Marginal Polytope of a Deformed Exponential Family

Giovanni Pistone

Collegio Carlo Alberto, Via Real Collegio 30, 10024 Moncalieri, Italy

Abstract

A deformed logarithm function called \(q\)-logarithm has received considerable attention by physicist after its introduction by C. Tsallis. J. Naudts has proposed a generalization called \(\phi\)-logarithm and he has derived the basic properties of \(\phi\)-exponential families. In this paper we study the related notion of marginal polytope in the case of a finite state space.

Keywords: \(\phi\)-logarithm, \(\phi\)-exponential family, marginal polytope

1. Introduction

In Sec. 2 we review the basic properties of deformed exponential families as they are discussed in Naudts (2011). We do not give here detailed references and refer to the bibliographical notes in this monograph. The presentation of exponential families we use is non-parametric as in Pistone (2009). In Sec. 3 we give our generalization of the notion of marginal polytope. The standard version is in Brown (1986).

2. Background

The deformed exponential function are usually introduced starting from the logarithm, see e.g. Naudts (2011, Ch. 10), with the aim to define a generalization of the entropy. Let \(\phi: \mathbb{R}_+ \rightarrow \mathbb{R}_+\) be a positive, increasing, absolutely continuous function. The \(\phi\)-logarithm is the function \(\ln_\phi (v) = \int_1^v \frac{dy}{\phi(y)},\ v \in \mathbb{R}_+\), which reduces to ordinary logarithm when \(\phi(v) = v\).

The deformed logarithm \(\ln_\phi\) is defined on \(\mathbb{R}_+\) and it is strictly increasing and concave. In the following we assume \(-\int_{-\infty}^1 \frac{dy}{\phi(y)} = \int_1^{+\infty} \frac{dy}{\phi(y)} = +\infty\) so that the range of \(\ln_\phi\) is the full real line \(\mathbb{R}\).
The \( \phi \)-exponential or deformed exponential is the inverse function \( \exp_{\phi} = \ln_{\phi}^{-1} \). It is increasing and convex and solves the differential equation \( y' = \phi(y), \ y(0) = 1 \). It is convenient to introduce the rate function

\[
\psi(u) = \frac{\phi(\exp_{\phi}(u))}{\exp_{\phi}(u)}.
\]

so that we have

\[
\exp_{\phi}'(u) = \phi(\exp_{\phi}(u)) = \psi(u) \exp_{\phi}(u).
\]

Viceversa, given a positive absolutely continuous rate function \( \psi: \mathbb{R} \to \mathbb{R}_{>0} \), such that \( \int_{-\infty}^{0} \psi(x)dx = \int_{0}^{\infty} \psi(x)dx = +\infty \) and \( \psi' + \psi^2 \geq 0 \), the solution of the differential equation \( y'(u) = \psi(u)y(u), \ y(0) = 1 \), is a deformed exponential \( \exp_{\phi} \) whose \( \phi \)-function is

\[
\phi(v) = \psi(\ln_{\phi}(v)), \quad v \in \mathbb{R}_{>0}.
\]

This deformed exponential is self-dual, \( \exp_{\phi}(u) \exp_{\phi}(-u) = 1 \), if, and only if, the rate function \( \psi \) is symmetric because

\[
\frac{d}{du} \exp_{\phi}(u) \exp_{\phi}(-u) = \\
\quad \psi(u) \exp_{\phi}(u) \exp_{\phi}(-u) - \psi(-u) \exp_{\phi}(u) \exp_{\phi}(-u) = \\
\quad (\psi(u) - \psi(-u)) \exp_{\phi}(u) \exp_{\phi}(-u).
\]

Example 1 (Kaniadakis). The deformed exponential defined in Kaniadakis (2001) with parameter is

\[
\exp_{\kappa}(u) = \exp \left( \int_{0}^{u} \frac{dy}{\sqrt{1 + \kappa^2 y^2}} \right), \quad u \in \mathbb{R}, \quad \kappa \in [0, 1[.
\]

It has

\[
\psi(y) = (1 + \kappa^2 y^2)^{-1/2}, \quad \phi(x) = \frac{2x}{x^\kappa + x^{-\kappa}}.
\]

Example 2 (Tsallis). The function \( \phi(y) = y^q \) does not satisfy our restrictive assumptions and has been used by Tsallis in 1994 to define his deformed logarithm. Given a symmetric function \( \sigma \), then \( \phi(y) = y\sigma(y^q, y^{-q}) \) is self-dual. Kaniadakis’ logarithm is an example, with \( \sigma(s, t) = 2/(s + t^{-1}) \).
Let \((\mathcal{X}, \mu)\) be a finite sample space with reference measure \(\mu\). We denote by \(L\) the vector space of real random variables on \(\mathcal{X}\). If \(p\) is any probability density of the sample space, \(L_0(p)\) denotes the vector space of \(p\)-centered random variable, i.e. \(u \in L\) belongs to \(L_0(p)\) if \(E_p[u] = \sum_{x \in \mathcal{X}} u(x)p(x)\mu(x) = 0\). Given a density \(p\) and random variables \(H_j \in L, j = 1, \ldots, m\), the \(\phi\)-exponential family of the statistics \(H_j\) is the parametrized set of densities

\[
p_\theta(x) = \exp_\phi \left( \sum_{j=1}^{m} \theta_j H_j(x) - \alpha(\theta) \right) p(x), \quad \theta \in \mathbb{R}^m, \tag{1}\]

where \(\alpha(\theta)\) is characterized by the normalization condition. In fact, the function

\[
\alpha \mapsto E_p \left[ \exp_\phi \left( \sum_{j=1}^{m} \theta_j H_j - \alpha \right) \right]
\]

is continuous and decreasing from \(+\infty\) to \(0\), so that for each \(\theta \in \mathbb{R}^m\) there exists a unique value \(\alpha(\theta)\) such that \(p_\theta\) in Eq. (1) is a density.

Two different sets of statistics \(H_j, j = 1, \ldots, m\) and \(H'_j, j = 1, \ldots, m'\) define the same statistical model if, and only if, the vector space generated by the centered random variables is the same,

\[
\operatorname{Span} (H_j - E_p[H_j], j = 1, \ldots, m) = \operatorname{Span} (H'_j - E_p[H'_j], j = 1, \ldots, m').
\]

According to Pistone (2009), it is more canonical to define the \(\phi\)-exponential model as the set of densities \(p_u\) of the form

\[
p_u = \exp_\phi (u - K(u)) p, \quad u \in V, \tag{2}\]

where \(V = \operatorname{Span} (H_j - E_p[H_j], j = 1, \ldots, m)\) is a linear sub-space of \(L_0(p)\) and

\[
K(u) = \alpha(\theta) - \sum_{j=1}^{m} \theta_j E_p[H_j], \quad u = \sum_{j=1}^{m} \theta_j (H_j - E_p[H_j]). \tag{3}\]

The quantity \(K(u)\) is in fact the divergence of \(p\) from \(p_u\) because from \(u - K(u) = \ln_\phi \left( \frac{q}{p} \right)\), \(E_p[u] = 0\), and the self-duality of the deformed logarithm, we have

\[
K(u) = E_p \left[ \ln_\phi \left( \frac{p}{q} \right) \right].
\]

3
The random variable $u \in V$ is a unique parameterization of $p_u$ as

$$u = \ln_\phi \left( \frac{q}{p} \right) - E_p \left[ \ln_\phi \left( \frac{q}{p} \right) \right].$$

The non-parametric derivative of the mapping $L_0: u \mapsto K(u)$ is obtained by derivation of the expected value of Eq. (2) in the direction $v \in L_0$. We use the notation $D K(u) v = \left. \frac{d}{dt} K(u + tv) \right|_{t=0}$. As $E\mu[p_u] = E_p[\exp_\phi(u - K(u))] = 1$, we obtain

$$E_p [D \exp_\phi(u - K(u)) v] = 0.$$ As we have

$$\psi(u - K(u)) = \psi \left( \ln_\phi \left( \frac{p_u}{p} \right) \right) = \phi \left( \frac{p_u}{p} \right)$$

we can write

$$E_{p_u} \left[ \phi \left( \frac{p_u}{p} \right) v \right] = E_{p_u} \left[ \phi \left( \frac{p_u}{p} \right) \right] D K(u) v.$$

The probability density

$$p_{\phi,u} = \frac{\phi \left( \frac{p_u}{p} \right)}{E_{p_u} \left[ \phi \left( \frac{p_u}{p} \right) \right]} p_u$$

is called the escort density and we have $D K(u) v = E_{\phi,u} \left[ v \right]$.

The second derivative of $u \mapsto \exp_\phi(u - K(u))$ in the directions $v$ and $w$ is the first derivative in the direction $w$ of $u \mapsto \exp_\phi(u - K(u))(v - DK(u)v)$, therefore it is equal to

$$\exp_\phi''(u - K(u))(v - DK(u)v)(w - DK(u)w) - \exp_\phi'(u - K(u)) D^2 K(u) vw.$$

The random variable in Eq. (4) has zero $p$-expectation, so that

$$D^2 K(u) vw = \frac{E_p \left[ \exp_\phi''(u - K(u))(v - DK(u)v)(w - DK(u)w) \right]}{E_p \left[ \exp_\phi'(u - K(u)) \right]}.$$

If $w = v \neq 0$, then $D^2 K(u) vw > 0$, therefore the functional $K$ is strictly convex. For $u = 0$ we obtain $D^2 K(0) vw = \text{Cov}_p(u,v)$. We do not have
a similar interpretation for \( u \neq 0 \), but see the discussion of the parallel transport in Pistone (2009, sec. 4) and of conformal transformations in Ohara and Amari (2011).

The convex conjugate of \( L_0(p) : u \mapsto K(u) \), is defined in the duality \((u^* , u) \mapsto E_p[u^*u]\) by

\[
H(u^*) = \sup \{ E_p[u^*u] - K(u) : u \in L_0(p) \}, \quad u^* \in L_0(p).
\]

The function \( L_0(p) \ni u \mapsto E_p[u^*u] - K(u) \) is concave and has derivative in the direction \( v \) equal to

\[
E_p[u^*v] - E_{\phi,u}[v] = E_p[u^*v] - E_p[p_{\phi,u}v].
\]

If we have a maximum at \( \hat{u} \) in Eq. (5), then \( \hat{u} \) satisfies \( p_{\phi,\hat{u}} = u^*p \).

For the model in Eq. (2) we define

\[
H_V(u^*) = \sup \{ E_p[u^*u] - K(u) : u \in V \}, \quad u^* \in L_0(p).
\]

In this case the directional derivative has to be zero for all \( v \in V \) and a maximum at \( \hat{u} \) implies that \( u^* \) has orthogonal projection on \( V \) equal to that of \( p_{\phi,\hat{u}}/p \).

3. Marginal polytope

In this section we consider the \( \phi \)-exponential family of Eq. (1) together with its non-parametric presentation, where we have a vector space \( V \) of \( p \)-centered random variables and the statistical model of Eq. (2). The random variables \( H_j - E_p[H_j], j = 1, \ldots, m \), span the space \( V \subset L_0(p) \) and the relation between the two parameterization \( \theta \in \mathbb{R}^m \) and \( u \in V \) are shown in (3). The marginal polytope of the \( \phi \)-model (also called convex support) is the convex hull \( M \) of the set \( \{ H(x) : x \in \mathcal{X} \} \subset R^m \), \( H = (H_1, \ldots, H_m) \). The function \( \alpha : \mathbb{R}^m \rightarrow \mathbb{R} \) is convex and has a convex conjugate \( \alpha^*(\eta) = \sup \{ \theta \cdot \eta - \alpha(\theta) : \theta \in \mathbb{R}^m \} \).

The following theorem is the deformed version of classical results e.g., Brown (1986, Th. 3.6). We use notions of convex analysis to be found in Rockafellar (1970).

**Theorem 1.** 1. The convex conjugate \( \alpha^* : \mathbb{R}^m \rightarrow \mathbb{R} \cup \{+\infty\} \) of \( \alpha \) is finite exactly on the marginal polytope \( M = \text{co} (\text{im} H) \).
2. The gradient mapping $\nabla \alpha : \mathbb{R}^m \to \mathbb{R}^m$ is onto the interior $M^\circ$ of the marginal polytope $M$.

3. $\alpha^*$ restricted to $M^\circ$ is the Legendre transform of $\alpha$ that is, $\alpha^*(\eta) = \theta \cdot \eta - \alpha(\theta)$ if $\eta = E_{\phi, \theta}[H]$.

Proof. 1. Assume first $\eta \in M$, namely $\eta = \sum_x \lambda(x)H(x)$, $\lambda(x) \geq 0$, $\sum_x \lambda(x) = 1$, and $H(x) = (H_1(x), \ldots, H_m(x))$. From the convexity of the $\exp_\phi$ function, we obtain

$$\exp_\phi (\theta \cdot \eta - \alpha(\theta)) = \exp_\phi \left( \sum_x \lambda(x) (\theta \cdot H(x) - \alpha(\theta)) \right) \leq \sum_x \lambda(x) \exp_\phi (\theta \cdot H(x) - \alpha(\theta))$$

As $\mu(x) > 0$, $x \in X$, $C = \max_x \lambda(x)/\mu(x)$ is finite and $\lambda(x) \leq C \mu(x)$, therefore

$$\exp_\phi (\theta \cdot \eta - \alpha(\theta)) \leq C \sum_x \mu(x) \exp_\phi (\theta \cdot H(x) - \alpha(\theta)) = C,$$

so that $\theta \cdot \eta - \alpha(\theta) \leq \ln_\phi(C)$ for all $\theta$.

Assume now $\eta \notin M$. As $M = \text{co}\{T(x): x \in X\}$ is a compact convex set, $\eta$ is strictly separated from $M$, that is, there exist an affine function $t \mapsto a \cdot t - a_0$, $a = (a_1, \ldots, a_m)$, such that $a \cdot H(x) \leq a_0$, $x \in X$, and $a \cdot \eta = a_0 + 1$. Along the sequence $\theta_n = na$, $n = 1, 2, \ldots$, we have

$$1 = \sum_x \exp_\phi (\theta_n \cdot H(x) - \alpha(\theta_n)) \mu(x) \leq \exp_\phi (na_0 - \alpha(\theta_n)),$$

so that

$$0 \leq na_0 - \alpha(\theta_n) = \theta_n \cdot \eta - n - \alpha(\theta_n),$$

which in turn implies $\theta_n \cdot \eta - \alpha(\theta_n) \to +\infty$ as $n \to \infty$.

2. Each $\eta = \nabla \psi(\theta)$ is of is an expected value with respect to the escort density, $\eta = E_{\phi, \theta}[H]$, therefore $\eta \in M^\circ$ because the escort density is strictly positive. Viceversa, if $\eta \in M^\circ$, let us assume first that the elements of $H$ are linearly independent so that the convex set $M$ is solid. In such a case, there exists a positive constant $\epsilon > 0$ such that $\eta + \epsilon u \in M^\circ$ for all unit vector $u$. Consider a tangent hyperplane $T_u(y) = 0$
of the $\epsilon$-ball centered at $\eta$, orthogonal to $u$, $T_u(y) = u \cdot (y - \eta) - \epsilon$. It follows that $T(\eta) = -\epsilon < 0$ and moreover there exists at least one $x_u \in \mathcal{X}$ such that $T(H(x_u)) > 0$, that is $\theta \cdot (H(x_u) - \eta) > \rho \epsilon$ for $\theta = \rho u$, $\rho \in \mathbb{R}$. We have

$$1 = \sum_x \exp_\phi (\theta \cdot H(x) - \alpha(\theta)) \mu(x) \geq \exp_\phi (\theta \cdot H(x_u) - \alpha(\theta)) \mu(x_u),$$

hence

$$\ln_\phi \left( \frac{1}{\mu(x_u)} \right) \geq \theta \cdot H(x_u) - \alpha(\theta) > \theta \cdot \eta + \rho \epsilon - \alpha(\theta).$$

therefore, for $\rho \to +\infty$,

$$\theta \cdot \eta - \alpha(\theta) < -\rho \epsilon \to -\infty.$$ 

The maximum of $\theta \mapsto \theta \cdot \eta - \alpha(\theta)$ is reached at some point $\hat{\theta}$ that satisfies $\eta = \nabla \alpha(\hat{\theta})$. The general case is obtained by considering a linear independent subset of $H_j$ and expressing the marginal polytope as an affine function of the reduced marginal polytope.

3. From the convexity of $\alpha$ it follows

$$\alpha(\theta) - \alpha(\hat{\theta}) \geq \nabla \alpha(\hat{\theta}) \cdot (\theta - \hat{\theta}) = \eta \cdot (\theta - \hat{\theta}).$$

By rearranging the terms,

$$\eta \cdot \hat{\theta} - \alpha(\hat{\theta}) \geq \eta \cdot \theta - \alpha(\theta),$$

therefore, $\alpha^*(\eta) = \eta \cdot \hat{\theta} - \alpha(\hat{\eta}).$

The non parametric version of item 1 of Th. 1 follows. We are not discussing here the other two items.

**Theorem 2.** The convex conjugate $H_V$ of $K$ is finite at $u^*$ if, and only if, $(u^* + 1)p$ is a density, that is $E_p[u^*] = 0$, $u^* + 1 \geq 0$. 

7
Proof. From Eq. (3) we have for $u \in V$

\[
E_p [u^* u] - K(u) = \sum_{j=1}^{m} \theta_j E_p [u^* (H_j - E_p [H_j])] - \alpha(\theta) + \sum_{j=1}^{m} \theta_j E_p [H_j]
\]

\[
= \sum_{j=1}^{m} \theta_j E_p [(u^* + 1) H_j] - \alpha(\theta)
\]

\[
= \eta \cdot \theta - \alpha(\theta),
\]

where $\eta_j = E_p [(u^* + 1) H_j]$, $j = 1, \ldots, m$. For such a $\eta$ we have $H_V(u^*) = \sup_{\eta}(\eta \cdot \theta - \alpha(\theta))$ which is finite if $\eta \in M$. As $\eta = \sum_x (u^*(x) + 1) H(x) p(x)$, $(u^* + 1)p$ must be a density.

4. Discussion

We have shown in Th. 1 that the basic properties of the marginal polytope carry over from the classical case to the deformed case. Moreover, we have provided in Th. 2 a non-parametric definition of the marginal polytope. This should be relevant in the discussion of the variational properties of the related deformed entropies. The results are restricted to the case of finite state space, while the non-parametric language prompts for a generalization in the direction of Pistone and Sempi (1995).

A new general non-parametric approach has been used in Vigelis and Cavalcante (2011) to ease the discussion of the dependence of the chart from the reference density $p$. Each density $q$ is represented as $\exp_\phi (u - K_{VC}(u) + \ln_\phi p)$ with respect to $\mu$, $u \in L_0(\mu)$. In such a case we have $\ln_\phi q = u - K_{VC}(u) + \ln_\phi p$, that is $K_{VC}(u) = E_{\mu} [\ln_\phi p - \ln_\phi q]$ instead of $K(u) = E_{\mu} [\ln_\phi \left( \frac{p}{q} \right)]$.

References

Brown, L. D., 1986. Fundamentals of statistical exponential families with applications in statistical decision theory. Institute of Mathematical Statistics, Hayward, CA.

Kaniadakis, G., 2001. Non-linear kinetics underlying generalized statistics. Physica A 296 (3-4), 405-425.
Naudts, J., 2011. Generalised Thermostatistics. Springer.

Ohara, A., Amari, S., 2011. Geometry of $q$-exponential family of probability distributions. Entropy 13 (6), 1170–1185.

Pistone, G., 2009. $\kappa$-exponential models from the geometrical viewpoint. The European Physical Journal B Condensed Matter Physics 71 (1), 29–37.

Pistone, G., Sempi, C., 1995. An infinite-dimensional geometric structure on the space of all the probability measures equivalent to a given one. Ann. Statist. 23 (5), 1543–1561.

Rockafellar, R. T., 1970. Convex analysis. Princeton Mathematical Series, No. 28. Princeton University Press, Princeton, N.J.

Vigelis, R. F., Cavalcante, C. C., 2011. On the $\phi$-family of probability distributions, http://arxiv.org/abs/1105.1118.