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ON THE CONVEXITY OF SOME DIVERGENCE MEASURES BASED ON ENTROPY FUNCTIONS

J. Burbea and C. Radhakrishna Rao

<u>Abstract</u> - Three measures of divergence between vectors in a convex set of an n-dimensional real vector space have been defined in terms of certain types of entropy functions, and their convexity property studied. Among other results, a classification of the α -order entropies is obtained by the convexity of these measures. These results have applications to the measurement of diversity of a discrete probability distribution and divergence between two distributions.

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1. INTRODUCTION

One of the most widely used index of diversity of a multinomial distribution, $x = (x_1, \dots, x_n), x_i \ge 0, \Sigma x_i = 1$, is the <u>Shannon entropy</u>, $H_n(x) = -\Sigma x_i \log x_i$ (Shannon [10]). The concavity of $H_n(x)$ provides a decomposition of the total diversity in a mixed distribution (x+y)/2 as

$$H_n(\frac{x+y}{2}) = \frac{1}{2}[H_n(x) + H_n(y)] + \frac{1}{2}J_n(x,y)$$
 (1.1)

The first component $2^{-1}[H_n(x) + H_n(y)]$ in (1.1) is the average diversity within the distributions, and the second component

$$J_{n}(x,y) = [-H(x) - H(y)] - 2[-H \frac{(x+y)}{2}]$$
(1.2)

which we call the <u>Jensen difference</u> arising out of the convex function -H(x) is non-negative, vanishes if and only if x = y, and thus provides a natural measure of divergence between the distributions x and y. (See Lewontin [6] and Rao [9] for some applications of $H_n(x)$ and $J_n(x,y)$ in biological studies). It is interesting to note that $J_n(x,y)$ considered as a function of (x,y) is convex, which meets the intuitive requirement that the average divergence between (x,y) and (z,w) is not less than that between their convex combination $\lambda(x,y) + \mu(z,w)$ where λ , $\mu \ge 0$ and $\lambda + \mu = 1$. The convexity of the divergence measure $J_n(x,y)$ is an additional attractive feature of the Shannon entropy $H_n(x)$ as a measure of diversity of a distribution. In this paper we consider the Jensen difference (1.2) arising from a generalized class of entropy functions including the α -order entropies due to Havrda and Charvát [3], which we call the J-divergence and examine its convexity. In particular, we show that the <u>J-divergence</u> (1.2) based on the α -order entropy

$$H_{n,\alpha}(x) = (\alpha - 1)^{-1} (1 - \Sigma x_i^{\alpha}), \ \alpha \neq 1$$
 (1.3)

defined on the convex set

$$S_n = \{(x_1, ..., x_n) \in I^n : \Sigma x_i = 1\}, I \equiv (0, 1)$$
 (1.4)

is convex on $S_n \times S_n$ if and only if $\alpha \in [1,2]$ for n > 2 and if and only if $\alpha \in [1,2]$ or [3,11/3] for n = 2. The last result is surprising and the proof is rather involved.

We define two other measures called the K and L-divergences (equations (2.4) and (2.5)) based on cross entropy functions (Good [2]) and study their convexity. These are similar to and include the divergence measure introduced by Jeffreys [4] for providing an invariant density of <u>a priori</u> probability and applied for the more general purpose of statistical inference by Kullback and Leibler [5].

As a by-product of these results we obtain some interesting inequalities (equations (4.3) and (5.7)).

We note that the J, K and L-divergences are semimetrics and not, in general, metrics as they may not satisfy the triangular inequality. However, by considering these

functions on a tangent space of a parametric space of probability distributions, one is led to a differential metric of a Riemannian geometry which induces a metric over the space of distribution functions. This was done earlier by Rao [7,8] where the differential metric is in terms of the information matrix of a parametric family of probability distributions. This metric has been recently studied by Atkinson and Mitchell [1]. Some extensions of this approach to more general convex functions along with other local properties of the J, K,L-divergences will be presented elsewhere. The present study is an investigation of the global properties of these divergence measures.

2. PRELIMINARIES AND NOTATION

Let ϕ be a C²-function on a domain D of \mathbb{R}^n . The Hessian of ϕ at $x \in D$ along the direction $u \in \mathbb{R}^n$ is defined by

$$\Delta_{\mathbf{u}} \phi(\mathbf{x}) \equiv \mathbf{d}^2 \phi(\mathbf{x}:\mathbf{u}) = \mathbf{u}^T \mathbf{M}_{\phi} \mathbf{u} ,$$

where M_{ϕ} is the n×n matrix whose entries are $\partial_{x_{j}} \partial_{x_{j}} \phi(x)$; i,j=1,...,n. This may also be written as

$$\Delta_{\mathbf{u}} \phi(\mathbf{x}) \equiv \mathbf{u}^{\mathbf{T}} [\partial_{\mathbf{x}_{\mathbf{i}}} \partial_{\mathbf{x}_{\mathbf{j}}} \phi] \mathbf{u}.$$

Sometimes it is convenient to consider a function ψ as a function on the cartestan product in $\mathbb{R}^n \times \mathbb{R}^n$. In this case we assume that $\psi = \psi(\cdot, \cdot)$ is a C²-function on D×D. The

Hessian, then, of ψ at $(x,y) \in D \times D$ along the direction $(u,v) \in \mathbb{R}^n \times \mathbb{R}^n$ is given by

$$\Delta_{(\mathbf{u},\mathbf{v})}\psi(\mathbf{x},\mathbf{y}) = \mathbf{u}^{\mathrm{T}}[\partial_{\mathbf{x}_{i}}\partial_{\mathbf{x}_{j}}\psi]\mathbf{u} + 2\mathbf{v}^{\mathrm{T}}[\partial_{\mathbf{x}_{i}}\partial_{\mathbf{y}_{j}}\psi]\mathbf{u} + \mathbf{v}^{\mathrm{T}}[\partial_{\mathbf{y}_{i}}\partial_{\mathbf{y}_{j}}\phi]\mathbf{v} \quad (2.1)$$

with the obvious meaning of the expressions involved.

Let D be a convex domain of \mathbb{R}^n . A function ϕ of class $C^2(D)$ is said to be convex on D if for every $(x,u) \in D \times \mathbb{R}^n$, $\Delta_u \phi(x) \ge 0$. The smoothness assumption $\phi \in C^2(D)$ can be, of course, weakened by only requiring that ϕ be continuous on D with $\Delta_u \phi(x) \ge 0$, where the partial derivatives are taken in the distributional sense. Alternatively, one may apply a standard regularization process. We briefly recall this concept. We choose a C^∞ -nonnegative function K whose compact support is inside the unit ball of \mathbb{R}^n and such that

$$\int K(x) dx = 1.$$

For $\varepsilon > 0$ we define

 $K_{\varepsilon}(x) \equiv \varepsilon^{-n}K(\varepsilon^{-1}x).$

Suppose f is locally integrable in the domain D of \mathbb{R}^n . We may assume that f = 0 outside a compact set and thus $f \in L_1(\mathbb{R}^n)$. We define

$$f_{\varepsilon}(y) \equiv (f \star K_{\varepsilon})(y) = \int f(x)K_{\varepsilon}(y-x)dx = \int K(x)f(y-\varepsilon x)dx$$

As is well known, $f_{\varepsilon} \in C^{\infty}(D)$. Moreover, if in addition f is continuous on D, then it is uniformly continuous on compacta of D and, $\lim_{\varepsilon \to 0} f_{\varepsilon} = f$ uniformly on compacta of D.

For a function ϕ which is continuous on a convex domain D, but not necessarily of class $C^2(D)$, to be <u>convex</u> (in the generalized sense) in D, we may only require that its regularization ϕ_{ϵ} , defined above, be convex in D, in the previously described restrictive sense. It is said to be <u>concave</u> if $-\phi$ is convex. Thanks to the above process of regularization we may always assume that the functions in question are sufficiently smooth.

Let ϕ be a C²-function on an interval I of R and consider the ϕ -entropy

$$H_{n,\phi}(x) = -\sum_{i=1}^{n} \phi(x_i), \quad x \in I^n$$
 (2.2)

as a function defined on I^n . The Jensen difference (1.2) based on (2.2), which will be referred to as the <u>J-divergence</u> between x and y, is

$$J_{n,\phi}(x,y) = \sum_{i=1}^{n} \{\phi(x_i) + \phi(y_i) - 2\phi[(x_i+y_i)/2]\}, (x,y) \in I^n \times I^n. \quad (2.3)$$

When the interval I does not contain the origin, we consider alternative measures which may be called the K and L-divergences,

$$K_{n,\phi}(x,y) = \sum_{i=1}^{n} (x_i - y_i) \left[\frac{\phi(x_i)}{x_i} - \frac{\phi(y_i)}{y_i} \right]$$
(2.4)

and

$$L_{n,\phi}(x,y) = \sum_{i=1}^{n} \left[x_i \phi(\frac{y_i}{x_i}) + y_i \phi(\frac{x_i}{y_i}) \right]$$
(2.5)

The Hessians of (2.3)-(2.5) can be computed using the formula (2.1). However, it is of some practical interest to

consider the divergence measures (2.3)-(2.5) as acting on the convex set S_n defined in (1.4). In this case, (2.2) can be written as

$$H_{n,\phi}(x:X) = H_{n-1,\phi}(x) + H_{1,\phi}(X)$$
 (2.6)

$$x = (x_1, \dots, x_{n-1}) \in I^{n-1}, \quad X = 1 - \sum_{i=1}^{n-1} x_i \in I.$$
 (2.7)

Then (2.3) may be written as

$$J_{n,\phi}(x:X,y:Y) = J_{n-1,\phi}(x,y) + J_{1,\phi}(X,Y)$$
(2.8)

where y, Y are defined in the same way as x, X. Similar expressions for the K and L-divergences (2.4) and (2.5) are also available.

Note that

$$\Delta_{u} H_{n,\phi}(\mathbf{x}:\mathbf{X}) = \Delta_{u} H_{n-1,\phi}(\mathbf{x}) + \Delta_{U} H_{1,\phi}(\mathbf{X})$$
(2.9)

and the Hessian of (2.3) subject to (2.7) is

$$\Delta_{u,v} J_{n,\phi} (x: X, y: Y) = \Delta_{u,v} J_{n-1,\phi} (x,y) + \Delta_{U,v} J_{1,\phi} (X,Y)$$
(2.10)

with similar expressions for the K and L-divergences, where

$$u = (u_1, \dots, u_{n-1}), v = (v_1, \dots, v_{n-1}) \in \mathbb{R}^{n-1}$$

and

$$U = \sum_{i=1}^{n-1} u_i, \qquad V = \sum_{i=1}^{n-1} v_i \in \mathbb{R}.$$

We denote by

$$\bar{S}_n = \{(x_1, \dots, x_n) \in \bar{I}^n : \Sigma x_i = 1\}; \bar{I} = [0,1], n \ge 2,$$

the closure of S_n defined in (1.4). For any real number α , we define

$$\phi_{\alpha}(\mathbf{x}) = \begin{cases} (\alpha - 1)^{-1} (\mathbf{x}^{\alpha} - \mathbf{x}), & \alpha \neq \mathbf{1} \\ \vdots & \vdots \\ \mathbf{x} \log \mathbf{x} & , & \alpha = 1 \end{cases}$$
(2.11)

over $x \in \mathbb{R}_+ \equiv (0, \infty)$, and when $\alpha \ge 0$, ϕ_{α} can be extended to x = 0 with the convention $0 \log 0 = 0$. Defining

$$H_{n,\alpha}(x) \equiv H_{n,\phi_{\alpha}}(x) , x \in S_{n}$$
(2.12)

we have

$$H_{n,1}(x) = -\Sigma x_i \log x_i, \qquad x \in \overline{S}_n, \qquad (2.13)$$

$$H_{n,\alpha}(x) = (\alpha - 1)^{-1} (1 - \Sigma x_i^{\alpha}), \quad x \in S_n, \quad \alpha \neq 1.$$
 (2.14)

We note that $H_{n,\alpha}$, for $\alpha \ge 0$ can be extended to the closure \overline{S}_n , which is the α -order entropy introduced by Havrda and Charvát [3], and that $H_{n,\alpha}$ tends to $H_{n,1}$ as $\alpha + 1$, which is the Shannon entropy H_n .

The J,K and L-divergences based on $H_{n,\alpha}$ are denoted by $J_{n,\alpha}, K_{n,\alpha}$ and $L_{n,\alpha}$ respectively. Their explicit expressions are as follows:

$$J_{\eta,\alpha}(x,y) = \begin{cases} (\alpha-1)^{-1} \Sigma \{x_i^{\alpha} + y_i^{\alpha} - 2[(x_i + y_i/2]^{\alpha}\}, & \alpha \neq 1 \\ \\ \sum \{x_i^{1} \log x_i + y_i^{1} \log y_i - (x_i + y_i) \log [(x_i + y_i)/2]\}, & \alpha = 1 \end{cases}$$
(2.15)

$$K_{n,\alpha}(x,y) = \begin{cases} (\alpha - 1)^{-1} \Sigma(x_{i} - y_{i})(x_{i}^{\alpha - 1} - y_{i}^{\alpha - 1}), & \alpha \neq 1 \\ \\ \Sigma(x_{i} - y_{i})(\log x_{i} - \log y_{i}), & \alpha = 1 \end{cases}$$
(2.16)

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and

$$L_{n,\alpha}(x,y) = \begin{cases} (\alpha-1)^{-1} \{ \sum x_{i}^{\alpha} y_{i}^{1-\alpha} + \sum x_{i}^{1-\alpha} y_{i}^{\alpha} - 2 \}, & \alpha \neq 1 \\ \\ \sum (x_{i} - y_{i})(\log x_{i} - \log y_{i}), & \alpha = 1 \end{cases}$$
(2.17)

Here $(x,y) \in S_n \times S_n$, and for $\alpha \ge 0$, $J_{n,\alpha}$ can be extended to $\overline{S}_n \times \overline{S}_n$. We note that $K_{n,1} = L_{n,1}$, and these expressions are the same as the divergence measure of Jeffreys [4] and Kullback and Liebler [5].

3. THE J-DIVERGENCE

The Hessian of $J_{n,\phi}$, in view of (2.1), is given by

$$^{\Delta}(u,v)^{J}_{n,\phi}(x,y) = \sum_{i=1}^{n} \{a(x_{i},y_{i})u_{i}^{2} + 2b(x_{i},y_{i})u_{i}v_{i} + a(y_{i},x_{i})v_{i}^{2}\}$$
(3.1)

where $x, y \in I^n$ with I being any interval of the line. Here, for $x, y \in I$,

$$b(x,y) = -\frac{1}{2} \phi''[(x+y)/2] \qquad (3.2)$$

and

$$a(x,y) = \phi''(x) + b(x,y) ; x,y \in I$$
. (3.3)

This shows that $J_{n,\phi}$ is convex (concave) on $I^n \times I^n$ if and only if $a(x,y) \ge 0$ (or $a(x,y) \le 0$) and

$$d(x,y) \equiv a(x,y)a(y,x) - [b(x,y)]^{2} \ge 0$$
 (3.4)

for every $(x,y) \in I \times I$.

Now, using (3.2)-(3.4) we deduce that for $x, y \in I$,

$$a(x,y) = \phi''(x) \phi'' [(x+y)/2] \{ \frac{1}{\phi''[(x+y)/2]} - \frac{1}{2} \frac{1}{\phi''(x)} \}$$

and

$$d(x,y) = \phi''(x) \phi''(y) \phi''[(x+y)/2]$$

× {
$$\frac{1}{\phi''[(x+y)/2]} - \frac{1}{2\phi''(x)} - \frac{1}{2\phi''(y)}$$
 }.

The expression in the last curly bracket is directly related to the Jensen difference of $(\phi'')^{-1}$. This with a closer examination of these expressions leads to the following basic result:

<u>Theorem 1</u>. $J_{n,\phi}$ is convex (concave) on $I^n \times I^n$ if and only if ϕ is convex (concave) and $(\phi'')^{-1}$ is concave (convex) on I.

As an application of the theorem we consider the following family of functions

$$g_{\alpha}(x) = a f_{\alpha}(x) + bx + c$$
 (3.5)

where a,b,c are arbitrary constants and $\{f_{\alpha}\}$ is a one parameter family of nonnegative functions defined on an interval I such that

$$f_{\alpha}^{"}(\mathbf{x}) = \alpha(\alpha - 1)f_{\alpha - 2}(\mathbf{x}) ; \mathbf{x} \in \mathbf{I}, \alpha \in \mathbf{R}.$$
 (3.6)

We shall fix a normalization

$$a\alpha(\alpha-1) \geq 0,$$
 (3.7)

from which it follows that g_{α} is convex on I for any $\alpha \in \mathbb{R}$. An immediate consequence of Theorem 1 is the following:

<u>Corollary 1</u>. Let the notation of (3.5)-(3.7) apply and consider $H_{n,g_{\alpha}}$ and $J_{n,g_{\alpha}}$ as formed in (2.2)-(2.3). Then, for any $\alpha \in \mathbb{R}$, $H_{n,g_{\alpha}}$ is concave on I^{n} while $J_{n,g_{\alpha}}$ is never concave on $I^{n} \times I^{n}$. Moreover, $J_{n,g_{\alpha}}$ is convex on $I^{n} \times I^{n}$ if and only if $(f_{\alpha-2})^{-1}$ is concave on I.

This corollary is appled to the following special case

$$f_{\alpha}(x) = x^{\alpha}$$
, $x \in \mathbb{R}_+$.

Writing $\beta = \alpha - 2$, we examine whether $h_{\beta} \equiv (f_{\beta})^{-1}$ is concave on \mathbb{R}_{+} . We have

$$h_{\beta}''(x) = \beta(\beta-1)x^{-\beta-2}$$
, $x \in \mathbb{R}_+$

and thus, h_{β} is concave if and only if $\beta \in [-1,0]$. This yields the following result:

Corollary 2. Let

$$g_{\alpha}(x) = ax^{\alpha} + bx + c, x \in \mathbb{R}_{+}$$

where a,b,c and α are constants with $a\alpha(\alpha-1) \ge 0$. Then $H_{n,g_{\alpha}}$ is concave on \mathbb{R}^{n}_{+} while $J_{n,g_{\alpha}}$ is never concave on $\mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$.

Moreover, $J_{n,g_{\alpha}}$ is convex on $\mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$ if and only if $\alpha \in [1,2]$ in which case $a \geq 0$.

Instead of g_{α} in this corollary we may take ϕ_{α} as in (2.11), and consequently:

<u>Corollary 3</u>. For any $\alpha \ge 0$, $H_{n,\phi_{\alpha}}$ is concave on \mathbb{R}^{n}_{+} and $J_{n,\phi_{\alpha}}$ is never concave on $\mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$. Moreover, $J_{n,\phi_{\alpha}}$ is convex on $\mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$ if and only if $\alpha \in [1,2]$.

Using this corollary and (2.6)-(2.10) we see that $J_{n,\alpha}$, for $n \ge 3$, is convex on $\overline{S}_n \times \overline{S}_n$ if and only if $\alpha \in [1,2]$. Of course, $J_{2,\alpha}$ is also convex on $\overline{S}_2 \times \overline{S}_2$ for every $\alpha \in [1,2]$. However, $J_{2,\alpha}$, interestingly, is also convex for other values of α , viz., in [3,11/3]. The proof of this fact is postponed to the next section. Meanwhile, we shall record the following corollary:

<u>Corollary 4</u>. For any $\alpha \ge 0$, $H_{n,\alpha}$ of (2.12) is concave on \overline{S}_n and $J_{n,\alpha}$ of (2.15) is never concave on $\overline{S}_n \times \overline{S}_n$. Moreover, for $n \ge 3$, $J_{n,\alpha}$ is convex on $\overline{S}_n \times \overline{S}_n$ if and only if $\alpha \in [1,2]$. Also, if $\alpha \in [1,2]$ then $J_{2,\alpha}$ is convex on $\overline{S}_2 \times \overline{S}_2$.

4. ADDITIONAL PROPERTIES OF THE J-DIVERGENCE

In order to deal with $J_{2,\alpha}$ on $\bar{S}_2 \times \bar{S}_2$ we shall apply Corollary 1 to the following family

$$f_{\alpha}(x) = x^{\alpha} + (1-x)^{\alpha} ; x \in I \equiv [0,1].$$

For this purpose we shall establish the following Lemma which is of some interest on its own right.

Lemma 1. The function

$$h_{\beta}(x) \equiv [f_{\beta}(x)]^{-1} = \{x^{\beta} + (1-x)^{\beta}\}^{-1} ; x \in I = [0,1],$$

has the following properties:

(i) for $\beta \in (-\infty, -1)$ and $\beta \in [2, \infty)$, h_{β} has inflection points on I; (ii) for $\beta \in (0, 1)$, h_{β} is (strictly) convex on I; (iii) for $\beta \in [-1, 0]$, h_{β} is concave on I; (iv) for $\beta \in [1, 5/3]$, h_{β} is concave on I while for $\beta \in (5/3, 2)$, h_{β} has inflection points on I.

Proof. We have

$$h_{\beta''} = f_{\beta}^{-3} [2(f_{\beta}')^2 - \beta(\beta - 1)f_{\beta}f_{\beta - 2}]$$

and item (ii) follows at once. To proceed with the other items, we study the sign of the function

$$2(f_{\beta}^{\prime})^{2} - \beta(\beta-1)f_{\beta}f_{\beta-2}$$

= $2\beta^{2}[x^{\beta-1} - (1-x)^{\beta-1}]^{2} - \beta(\beta-1)[x^{\beta-2} + (1-x)^{\beta-2}][x^{\beta} + (1-x)^{\beta}].$

This function is symmetric about the point x = 1/2 and it is therefore more convenient to introduce the new variable, y=(1-x)/x with $y \in [0,1]$. This corresponds to $x \in [1/2,1]$ and by symmetry y may also be allowed to range in $[1,\infty]$. With this new variable, the sign of the above function is the same as that of

$$\mathbf{F}_{\beta}(\mathbf{y}) \equiv \beta \{ 2\beta (1-y^{\beta-1})^2 - (\beta-1)(1+y^{\beta}) (1+y^{\beta-2}) \} .$$

This may be also written as

$$F_{\beta}(y) = \beta\{(\beta+1)(1-y^{\beta-1})^2 - (\beta-1)y^{\beta-2}(1+y)^2\}.$$
 (4.1)

When $\beta \in [-1,0]$ it follows from (4.1) that $F_{\beta}(y) \leq 0$ and therefore item (iii) follows. As for item (i), we see from (4.1) that

$$F_{\beta}(0) = +\infty$$
, $F_{\beta}(1) = 4\beta(1-\beta) < 0$ for $\beta \in (-\infty, -1)$,
 $F_{2}(0) = 4$, $F_{2}(1) = -8$

and

$$F_{\beta}(0) = \beta(\beta+1) > 0$$
, $F_{\beta}(1) = -4\beta(\beta-1) < 0$, for $\beta \in (2,\infty)$.

Consequently, item (i) follows. We turn now to item (iv). Here $F_1(\underline{v}) \equiv 0$ and we shall therefore assume that $\beta \in (1,2)$. A differentiation of (4.1) gives

$$\mathbf{F}'_{\beta}(\mathbf{y}) = \beta(\beta-1)\mathbf{y}^{\beta-3} \{2(\beta+1)\mathbf{y}^{\beta}-\beta\mathbf{y}^{2}-4\beta\mathbf{y}+2-\beta\}.$$

The sign of this derivative is determined by

$$G_{\beta}(y) \equiv 2(\beta+1)y^{\beta} - \beta y^2 - 4\beta y + 2 - \beta$$
.

Now,

$$G_{\beta}(0) = 2 - \beta > 0$$
, $G_{\beta}(1) = -4(\beta - 1) < 0$,

and hence $G_{\beta}(y_{\beta}) = 0$ for some $y_{\beta} \in (0,1)$. Next, we have

$$G'_{\beta}(y) = 2\beta\{(\beta+1)y^{\beta-1} - y - 2\}$$
.

However, by Bernoulli's inequality

$$y + 2 - (\beta + 1)y^{\beta - 1} = y + 2 - (\beta + 1)[1 - (1 - y)]^{\beta - 1}$$

$$\geq y + 2 - (\beta + 1)[1 - (\beta - 1)(1 - y)]$$

$$= (2 - \beta^{2})y + \beta(\beta - 1).$$

The last expression describes a straight line passing through the points $(0, \beta^2 - \beta)$ and $(1, 2-\beta)$ and therefore

$$y+2 - (\beta+1)y^{\beta-1} > 0$$
 for $y \in (0,1)$

Consequently, y_{β} is the only root of $G_{\beta}(y) = 0$ in (0,1) and, moreover, $F_{\beta}(y)$ has a <u>single maximum</u> at $y_{\beta} \in (0,1)$. The root y_{β} lies in the variety.

$$2(\beta+1)y^{\beta} = \beta y^{2} + 4\beta y + \beta - 2 . \qquad (4.2)$$

We replace y^{β} in (4.1) by the quadratic expression in (4.2). This, after some manipulations, results in

$$H_{\beta}(y) \equiv -4 \frac{\beta+1}{\beta^2} y^2 F_{\beta}(y) = (\beta-2)y^4 + 8(\beta-1)y^3 + 2(7\beta-6)y^2 + 8(\beta-1)y + \beta-2$$

and, hence, we seek β for which $H_{\beta}(y_{\beta}) \ge 0$. However, we can factor $H_{\beta}(y)$ in the form of

$$H_{\beta}(y) = (\beta-2)(1+y)^2 [y-B(\beta)][y-B(\beta)^{-1}]$$

where

$$B(\beta) \equiv (2-\beta)^{-1} \{3\beta-2-2[2\beta(\beta-1)]^{\frac{1}{2}}\}.$$

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. . .

Since $\beta \in (1,2)$, we clearly have $0 < B(\beta) < 1 < B(\beta)^{-1}$. Hence, $H_{\beta}(y_{\beta}) \ge 0$ if and only if

$$y_{\beta} \geq B(\beta)$$
.

This condition is equivalent to the requirement that $F_{\beta}[B(\beta)] \ge 0$. This requirement is determined by the region of non-negativity of the function $K(\beta)$ defined below. This interesting function is defined as follows:

$$\mathbf{K}(\beta) \equiv \mathbf{2}(\beta+1)\mathbf{B}(\beta)^{\beta} - \beta \mathbf{B}(\beta)^{2} - 4\beta\mathbf{B}(\beta) + 2 - \beta \quad ; \quad \beta \in (1,2).$$

We have

K(1)=K(2)=0; $K'(1)=+\infty$, K'(2)=0.

Moreover, a direct calculation shows that K(5/3) = 0 and that $\beta = 5/3$ is the cut-off point of the region of non-negativity. Thus $K(\beta) > 0$ for all $\beta \in (1, 5/3)$, K(5/3) = 0 and $K(\beta) < 0$ for all $\beta \in (5/3, 2)$, (see Figure 1). The proof of the lemma is now complete.

Before proceeding any further we shall record an interesting consequence of this lemma, or rather from the proof of the lemma.

<u>Corollary 5</u>. For any $\gamma \in [0, 2/3]$ the following inequality holds for all $t \in (-\infty, \infty)$

$$\left(\frac{\sinh\gamma t}{\cosh t}\right)^2 \leq \frac{\gamma}{\gamma+2} \quad . \tag{4.3}$$

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<u>Proof</u>. From (4.1) we know that $F_{\beta}(y) \leq 0$ for $\beta \in [1, 5/3]$ and, therefore,

$$(\beta+1)(1-y^{\beta-1})^2 \leq (\beta-1)y^{\beta-2}(1+y)^2.$$

This was proved for $y \in [0,1]$. However, this inequality is invariant under the substitution $y \neq y^{-1}$ and, therefore, it is valid for all $y \in (0,\infty)$. Setting $y^{\frac{1}{2}} = e^{t}$ and $\beta = \gamma + 1$ concludes the proof.

Corresponding to Theorem 1 and Corollaries 1 and 2, Lemma 1 leads to :

Theorem 2. Let

$$g_{\alpha}(x) = af_{\alpha}(x) + bx + c$$
, $x \in I = [0,1]$,

where a,b,c and α are constants with $a\alpha(\alpha-1) > 0$ and

$$f_{\alpha}(x) = x^{\alpha} + (1-x)^{\alpha}$$
.

Then $H_{n,g_{\alpha}}$ is convex on I^n . Moreover, $J_{n,g_{\alpha}}$ is never concave on $I^n \times I^n$. It is convex there if and only if $\alpha \in [1,2]$ or $\alpha \in [3,11/3]$, in which case $a \ge 0$.

Theorem 2 enables us to strengthen the result of Corollary 4 on the Jensen difference of the α -order entropy with the following additional feature:

Corollary 6. $J_{2,\alpha}$ is convex on $\overline{S}_2 \times \overline{S}_2$ if and only if $\alpha \in [1,2]$ or $\alpha \in [3,11/3]$.

In correspondence with (2.11) we define

$$g_{\alpha}(x) = \begin{cases} (\alpha-1)^{-1} [x^{\alpha} + (1-x)^{\alpha}] , & \alpha \neq 1 \\ \\ x \log x + (1-x) \log(1-x) , & \alpha \neq 1 \end{cases}$$
(4.4)

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for $x \in I \equiv [0,1]$. We also define

$$G_{n,\alpha}(x) \equiv H_{n,g_{\alpha}}(x) , x \in S_{n},$$
 (4.5)

and call $G_{n,\alpha}(x)$, $x \in S_n$, the <u>paired entropy of order α </u>. Using (2.11) - (2.14), we clearly have the following relationships:

$$G_{n,\alpha}(x) = H_{n,\alpha}(x) + H_{n,\alpha}(1-x) - (\alpha-1)^{-1} ; \alpha \neq 1, x \in S_n$$

$$G_{n,1}(x) = H_{n,1}(x) + H_{n,1}(1-x) ; x \in \overline{S}_n$$
We shall write

$$I_{n,\alpha}(x,y) \equiv J_{n,g_{\alpha}}(x,y) ; (x,y) \in S_n \times S_n$$
(4.6)

for the Jensen difference of g_{α} of (4.4). From Theorems 1, 2 and (2.6)-(2.10) we conclude :

<u>Theorem 3</u>. Let the notation of (4.4)-(4.6) apply with $\alpha \ge 0$. Then:

- (i) $G_{n,\alpha}$ is concave on \overline{S}_n ;
- (ii) $I_{n,\alpha}$ is never concave on $\bar{S}_n \times \bar{S}_n$;

(iii) $I_{n,\alpha}$ is convex on $\overline{S}_n \times \overline{S}_n$ if and only if $\alpha \in [1,2]$ or $\alpha \in [3,11/3]$.

In particular,

(iv) $G_{n,1}$ is concave on \overline{S}_n and $I_{n,1}$ is convex on $\overline{S}_n \times \overline{S}_n$.

Item (iv) of this theorem is a limiting case of the previous items as $\alpha \rightarrow 1$. It could also be directly deduced from Theorem 4. Indeed, from (4.4), $g''_1(x) = [x(1-x)]^{-1} > 0$ which

shows that g_1 is convex on (0,1). Furthermore, $F = (g_1'')^{-1}$ is given by $F(x) = x - x^2$ and thus F''(x) = -2 < 0. Therefore, $(g_1'')^{-1}$ is concave on [0,1] and Theorem 1 applies.

It may be noted that we could base our analysis of sections 3 and 4 on a more generalized form of the Jensen difference

$$J_{\phi}^{(\alpha,\beta)}(x,y) = 2[\alpha \phi(x) + \beta \phi(y) - \phi(\alpha x + \beta y)]$$
(4.7)

with $\alpha, \beta \ge 0$, $\alpha + \beta = 1$, so that (4.7) reduces to J_{ϕ} when $\alpha = \beta$. However, this does not constitute a major generalization and the results obtained for J_{ϕ} can also be derived for $J_{\phi}^{(\alpha,\beta)}$ after a minor modification of the argument.

5. THE K-DIVERGENCE

We briefly discuss the K-divergence $K_{n,\phi}$ defined in (2.4) and its relationship with the J-divergence $J_{n,\phi}$. To do this we define

$$\psi(\mathbf{x}) \equiv \phi(\mathbf{x})/\mathbf{x} ; \mathbf{x} \in \mathbf{R}_{\perp} . \tag{5.1}$$

We start with the following simple proposition:

<u>Proposition 1</u>. $K_{n,\phi}$ is non-negative on $\mathbb{R}^n_+ \times \mathbb{R}^n_+$ if and only if ψ is increasing on \mathbb{R}_+ .

Proof. This is equivalent to the specialized statement with

n=1 which in turn is straightforward.

The following theorem establishes a comparison between $K_{n,\,\phi} \text{ and } J_{n,\,\phi}:$

<u>Theorem 4</u>. Assume that ψ is increasing and concave on I. Then, for any $(x,y) \in \mathbb{R}^n_+ \times \mathbb{R}^n_+$,

$$J_{n,\phi}(x,y) \leq K_{n,\phi}(x,y)$$

with equality if and only if x = y.

<u>Proof.</u> Again, this statement is equivalent to the specialized case of n=1. Accordingly, we consider the function

$$F(x,y) \equiv J_{1,\phi}(x,y) - K_{1,\phi}(x,y) \quad ; \quad (x,y) \in \mathbb{R}_{+} \times \mathbb{R}_{+}$$

This may be written as

$$\frac{\mathbf{F}(\mathbf{x},\mathbf{y})}{\mathbf{x}+\mathbf{y}} = \frac{\mathbf{y}}{\mathbf{x}+\mathbf{y}} \ \psi(\mathbf{x}) + \frac{\mathbf{x}}{\mathbf{x}+\mathbf{y}} \ \psi(\mathbf{y}) - \psi[(\mathbf{x}+\mathbf{y})/2]$$
$$\leq \psi\left(\frac{\mathbf{y}\mathbf{x}}{\mathbf{x}+\mathbf{y}} + \frac{\mathbf{x}\mathbf{y}}{\mathbf{x}+\mathbf{y}}\right) - \psi\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right)$$
$$= \psi\left(\frac{2\mathbf{x}\mathbf{y}}{\mathbf{x}+\mathbf{y}}\right) - \psi\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right) \le 0.$$

The first inequality follows from the concavity of ψ while the second inequality is due to the fact that ψ is increasing on \mathbb{R}_+ . The equality statement also follows and the proof is complete.

The Hessian of $K_{n,\phi}$, in accordance with (2.1), is given

$$\Delta_{(u,v)} K_{n,\phi}(x,y) = \sum_{i=1}^{n} \{a(x_i,y_i)u_i^2 + 2b(x_i,y_i)u_iv_i + a(y_i,x_i)v_i^2\}$$
(5.2)

where $x, y \in \mathbb{R}^n_+$ and for $x, y \in \mathbb{R}_+$,

$$a(x,y) = \phi''(x) - y \psi''(x)$$
 (5.3)

and

$$b(x,y) = -[\psi'(x) + \psi'(y)]$$
 (5.4)

with ψ as given in (5.1). It follows, therefore, that $K_{n,\phi}$ is convex if and only if $a(x,y) \ge 0$ and

$$d(\mathbf{x},\mathbf{y}) \equiv a(\mathbf{x},\mathbf{y})a(\mathbf{y},\mathbf{x}) - [b(\mathbf{x},\mathbf{y})]^2 \ge 0 \quad ; \quad \mathbf{x},\mathbf{y} \in \mathbb{R}_+ \quad (5.5)$$

From (5.3) we see that $a(x,y) \ge 0$ whenever ϕ is convex and ψ is concave on \mathbb{R}_+ . We have:

Theorem 5. Assume that ϕ is convex and ψ is concave on \mathbb{R}_+ . Then:

- (i) ψ is increasing on \mathbb{R}_{\perp} ;
- (ii) $K_{n,\phi}(x,y) \ge J_{n,\phi}(x,y) \ge 0$ for every $(x,y) \in \mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$. Equality in one of the inequalities entails equalities in both inequalities. This occurs if and only if x=y.

If, in addition, (5.5) holds, then:

- (iii) $\mathbb{K}_{n,\phi}$ is convex on $\mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$;
- (iv) $\mathbb{K}_{n,\phi}$ is convex on $S_n \times S_n$.

Proof. Using (5.1) we have

$$\psi'(\mathbf{x}) = -\frac{1}{\mathbf{x}} \left[\psi(\mathbf{x}) - \phi'(\mathbf{x}) \right]$$

by

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and thus

$$\psi''(\mathbf{x}) = -\frac{1}{\mathbf{x}} \left[\psi'(\mathbf{x}) - \phi''(\mathbf{x}) \right] + \frac{1}{\mathbf{x}^2} \left[\psi(\mathbf{x}) - \phi'(\mathbf{x}) \right]$$
$$= -\frac{1}{\mathbf{x}} \left[2\psi'(\mathbf{x}) - \phi''(\mathbf{x}) \right] .$$

Therefore

$$2\psi'(x) = -x\psi''(x)+\phi''(x) > 0$$

and (i) follows. The fact that $J_{n,\phi}(x,y) \ge 0$ and its equality statement is a result of ϕ being convex. Also, $K_{n,\phi}(x,y) \ge J_n(x,y)$ and its equality statement follows from item (i) because of Porposition 1 and Theorem 4. This proves item (ii). Item (iii) follows from item (i) and the preceeding discussion. Item (iv) follows from (iii), (5.2) and formulae similar to (2.6) - (2.10). This concludes the proof.

The following hold:

Theorem 6. Let $\alpha \in [1,2]$. Then:

(i) $K_{n,\phi_{\alpha}}(x,y) \ge J_{n,\phi_{\alpha}}(x,y) \ge 0$ for every $(x,y) \in \mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$. Equality in one of the inequalities occurs if and only if x=y. The same applies to $K_{n,\alpha}(x,y) \ge J_{n,\alpha}(x,y) \ge 0$ for every $(x,y) \in S_{n} \times S_{n}$.

(ii) $K_{n,\phi_{\alpha}}$ is convex on $\mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$ and $K_{n,\alpha}$ is convex on $S_{n} \times S_{n}$.

<u>Proof</u>. In this case ϕ_{α} is convex and ψ_{α} is concave on \mathbb{R}_{+} and, therefore, we may use Theorem 5. To do so, we have to validate (5.5), i.e., we have to show that the discriminant function

 $\mathbf{d}_{\alpha}(\mathbf{x},\mathbf{y}) \equiv [\alpha \mathbf{x}^{\alpha-2} - (\alpha-2)\mathbf{y}\mathbf{x}^{\alpha-3}][\alpha \mathbf{y}^{\alpha-2} - (\alpha-2)\mathbf{x}\mathbf{y}^{\alpha-3}] - (\mathbf{x}^{\alpha-2} + \mathbf{y}^{\alpha-2})^2$

is non-negative on $\mathbb{R}_{+} \times \mathbb{R}_{+}$. Here, $d_{1}(x,y) \equiv d_{2}(x,y) \equiv 0$; we may, therefore, assume that $\alpha \in (1,2)$. Since $d_{\alpha}(x,x)=0$ and $d_{\alpha}(x,y)=d_{\alpha}(y,x)$ it is sufficient to assume that y > x > 0. In this way, we have

$$d_{\alpha}(x,y) = x^{2\alpha-4} f_{\alpha}(t) ; t \in y/x,$$

where

$$f_{\alpha}(t) \equiv t^{\alpha-3} [\alpha t - (\alpha - 2)] [\alpha - (\alpha - 2)t] - (1 + t^{\alpha - 2})^2 .$$
 (5.6)

We must show that $f_{\alpha}(t) \geq 0$ for $t \in (1, \infty)$. After some simplifications, we obtain

$$f'_{\alpha}(t) = (2-\alpha)t^{\alpha-4}g_{\alpha}(t)$$

with

$$g_{\alpha}(t) \equiv \alpha(\alpha-1)t^{2} - 2(\alpha-1)^{2}t - \alpha(3-\alpha) + 2t^{\alpha-1}$$

Therefore,

$$g'_{\alpha}(t) = 2(\alpha-1)[\alpha(t-1)+1+t^{\alpha-2}] > 0$$
; $t \in (1,\infty), \alpha \in (1,2)$,

Hence g_{α} is increasing on $(1,\infty)$ and since $g_{\alpha}(1) = 0$, we conclude that $g_{\alpha}(t) > 0$. Therefore, $f'_{\alpha}(t) > 0$ or that f_{α} is increasing on $(0,\infty)$. However, $f_{\alpha}(1) = 0$ and thus $f_{\alpha}(t) > 0$ for $t \in (1,\infty)$. This concludes the proof.

From the proof of this theorem we also deduce the following inequality:

<u>Corollary 6</u>. Let $\beta \in [0, 1/2]$ Then, for every $s \in (-\infty, \infty)$,

$$\cosh^{2}\beta s \leq [\beta^{2} + (1-\beta^{2})][1 + \frac{2\beta(1-\beta)}{\beta^{2} + (1-\beta)^{2}} \cosh \beta].$$
(5.7)

<u>Proof</u>. For $\alpha \in [1,2]$ we have shown that f_{α} of (5.6) satisfies $f_{\alpha}(t) \geq 0$ for every $t \in [1,\infty)$. This is equivalent to

$$[\alpha t - (\alpha - 2)][\alpha t^{-1} - (\alpha - 2)] \ge [t^{(2-\alpha)/2} + t^{-(2-\alpha)/2}]$$

for every $t \in [1,\infty)$. Since this inequality is invariant under the transition $t \rightarrow t^{-1}$, it holds for every $t \in (0,\infty)$. Putting $t = e^{S}$ and $\beta = (2-\alpha)/2$ concludes the proof.

6. THE L-DIVERGENCE

The Hessian of $L_{n,\phi}(x,y)$ defined in (2.5), in view of (2.1), is

 $\Delta_{(u,v)} L_{n,\phi}(x,y) = \sum_{i=1}^{n} \{a(x_{i},y_{i})u_{i}^{2} + 2b(x_{i},y_{i})u_{i}v_{i} + a(y_{i},x_{i})v_{i}^{2}\}$ where $(x,y) \in \mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$. Here

$$a(x,y) = \frac{1}{y} \phi''(\frac{x}{y}) + (\frac{y^2}{x^2} \phi''(\frac{y}{x})$$

and

$$b(x,y) = -\frac{x}{y^2} \phi''(\frac{x}{y}) - \frac{y}{x^2} \phi''(\frac{y}{x}) ; x, y \in \mathbb{R}_+$$

In this case, the discriminant

$$d(x,y) = a(x,y)a(y,x) - [b(x,y)]^2$$

is identically zero on $\mathbb{R}_+ \times \mathbb{R}_+$. This, together with formulae similar to (2.6)-(2.10), leads to:

Theorem 7. The following hold:

- (i) $L_{n,\phi}(x,y) \ge 0$ for every $n \ge 1$ and every $(x,y) \in \mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$ if and only if the function $\psi(t) \equiv t \phi(t^{-1}) + \phi(t)$ is non-negative for all $t \in \mathbb{R}_{+}$;
- (ii) $L_{n,\phi}$ is convex on $\mathbb{R}^{n}_{+} \times \mathbb{R}^{n}_{+}$ if and only if $\psi(t) \equiv t \phi(t^{-1}) + \phi(t)$ is convex on \mathbb{R}_{+} .

Proof. As for item (i), we have

$$L_{n,\phi}(x,y) = \sum_{i=1}^{n} \frac{1}{x_i} \psi(t_i) ; t_i = y_i/x_i$$

and $L_{1,\phi}(x,y) = x^{-1}\psi(t)$, t = y/x. Thus (i) follows. As for item (ii), since $d(x,y) \equiv 0$ for every $(x,y) \in \mathbb{R}_+ \times \mathbb{R}_+$ we have that $D_{n,\phi}$ is convex on $\mathbb{R}^n_+ \times \mathbb{R}^n_+$ if and only if

$$a(x,y) = \frac{y^2}{x^3} \left\{ \frac{x^3}{y^3} \phi''(\frac{x}{y}) + \phi''(\frac{y}{x}) \right\} \ge 0 \quad ; \quad (x,y) \in \mathbb{R}_+ \times \mathbb{R}_+.$$

Putting t = y/x this condition becomes

$$t^{-3}\phi''(t^{-1}) + \phi''(t) \ge 0$$
; $t \in \mathbb{R}_+$.

This means that $\psi''(t) \ge 0$ and the theorem follows.

<u>Corollary 7</u>. For any $\alpha \ge 0$, $L_{n,\alpha}$ is a non-negative convex function on $S_n \times S_n$.

<u>Proof.</u> We use Theorem 7 and formulae similar to (2.6)-(2.10) for $\Delta_{(u,v)}L_{n,\alpha}(x,y)$ on $S_n \times S_n$. We start with

and the second second

 $\alpha = 1$. In this case

$$\phi_1(t) = t \log t$$
, $\psi_1(t) \equiv t \phi_1(t^{-1}) + \phi_1(t)$; $t \in \mathbb{R}_+$,

and thus

$$\psi_1(t) = (t-1)\log t \ge 0$$
, $\psi''_1(t) = (t^{-1} + t^{-2}) > 0$, $t \in \mathbb{R}_+$.

On the other hand, for $\alpha \neq 1$,

$$\phi_{\alpha}(t) = (\alpha - 1)^{-1}(t^{\alpha} - t), \quad \psi_{\alpha}(t) \equiv t\phi_{\alpha}(t^{-1}) + \phi_{\alpha}(t); \quad t \in \mathbb{R}_{+}.$$

Therefore, for $\alpha \ge 0$, $\alpha \ne 1$,

$$\psi_{\alpha}(t) = (\alpha - 1)^{-1} t^{1 - \alpha} (t^{\alpha - 1} - 1) (t^{\alpha} - 1) \ge 0 \quad ; \quad t \in \mathbb{R}_{+}$$

and

$$\psi''_{\alpha}(t) = \alpha \left(t^{\alpha-2} + t^{-\alpha-1}\right) \ge 0 \quad ; \quad t \in \mathbb{R}_{+} \quad .$$

This concludes the proof.

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