model belongs to the exponential family with two parameters.

### IV. ESCORT DISTRIBUTIONS

Given a model with probability distribution $p_\theta(i)$, any other probability distribution $P_\theta(i)$, depending on the same parameters, is an escort distribution for the given $p_\theta(i)$. However, of interest are pairs of distributions $p_\theta(i), P_\theta(i)$ which satisfy some special relation. In [2] the well-known inequality of Cramer and Rao was generalised to pairs of probability distributions and a sufficient condition was given that, when satisfied, makes the inequality optimal. The usual inequality of Cramer and Rao is optimal in case of a distribution belonging to the exponential family. Hence it is natural to say that escort probabilities, optimising the generalised version of the inequality of Cramer and Rao, generalise the notion of exponential family. This statement is elaborated in the next section.

The concept of escort probability distributions is borrowed from the theory of fractals, see [4]. It goes back to the thermodynamical analysis [2] of multifractals [6], now twenty years ago.

Given a probability distribution $p(i)$ which does not depend on any parameters, one can construct a parameter-dependent family $p_\theta(i)$ by

$$
p_\theta(i) = \frac{1}{\sum_j p(j)\theta} p(i)^\theta.
$$

(8)

Clearly is $p_1 = p$. A short calculation gives

$$
\frac{\partial}{\partial \theta^j} p_\theta = p_\theta \left( \frac{\partial G}{\partial \theta} - H(i) \right)
$$

(9)

with

$$
G(\theta) = -\ln \sum_i p(i)^\theta \quad \text{and} \quad H(i) = -\ln p(i).
$$

(10)
One can indeed write
\[ p_\theta(i) = \exp(G(\theta) - \theta H(i)). \] (11)
This shows that the multifractal model belongs to the exponential family.
In the present terminology, \( p_\theta \) is an escort of itself, not of \( p \), as said in [4]. But except for this slight change in the meaning of the word escort, the present concept generalises that of the multifractal context. Also the thermodynamical formalism, developed in the theory of multifractals, coincides with that found in [2].

V. GENERALISED INEQUALITY OF CRAMER AND RAO

Here we follow [2], with changes in presentation. Introduce the notations
\[ \langle A \rangle_\theta = \sum_i p_\theta(i) A(i) \quad \text{and} \quad \langle\langle A \rangle\rangle_\theta = \sum_i P_\theta(i) A(i). \] (12)
The notion of score variables, used in statistics, is generalised to
\[ X_k(i) = \frac{1}{P_\theta(i)} \frac{\partial}{\partial \theta} p_\theta(i). \] (13)
Let \( H_k \) be variables for which a function \( F(\theta) \) exists such that
\[ \langle H_k \rangle_\theta = \frac{\partial}{\partial \theta} F(\theta). \] (14)
Then the generalised inequality of Cramer and Rao, valid for arbitrary \( u^k \) and \( v^l \), reads
\[ u^k u^l \left( \langle\langle H_k H_l \rangle\rangle_\theta - \langle\langle H_k \rangle\rangle_\theta \langle\langle H_l \rangle\rangle_\theta \right) v^m v^n \langle\langle X_m X_n \rangle\rangle_\theta \geq \left[ u^k u^l \frac{\partial^2}{\partial \theta^k \partial \theta^l} F(\theta) \right]^2. \] (15)
The inequality is said to be optimal if equality holds whenever \( u = v \).
A sufficient condition for optimality is that a function \( Z(\theta) \) exists which is such that
\[ \frac{1}{Z(\theta)} \langle\langle X_k X_l \rangle\rangle_\theta = Z(\theta) \left( \langle\langle H_k H_l \rangle\rangle_\theta - \langle\langle H_k \rangle\rangle_\theta \langle\langle H_l \rangle\rangle_\theta \right) = -\frac{\partial}{\partial \theta} \langle\langle H_l \rangle\rangle_\theta. \] (16)
An slightly stronger condition is that functions \( Z(\theta) > 0 \) and \( G(\theta) \) exist for which
\[ \frac{\partial}{\partial \theta} p_\theta(i) = Z(\theta) P_\theta(i) \left( \frac{\partial G}{\partial \theta} - H_k(i) \right). \] (17)
See Appendix A. It is the latter condition that is used to define generalised exponential families.

VI. GENERALISED EXPONENTIAL FAMILIES

Obvious solutions of (17) are of the form
\[ p_\theta(i) = c(i) f_i \left( G(\theta) - \theta^k H_k(i) \right) \] (18)
\[ P_\theta(i) = \frac{c(i)}{Z(\theta)} f_i \left( G(\theta) - \theta^k H_k(i) \right) \] (19)
\[ Z(\theta) = \sum_i c(i) f_i \left( G(\theta) - \theta^k H_k(i) \right). \] (20)
where \(c(i)\) is a positive constant and where \(f_i(x)\) is a positive non-decreasing (stochastic) function. \(f'(i)\) is the derivative of \(f_i(x)\) (For convenience, the dependence of \(f_i(x)\) on the stochastic variable \(i\) is written as an index; when possible the dependence on \(i\) is omitted). The normalisation \(G(\theta)\) must be such that

\[
\sum_i c(i) f_i \left( G(\theta) - \theta^k H_k(i) \right) = 1. \tag{21}
\]

A function \(\phi_i(y)\) is defined by

\[
\phi_i(y) = f_i' \left( f_i^{-1}(y) \right), \tag{22}
\]

with \(f_i^{-1}(y)\) the inverse of the function \(f_i(x)\). Then one has

\[
\frac{1}{c(i)} p_\theta(i) = \frac{1}{Z(\theta)} \phi_i \left( \frac{1}{c(i)} p_\theta(i) \right). \tag{23}
\]

The only function which is its own derivative is the exponential function. Hence, with \(f_i(x) = \exp(x)\) one finds \(\phi(x) = x\), \(Z(\theta) = 1\), and \(p_\theta(i) = p_\theta(i)\). In this case one recovers a distribution belonging to the exponential family.

VII. IDENTITIES

A well-known trick of statistical physics is the calculation of averages by taking derivatives of \(-\log Z\). E.g., in the Ising model is

\[
-\frac{\partial}{\partial \beta} \log Z = \frac{\partial G}{\partial \beta} = \langle H \rangle_\theta \quad \text{and} \quad -\frac{\partial}{\partial h} \log Z = \frac{\partial G}{\partial h} = \langle H^2 \rangle_\theta. \tag{24}
\]

As a consequence, the main problem of equilibrium statistical physics is often the evaluation of the partition sum \(Z\) to a closed form expression.

The trick works for all generalised exponential families, and is based on the identity

\[
\frac{\partial G}{\partial \theta^k} = \langle H^k \rangle_\theta. \tag{25}
\]

The latter follows from conservation of probability. Indeed, one calculates

\[
0 = \frac{\partial}{\partial \theta^k} \sum_i p_\theta(i) = \sum_i Z(\theta) p_\theta(i) \left( \frac{\partial G}{\partial \theta^k} - H_k(i) \right) = Z(\theta) \left( \frac{\partial G}{\partial \theta^k} - \langle H_k \rangle_\theta \right). \tag{26}
\]

It may be disappointing that the quantities that one can calculate via \(25\) are \(\langle H^k \rangle_\theta\), and not the physically relevant \(\langle H_k \rangle_\theta\). However, the derivatives of the latter are static susceptibilities, up to a sign, and are given by

\[
\frac{\partial}{\partial \theta^k} \langle H_k \rangle_\theta = -Z(\theta) \left( \langle H^k H_l \rangle_\theta - \langle H_k \rangle_\theta \langle H_l \rangle_\theta \right). \tag{27}
\]

Hence, the static susceptibilities are controlled by the pair correlations of the escort distribution, showing the physical relevance of the latter. Note that the bracket in the r.h.s. of \(27\) coincides with the generalised Fisher information matrix — see \(2\).

The existence of the identities \(25\) and \(27\) makes it attractive to use generalised exponential families. This is illustrated below in case of the percolation model.
VIII. SITE PERCOLATION

In the site percolation problem the points of a lattice are occupied with probability $p$, independent of each other. The origin of the lattice is either unoccupied, with probability $p\emptyset$, or it belongs to a cluster of occupied sites. This cluster is finite with probability one if the density $p$ is less than the percolation threshold $p_c$. Two clusters of the same size can have a different shape (these shapes are called lattice animals). The probability that the origin belongs to a cluster of shape $i$ is denoted $p(i)$ and is given by

$$p(i) = c(i)p^{s(i)}(1-p)^{t(i)},$$

(28)

where $c(i)$ is the number of clusters of shape $i$, $s(i)$ is the number of sites, and $t(i)$ is the number of perimeter sites. The latter are unoccupied sites that have at least one site of the cluster as a neighbour. Identify shape 0 with the absence of a cluster at the origin. Then (28) holds with $c(0) = 1$, $s(0) = 0$ and $t(0) = 1$.

The probability that the origin belongs to an infinite cluster is denoted $p(\infty)$. It vanishes for $p < p_c$ and is strictly positive for $p > p_c$. It satisfies

$$p(\infty) + \sum_i p(i) = 1.$$  

(29)

For simplicity of notation we convene that $s(\infty) = t(\infty) = 0$ instead of the more obvious infinite value.

It is possible to write (28) into the form

$$p_\theta(i) = c(i)\exp \left( \frac{G(\theta) - \theta H(i)}{} \right) (s(i) + t(i))$$

(30)

with parameter $\theta$ defined by

$$\theta = \ln\frac{p}{1-p},$$

(31)

with Hamiltonian

$$H(i) = \frac{t(i)}{s(i) + t(i)},$$

(32)

and with normalisation

$$G(\theta) = -\ln(1 + e^{-\theta}) = \ln p.$$  

(33)

This suggests the introduction of a stochastic function $f$ defined by

$$f_i(G) = \exp((s(i) + t(i))G) \quad \text{if } i < \infty$$

$$f_\infty(G) = 1 - \sum_{i \neq \infty} c(i)f_i(G + H(i) \ln(e^G - 1)).$$

(34)

Introduce further conventions $c(\infty) = 1$ and $H(\infty) = 0$. Then the probability distribution is of the form (18). Note that the derivative of $f$ is given by

$$f'_i(G) = (s(i) + t(i))f_i(G) \quad \text{if } i \neq \infty$$

$$f'_\infty(G) = \frac{1}{1 - e^G \frac{\partial}{\partial \theta} p_\theta(\infty)} \bigg|_{G = G(\theta)}.$$  

(35)

(36)

The optimal escort probability distribution is therefore given by

$$P_\theta(i) = \frac{1}{Z(\theta)}(s(i) + t(i))p_\theta(i) \quad \text{if } i \neq \infty$$

$$P_\theta(\infty) = \frac{1}{Z(\theta)} \frac{1}{1-p} \frac{\partial}{\partial \theta} p_\theta(\infty),$$  

(37)

(38)

with appropriate normalisation $Z(\theta)$, given by

$$Z(\theta) = (s + t)\theta + \frac{1}{1 - p} \frac{\partial}{\partial \theta} p_\theta(\infty).$$

(39)
IX. PERCOLATION IDENTITIES

The identity one can derive from (25) reads

$$\langle \langle H \rangle \rangle_\theta = \frac{dG}{d\theta} = 1 - p. \quad (40)$$

Using the definition of the Hamiltonian and of the escort probability one finds

$$\langle \langle H \rangle \rangle_\theta = \frac{1}{Z(\theta)} \langle t \rangle_\theta. \quad (41)$$

Combining (39, 40, 41) the identity becomes

$$\frac{\partial}{\partial \theta} p(\infty) = \langle M \rangle_\theta,$$

with

$$M(i) = pt(i) - (1 - p)s(i). \quad (42)$$

This result is known — see (44a) of [3]. The variable $M$ acts as an order parameter. Its average value vanishes for $p < p_c$. It is non-zero for $p > p_c$ and diverges as $(p - p_c)^{\beta - 1}$ when $p$ decreases towards $p_c$.

In the present approach the relevant susceptibility is

$$\chi = -\frac{d}{d\theta} \langle H \rangle_\theta = -\frac{d}{d\theta} (\frac{t}{s + t})_\theta. \quad (43)$$

Using (27) this becomes

$$\chi = Z(\theta) \left( \langle \langle H^2 \rangle \rangle_\theta - \langle \langle H \rangle \rangle_\theta^2 \right)$$

$$= \langle HM \rangle_\theta$$

$$= \langle \frac{1}{s + t} M^2 + (1 - p)M \rangle_\theta. \quad (44)$$

It is expected to diverge as $|p - p_c|^{-\gamma}$ when $p$ approaches the percolation threshold.

X. DISCUSSION

In non-extensive thermostatistics average energy is often calculated using the escort probability distribution. Next, entropy is maximised under the constraint that the escort averaged energy $\langle \langle H \rangle \rangle$ has some given value $U$ — see [1]. The main point of the present paper is that $\langle \langle H \rangle \rangle$ and $\langle \langle H^2 \rangle \rangle$ can be used as part of the identities (25, 27). They provide a convenient way of obtaining relevant information about the model under study. This approach has been illustrated by taking site percolation as an example.

The presentation has been purely classical, avoiding quantum statistics. A first attempt to treat the quantum case is found in [8]. The probability distribution and its escort should be replaced by a pair of density operators $\rho$ and $\sigma$. However, the possibility that $\rho$ and $\sigma$ do not commute prevents a straightforward translation of the classical formalism to the quantum context.

APPENDIX A: OPTIMALITY OF (16) AND IMPLICATION OF (16) BY (17)

Let us first show that (16) implies optimality of inequality (15). From (16) follows

$$\frac{\partial}{\partial \theta^k} \langle H_i \rangle_\theta = \frac{\partial}{\partial \theta^k} \langle H_k \rangle_\theta. \quad (A1)$$

Hence, a function $F(\theta)$ exists such that

$$\langle H_k \rangle_\theta = \frac{\partial F}{\partial \theta^k}. \quad (A2)$$
Using (16) the inequality then becomes

\[ u^k v^l \frac{\partial^2 F}{\partial \theta^k \partial \theta^l} v^m v^n \frac{\partial^2 F}{\partial \theta^m \partial \theta^n} \geq \left[ u^k v^l \frac{\partial^2 F}{\partial \theta^k \partial \theta^l} \right]^2. \]  

(A3)

Obviously, this is an equality when \( u = v \). Hence, the inequality is satisfied optimally.

Finally, assume (17) holds and prove (16). Condition (17) implies that

\[ 0 = \sum_i \frac{\partial}{\partial \theta^k} p_\theta(i) \]

\[ = Z(\theta) \left( \frac{\partial G}{\partial \theta^k} - \langle \langle H_k \rangle \rangle_\theta \right). \]  

(A4)

and

\[ X_k(i) = Z(\theta) \left( \frac{\partial G}{\partial \theta^k} - H_k \right) = -Z(\theta) (H_k - \langle \langle H_k \rangle \rangle_\theta). \]  

(A5)

Hence, the first equality of (16) follows. On the other hand is

\[ \frac{\partial}{\partial \theta^k} \langle H_l \rangle_\theta = Z(\theta) \sum_i P_\theta(i) \left( \frac{\partial G}{\partial \theta^k} - H_k \right) H_l(i) \]

\[ = -Z(\theta) \left[ \langle \langle H_k H_l \rangle \rangle_\theta - \langle \langle H_k \rangle \rangle_\theta \langle \langle H_l \rangle \rangle_\theta \right]. \]  

(A6)

This proves the remaining equality.

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