Escort density operators and generalized quantum information measures

Jan Naudts
Departement Fysica, Universiteit Antwerpen,
Universiteitsplein 1, 2610 Antwerpen, Belgium
E-mail Jan.Naudts@ua.ac.be

August 21, 2018

Abstract

Parametrized families of density operators are studied. A generalization of the lower bound of Cramér and Rao is formulated. It involves escort density operators. The notion of $\phi$-exponential family is introduced. This family, together with its escort, optimizes the generalized lower bound. It also satisfies a maximum entropy principle and exhibits a thermodynamic structure in which entropy and free energy are related by Legendre transform.

1 Introduction

The exponential family of probability distributions plays a central role in statistical mechanics, where it is called the Boltzmann-Gibbs distribution. In a previous paper [1] the author has proposed a generalization of this family, involving the notion of deformed exponential functions. It is called the $\phi$-exponential family because it involves a function $\phi$, which is used to deform the exponential function. The present paper extends this work to the quantum-mechanical context, solving some of the difficulties resulting from working with non-commuting operators. Other difficulties that can arise (unbounded operators, operators that are not trace-class, ...) are not discussed at all. However, none of the latter technicalities arise if the Hilbert space $\mathcal{H}$ of quantum-mechanical wavefunctions is assumed to be finite dimensional.

The motivation for this work is twofold. At one hand the canonical ensemble, although dominant, is not the only ensemble that occurs in statistical physics. Hence the present generalization might have practical applications. In fact, in nonextensive thermostatistics [2], which involves the $\phi$-exponential family with $\phi(u) = u^q$, many such applications are claimed. But because of the generality of the present approach applications in statistics and in information theory are possible as well. At the other hand the formulation of a generalization might
provide new insights into the existing theory. Of particular interest is a better understanding of the problems around the definition of a quantum information manifold — see [3] for a recent attempt in this direction. Further work is needed both on the fundamental level and in the direction of finding applications.

The paper is organised as follows. The next section generalizes the well-known lower bound of Cramér and Rao in quantum context. In Section 3 a sufficient condition for optimality of this lower bound is presented. Section 4 introduces the φ-exponential family of density operators. In Section 5 appropriate notions of entropy and of relative entropy are defined. Section 6 contains the obvious example of powerlaw distributions. In Section 7 the φ-exponential family is shown to satisfy a maximum entropy principle. The associated structure of Legendre transforms is revealed. The final section contains a short discussion of results.

2 Escort density operators and the lower bound of Cramér and Rao

Fix a Hilbert space $\mathcal{H}$. Recall that a density operator $\rho$ of $\mathcal{H}$ is a positive operator which is trace-class, with trace equal to 1. Let us consider families of density operators $(\rho_\theta)_{\theta \in D}$, with parameters $\theta = (\theta^1, \ldots, \theta^N)$ in some open domain $D$, subset of $\mathbb{R}^N$. It is assumed that $\rho_\theta$, seen as a function of its parameters $\theta$, is sufficiently smooth so that its derivatives $\partial \rho_\theta / \partial \theta^k$ are well-defined operators.

Consider two families of density operators $(\rho_\theta)_{\theta \in D}$ and $(\sigma_\theta)_{\theta \in D}$ with common parameter domain $D$. The two families are not related any further. Still, $\sigma_\theta$ is called the escort density operator of $\rho_\theta$. Averages with respect to the two families of density operators are denoted by

$$\langle A \rangle_\theta = \text{Tr} \rho_\theta A \quad \text{resp.} \quad [A]_\theta = \text{Tr} \sigma_\theta A. \quad (1)$$

For simplicity let us assume that $\sigma_\theta$ is invertible. A generalized Fisher information $g(\theta)$ is defined by

$$g_{kl}(\theta) = \frac{\text{Tr}}{\sigma_\theta} \frac{\partial \rho_\theta}{\partial \theta^k} \frac{\partial \rho_\theta}{\partial \theta^l} = \left[ \frac{1}{\sigma_\theta} \frac{\partial \rho_\theta}{\partial \theta^k} \right]^{\dagger} \left( \frac{1}{\sigma_\theta} \frac{\partial \rho_\theta}{\partial \theta^l} \right)_{\theta}. \quad (2)$$

The $N$-by-$N$-matrix may contain complex entries. However, it is positive-definite.

Let be given bounded self-adjoint operators $H_1, \cdots, H_N$ and assume that a function $F(\theta)$ exists for which

$$\langle H_k \rangle_\theta = \frac{\partial F}{\partial \theta^k}, \quad k = 1, \cdots, N. \quad (3)$$

In physical applications these operators $H_k$ are the macroscopic observables like Hamiltonian, total magnetization, particle number, ... . The parameters
\( \theta_k \) could be inverse temperature, external magnetic field, chemical potential (multiplied with inverse temperature), \( \ldots \). The function \( F \) is minus the Massieu function (free energy multiplied with inverse temperature). The well-known lower bound of Cramér and Rao can now be generalized as follows

**Proposition** For arbitrary complex numbers \( u^k \) and \( v^m \) is

\[
\frac{|u^k \bar{u}^l ([H_k H_l]_\theta - [H_k]_\theta [H_l]_\theta)|^2}{|\pi^m v^n \frac{\partial^2 F}{\partial \theta^m \partial \theta^n}|^2} \geq \frac{1}{|\pi^m v^n \varphi_{mn}(\theta)|^2}.
\]

(4)

**Proof** The proof is based on Schwarz’s inequality. Let

\[
X_k = \frac{1}{\sigma_\theta} \frac{\partial \rho}{\partial \theta^k} \quad \text{and} \quad Y_k = H_k - [H_k]_\theta.
\]

(5)

Then one has

\[
|\pi^k v^m [Y_k X_m^\dagger]|^2 \leq |u^k \bar{u}^l [Y_k Y_l]_\theta \pi^n v^m [X_n X_m^\dagger]|. \quad (6)
\]

The l.h.s. evaluates to

\[
\frac{|u^k v^m [Y_k X_m^\dagger]|^2}{|\pi^k v^m [Y_k X_m^\dagger]|^2} = \frac{|u^k v^m \left([H_k - [H_k]_\theta] \frac{\partial \rho}{\partial \theta^m} \frac{1}{\sigma_\theta}\right)|^2}{|u^k v^m \text{Tr} [H_k - [H_k]_\theta] \frac{\partial \rho}{\partial \theta^m}|^2} = \frac{|u^k v^m \frac{\partial}{\partial \theta^m} [H_k]_\theta|^2}{|u^k v^m \frac{\partial^2 F}{\partial \theta^m \partial \theta^k}|^2}. \quad (7)
\]

Evaluation of the r.h.s. of (6) is straightforward. The result can be written as (1).

\( \square \)

### 3 Optimal escort families

The lower bound (4) is said to be optimal if equality holds whenever \( u^k = v^k \) for all \( k \). The exponential family is known to optimize the usual version of the lower bound of Cramér and Rao. Escort density operators are allowed in the generalized lower bound (4). One can therefore expect that other families than the exponential one can optimize the lower bound provided that the escort family is chosen in a suitable way. Explicit examples of such families are discussed in the next section. Here, a sufficient condition for optimizing (1) is derived.
Proposition A sufficient condition under which the escort family \((\sigma_\theta)_{\theta \in D}\) optimizes \(\Phi\) is that there exists functions \(G(\theta)\) and \(Z(\theta)\) such that
\[
\sigma_\theta^{-1} \frac{\partial \rho_\theta}{\partial \theta^k} = \sigma_\theta^{-1} \frac{\partial \rho_\theta}{\partial \theta^k} = Z(\theta) \frac{\partial}{\partial \theta^k} \left(G(\theta) - \theta^l H_l\right).
\] (8)

Proof In order to show this point first notice that
\[
\text{Tr} \sigma_\theta \left(\sigma_\theta^{-1} \frac{\partial \rho_\theta}{\partial \theta^k}\right) = \frac{\partial}{\partial \theta^k} \text{Tr} \rho_\theta = 0.
\] (9)

Hence, (8) implies that
\[
\frac{\partial G}{\partial \theta^k} = [H_k]_\theta.
\] (10)

One then calculates
\[
g_{kl}(\theta) = \text{Tr} \frac{1}{\sigma_\theta} \frac{\partial \rho_\theta}{\partial \theta^k} \frac{\partial \rho_\theta}{\partial \theta^l} = Z(\theta)^2 \text{Tr} \sigma_\theta \left([H_k]_\theta - H_k\right) \left([H_l]_\theta - H_l\right)
\]
\[
= Z(\theta)^2 \left([H_k H_l]_\theta - [H_k]_\theta [H_l]_\theta\right).
\] (11)

On the other hand is, using (8),
\[
\frac{\partial^2 F}{\partial \theta^k \partial \theta^l} = \frac{\partial}{\partial \theta^k} \left[H_l\right] = \text{Tr} \frac{\partial \rho_\theta}{\partial \theta^k} H_l = Z(\theta) \text{Tr} \sigma_\theta \left(\frac{\partial G}{\partial \theta^k} - H_k\right) H_l
\]
\[
= Z(\theta) \left([H_k]_\theta [H_l]_\theta - [H_k H_l]_\theta\right).
\] (12)

Combining (11,12) gives
\[
u_{(H_k, H_l)} \left([H_k H_l]_\theta - [H_k]_\theta [H_l]_\theta\right) = \frac{1}{\pi u^n g_{mn}(\theta)} \frac{\partial^2 F}{\partial \theta^k \partial \theta^l} \left(H_k, H_l\right)\] (13)

4 \(\phi\)-exponential family
Fix a positive nondecreasing function \(\phi(u)\), defined for \(u \geq 0\). Use it to define another function, denoted \(\exp_\phi(u)\), by the relations
\[
\frac{d}{du} \exp_\phi(u) = \phi \left(\exp_\phi(u)\right) \quad \text{and} \quad \exp_\phi(0) = 1.
\] (14)
It is called a deformed exponential \[4\]. Its inverse \(\ln_\phi(u)\) is a deformed logarithm.

As before, a set of Hamiltonians \(H_1, \ldots, H_N\) is fixed. The \(\phi\)-exponential family is defined in terms of these Hamiltonians by

\[
\rho_\theta = \exp_\phi \left(G(\theta) - \theta^k H_k \right).
\]

(15)

It is assumed that these operators \(\rho_\theta\) are trace-class. Normalization \(\text{Tr} \rho_\theta = 1\) determines the function \(G(\theta)\).

Assume in what follows that the operators \(H_1, \ldots, H_N\) are two-by-two commuting. This condition is needed for easy calculation of the derivatives \(\partial \rho_\theta / \partial \theta^k\).

With this assumption there exists a common orthonormal basis of eigenvectors \((\psi_n)_n\)

\[
H_k \psi_n = \epsilon_k(n) \psi_n.
\]

(16)

Then also \(\rho_\theta\) is diagonal in the same basis and one has

\[
\rho_\theta \psi_n = \exp_\phi \left(G(\theta) - \theta^k \epsilon_k(n) \right) \psi_n.
\]

(17)

and

\[
\frac{\partial \rho_\theta}{\partial \theta^k} \psi_n = \phi \left( \exp_\phi \left(G(\theta) - \theta^k \epsilon_k(n) \right) \left( \frac{\partial G}{\partial \theta^k} - \epsilon_k(n) \right) \right) \psi_n
\]

\[
= \phi(\rho_\theta) \left( \frac{\partial G}{\partial \theta^k} - H_k \right) \psi_n.
\]

(18)

Using this last result it is now straightforward to verify that the condition for optimality \[8\] is satisfied with escort family and normalization given by

\[
\sigma_\theta = \frac{1}{Z(\theta)} \phi(\rho_\theta) \quad \text{and} \quad Z(\theta) = \text{Tr} \phi(\rho_\theta).
\]

(19)

5 Entropy and relative entropy functionals

The \(\phi\)-exponential family is the basis for formulating a generalized thermodynamics \[5, 6\]. The derivation of the thermodynamical structure requires the introduction of an entropy functional \(I_\phi(\rho)\) and of relative entropy \(I_\phi(\rho||\sigma)\). The classical version of these quantities is found in \[1\], although the way of presenting here is slightly different.

An appropriate definition of entropy is

\[
I_\phi(\rho) = - \int_0^1 dx \text{Tr} \rho \ln_\phi(x \rho) + \int_0^1 dx \ln_\phi(x),
\]

(20)

Let us shortly analyse this expression. Introduce a function \(\xi\) given by

\[
\frac{1}{\xi(u)} = \int_0^1 dx \frac{x}{\phi(xu)} = \frac{1}{u} \left( \ln_\phi(u) - \frac{1}{u} \int_u^a dw \ln_\phi(w) \right)
\]

(21)
Note that $\xi(u)$ is a positive increasing function of $u$. One has

$$I_\phi(\rho) = -\text{Tr} \rho \ln \xi(\rho). \quad (22)$$

This expression looks familiar. In case of the natural logarithm is $\phi(x) = x$. This implies that also $\xi(x) = x$. Then (22) reduces to the conventional definition.

From (22) follows also that $I_\phi(\rho) \geq 0$ because $\ln \xi(\rho) \leq 0$.

Relative entropy, also called divergence, is defined by

$$I_\phi(\rho||\sigma) = I_\phi(\sigma) - I_\phi(\rho) - \text{Tr} (\rho - \sigma) \ln \phi(\sigma). \quad (23)$$

Its basic property is the following.

**Proposition** For any pair of density operators $\rho$ and $\sigma$ is

$$I_\phi(\rho||\sigma) \geq 0 \quad (24)$$

**Proof** From

$$\frac{d}{du} u \ln \xi(u) = \int_0^1 dx x \int_1^u dv \left( \frac{1}{\phi(xv)} - \frac{1}{\phi(xu)} \right) \quad (25)$$

follows that the function $f(u) = u \ln \xi(u)$ is convex. Hence Klein’s inequality (see e.g. [7], 2.5.2)

$$\text{Tr} \left( f(\rho) - f(\sigma) - (\rho - \sigma) f'(\sigma) \right) \geq 0 \quad (26)$$

implies

$$- I_\phi(\rho) + I_\phi(\sigma) - \text{Tr} (\rho - \sigma) \left( \ln \xi(\sigma) + \frac{\sigma}{\xi(\sigma)} \right) \geq 0. \quad (27)$$

The proof follows now from the identity

$$\ln_\phi u = \ln \xi(u) + \frac{u}{\xi(u)} - \frac{1}{\xi(1)}. \quad (28)$$

□

This result can be used to prove concavity of the entropy functional $I_\phi(\rho)$.

**Corollary** For any $\lambda$ satisfying $0 \leq \lambda \leq 1$ is

$$I_\phi(\lambda \sigma + (1 - \lambda) \rho) \geq \lambda I_\phi(\sigma) + (1 - \lambda) I_\phi(\rho). \quad (29)$$

**Proof** Let $\tau = \lambda \sigma + (1 - \lambda) \rho$. Applying twice the proposition, in combination with definition (23), one obtains

$$I_\phi(\tau) - I_\phi(\rho) \geq \text{Tr} (\rho - \tau) \ln_\phi(\tau)$$
\[ I_\phi(\tau) - I_\phi(\sigma) \geq \text{Tr} (\sigma - \tau) \ln_\phi(\tau). \] (30)

By taking a convex combination of these two expressions (29) follows. □

Finally, note that a short calculation shows that

\[ I_\phi \left( \rho + u^k \frac{\partial \rho}{\partial \theta^k} \right) + I_\phi \left( \rho + u^k \frac{\partial \rho}{\partial \theta^k} \right) = \frac{1}{Z(\theta)} u^k u^l g_{kl}(\theta) + o(u^2). \] (31)

This expression links relative entropy to generalized Fisher information.

6 Example

The obvious example is obtained by taking \( \phi(u) = u^q \), with \( 0 < q < 2 \) (\( q = 1 \) corresponds with the standard case). In this case the notations \( \ln_q \) and \( \exp_q \) are used instead of \( \ln_\phi \) resp. \( \exp_\phi \). A short calculation gives

\[ \ln_q(u) = \frac{1}{1-q} \left( u^{1-q} - 1 \right). \] (32)

This particular definition of deformed logarithm has been introduced in [8]. An easy integration gives \( \xi(u) = (2-q)u^q \). Hence, in this case the functions \( \phi \) and \( \xi \) differ only by a constant factor. The resulting entropy functional is

\[ I_\phi(\rho) = -\frac{1}{2-q} \text{Tr} \rho \ln_q(\rho) = \frac{1}{2-q} \frac{1}{q-1} \left( \text{Tr} \rho^2 - q - 1 \right). \] (33)

This is, up to some changes in notation and a proportionality factor \( 1/(q-1) \), the entropy studied in the context of Tsallis’ thermostatistics [2]. The corresponding expression for relative entropy is

\[ I_\phi(\rho|\sigma) = \frac{1}{(q-1)(2-q)} \text{Tr} \left( (q-1)\sigma^{2-q} - \rho^{2-q} + (2-q)\rho\sigma^{1-q} \right). \] (34)

7 Variational principle and duality

Let us now show that the \( \phi \)-exponential family satisfies a maximum entropy principle.

**Proposition** Let \( \{\rho_\theta\} \) be a \( \phi \)-exponential family of density operators with two-by-two commuting Hamiltonians \( H_1, \cdots, H_N \), and with averages \( \langle H_k \rangle_\theta \) equal to the gradients of the potential \( F(\theta) \). There exists a constant \( F_0 \) such that

\[ F(\theta) = F_0 + \min_{\rho} \{ \text{Tr} \rho \theta^k H_k - I_\phi(\rho) \}. \] (35)

The minimum is attained for \( \rho = \rho_\theta \). In particular, \( F(\theta) \) is a convex function of \( \theta \) and \( \rho = \rho_\theta \) maximizes \( I_\phi(\rho) \) under the constraint that \( \text{Tr} \theta^k \rho H_k = \text{Tr} \theta^k \rho_\theta H_k \).
Proof From \( I(\rho||\rho_0) \geq 0 \) follows

\[
0 \leq I_\phi(\rho_0) - I_\phi(\rho) - \text{Tr} (\rho - \rho_0) \ln_\phi(\rho_0).
\] (36)

But one has

\[
\ln_\phi(\rho_0) = G(\theta) - \theta^k H_k.
\] (37)

Hence one obtains

\[
0 \leq I_\phi(\rho_0) - I_\phi(\rho) + \text{Tr} (\rho - \rho_0) \theta^k H_k.
\] (38)

This proves that for all \( \rho \)

\[
\text{Tr} \rho_0 \theta^k H_k - I_\phi(\rho_0) \leq \text{Tr} \rho \theta^k H_k - I_\phi(\rho).
\] (39)

Next note that

\[
\frac{\partial F}{\partial \theta^k} = \langle H_k \rangle_{\theta} = \frac{\partial}{\partial \theta^k} \left( \theta^l \langle H_l \rangle_{\theta} - I_\phi(\rho_0) \right)
\] (40)

because one has

\[
\frac{\partial}{\partial \theta^k} I_\phi(\rho_0) = -\frac{\partial}{\partial \theta^k} \text{Tr} \rho_0 \ln_\xi \rho_0
\]
\[
= -\text{Tr} \left( \ln_\xi \rho_0 + \frac{1}{\xi(\rho_0)} \rho_0 \right) \frac{\partial}{\partial \theta^k} \rho_0
\]
\[
= -\text{Tr} \left( \ln_\phi \rho_0 \right) \frac{\partial}{\partial \theta^k} \rho_0
\]
\[
= -\text{Tr} \left( G(\theta) - \theta^l H_l \right) \frac{\partial}{\partial \theta^k} \rho_0
\]
\[
= \theta^k \frac{\partial}{\partial \theta^k} \langle H_l \rangle_{\theta}.
\] (41)

From (40) follows that there exists a constant \( F_0 \) for which

\[
F(\theta) = F_0 + \theta^l \langle H_l \rangle_{\theta} - I_\phi(\rho_0)
\] (42)

holds for all \( \theta \). This finishes the proof.

\[\Box\]

Introduce dual coordinates \( \eta_k \) (dual to \( \theta_k \)) by (see (3))

\[
\eta_k = \langle H_k \rangle_{\theta} = \frac{\partial F}{\partial \theta^k}.
\] (43)

They satisfy (use (11, 12))

\[
\frac{\partial \eta_k}{\partial \theta^l} = \frac{\partial^2 F}{\partial \theta^k \partial \theta^l} = Z(\theta) \left( [H_k]_{\theta} [H_l]_{\theta} - [H_k H_l]_{\theta} \right) = -\frac{1}{Z(\theta)} g_{kl}(\theta).
\] (44)

8
These are the orthogonality relations between the two sets of coordinates. The dual of relation (43) is

\[ \theta^k = \frac{\partial}{\partial \eta^k} I_\phi(\rho_\theta). \] (45)

Indeed, using (41, 44) one obtains

\[ \frac{\partial}{\partial \eta^k} I_\phi(\rho_\theta) = \frac{\partial \theta^l}{\partial \eta^k} \frac{\partial}{\partial \theta^l} I_\phi(\rho_\theta) = -Z(\theta)g^{kl} \frac{\partial^2 F}{\partial \theta^l \partial \theta^m} \theta^m, \] (46)

where \( g^{kl} \) is the inverse matrix of \( g_{kl} \). Next use (11) to obtain (45).

Let \( E(\eta) = I_\phi(\rho_\theta) \). Then one can write (42) as (putting \( F_0 = 0 \))

\[ F(\theta) + E(\eta) = \theta^k \eta_k. \] (47)

This shows that \( F(\theta) \) and \( E(\eta) \) are each others Legendre transform. This generalizes the well-known result of standard thermostatistics that free energy is the Legendre transform of equilibrium entropy.

8 Summary and discussion

This paper introduces the notion of \( \phi \)-exponential family of density operators \( \rho_\theta \). It depends on an arbitrary non-decreasing non-negative function \( \phi \) of the positive reals and on a set of Hamiltonians \( H_k \). The analogy with the standard exponential family is enhanced by using the notion of deformed exponential function \( \exp_{\phi} \). The definition is motivated by showing that the \( \phi \)-exponential family, together with a family of escort density operators, optimizes a generalized version of the well-known lower bound of Cramér and Rao.

Generalized definitions of entropy (20) and of relative entropy (23) have been given. The definitions are such that the \( \phi \)-exponential family of density operators satisfies a maximum entropy principle and that the function \( F(\theta) \) and entropy \( I_\phi(\rho_\theta) \) are each others Legendre transforms. The relation between \( F(\theta) \) and relative entropy is

\[ \theta^k \text{Tr} \rho H_k - I_\phi(\rho) = F(\theta) + I_\phi(\rho_\theta). \] (48)

The latter has the interpretation that free energy is minimal in equilibrium (i.e., when \( \rho = \rho_\theta \)).

The assumption has been made that the Hamiltonians \( H_k \) are two-by-two commuting. As a consequence, the quantum information ‘manifold’ \( (\rho_\theta)_\theta \) is still abelian. This is clearly too restrictive for a fully quantum-mechanical theory. Further work is needed to remove this restriction.

References

[1] J. Naudts, Estimators, escort probabilities, and phi-exponential families in statistical physics, arXiv:math-ph/0402005
[2] C. Tsallis, Possible Generalization of Boltzmann-Gibbs Statistics, J. Stat. Phys. 52, 479-487 (1988).

[3] R.F. Streater, Duality in quantum information geometry, Open Sys. & Information Dyn. 11, 71-77 (2004).

[4] J Naudts, Deformed exponentials and logarithms in generalized thermostatistics, arXiv:cond-mat/0203489, Physica A316, 323-334 (2002).

[5] J. Naudts, Generalized thermostatistics and mean-field theory, arXiv:cond-mat/0211444 Physica A332, 279-300 (2004).

[6] J. Naudts, Generalized thermostatistics based on deformed exponential and logarithmic functions, arXiv:cond-mat/0311438 Physica A340, 32-40 (2004).

[7] D. Ruelle, Statistical Mechanics (W.A. Benjamin Inc., 1969)

[8] C. Tsallis, What are the numbers that experiments provide? Quimica Nova 17, 468 (1994).