The Maximal Extension of the Strict Concavity Region on the Parameter Space for Sharma-Mittal Entropy Measures

R. P. Mondaini and S. C. de Albuquerque Neto

1 Introduction

The present work aims to complement a previous publication [1] where we have derived the Generalized Khinchin-Shannon (GKS) Inequalities [2] associated to Sharma-Mittal Entropy measures. We introduce here the result of maximal extension of the strict concavity region of this class of entropy measures. In Sect. 2, we present the state of art of the work with the Sharma-Mittal class as well as the Information measures associated to it. All the limit processes are then described carefully together with the consequences of these definitions and their properties with respect to the assumption of strict concavity. We think that the notation which has been adopted could appear as awkward, however it is very efficient for the derivation of all formulae to be presented here and specially for the proof of strict concavity of Sect. 3. A complete derivation is then done of the greatest lower bound of the successive epigraph regions, which leads to establish the maximal extension of the previously adopted strict concavity region of the scientific literature. In Sect. 4, we then derive some interesting additional matters to a subject already published in ref. [1], in terms of the difference between escort conditional probabilities and conditional escort probabilities. Some necessary development seems to be worthwhile here for a perfect understanding of the results based on the structure and properties of the probabilistic space and this is presented in appendices at the end of the paper.

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2 The Sharma-Mittal Class of Entropy Measures

The usual expression of the Sharma-Mittal entropy measures [3], is given by:

$$(SM)^{(s,r)}_{j_1\dots j_t} = \frac{(\alpha_{j_1\dots j_t})^{\frac{1-r}{1-s}} - 1}{1-r} \tag{1}$$

These entropies are here defined on arrays of t columns of m rows each and the $\alpha_{j_1\dots j_t}$ symbols are written as:

$$\alpha^{(s)}_{j_1\dots j_t} = \sum_{a_1,\dots,a_t} \Big(p_{j_1\dots j_t}(a_1, \dots, a_t)\Big)^s \tag{2}$$

where $p_{j_1\dots j_t}(a_1, \dots, a_t)$ stands for the probability of occurrence of t-sets of ordered values $(a_1, \dots, a_t)$ in t columns $j_1, \dots, j_t$ of a distribution obtained from an array of m rows and n columns (see Appendix 1).

All the values $a_1, \dots, a_t$, are running over the values $1, \dots, W$ and the j-values are ordered as [4]:

$$j_1 < j_2 < \dots < j_n$$

and we have,

$$\begin{aligned} j_1 &= 1, \dots, n-t+1 \\ j_2 &= j_1 + 1, \dots, n-t+2 \\ &\dots\dots\dots\dots\dots\dots \\ j_{t-1} &= j_{t-2} + 1, \dots, n-1 \\ j_t &= j_{t-1} + 1, \dots, n \end{aligned} \tag{3}$$

There are then $\binom{n}{t} = \frac{n!}{t!(n-t)!}$ geometrical objects $p_{j_1\dots j_t}$ and each of them has W^t correspondents $p_{j_1\dots j_t}(a_1, \dots, a_t)$.

For an equiprobable distribution [4],

$$p_{j_1\dots j_t}(a_1, \dots, a_t) = W^{-t}\,, \tag{4}$$

we then get

$$\alpha_{j_1\dots j_t}(W^{-t}) = W^t (W^{-t})^s = W^{t(1-s)}\,,\ \forall t \tag{5}$$

and the corresponding value of the $(SM)_{j_1 \ldots j_t}$ entropy will be written as:

$$(SM)^{(r)}_{j_1 \ldots j_t}(W^{-t}) = \frac{\left(W^{t(1-s)}\right)^{\frac{1-r}{1-s}} - 1}{1-r} = \frac{W^{t(1-r)} - 1}{1-r}\,. \tag{6}$$

We also introduce an associated Information measure:

$$I^{(s,r)}_{j_1 \ldots j_t} = -\frac{(SM)_{j_1 \ldots j_t}}{(\alpha_{j_1 \ldots j_t})^{\frac{1-r}{1-s}}} \tag{7}$$

For an equiprobable distribution, Eq. (4), this can be written as:

$$I^{(s,r)}_{j_1 \ldots j_t}(W^{-t}) = -\frac{\frac{W^{t(1-r)} - 1}{1-r}}{W^{t(1-r)}} = \frac{1 - W^{t(1-r)}}{(1-r)W^{t(1-r)}} \tag{8}$$

We then list some special cases of entropies of the Sharma-Mittal class [3, 5–7] together with their equiprobable versions:

(a) The Havrda-Charvat entropy measure [5], with $r = s$

$$(HC)^{(s)}_{j_1 \ldots j_t} = \frac{\alpha_{j_1 \ldots j_t} - 1}{1-s} \tag{9}$$

$$(HC)^{(s)}_{j_1 \ldots j_t}(W^{-t}) = \frac{W^{t(1-s)} - 1}{1-s} \tag{10}$$

(b) The Landsberg-Vedral entropy measure [6], with $r = 2 - s$

$$(LV)^{(s)}_{j_1 \ldots j_t} = \frac{\alpha_{j_1 \ldots j_t} - 1}{(1-s)\alpha_{j_1 \ldots j_t}} = \frac{(HC)^{(s)}_{j_1 \ldots j_t}}{\alpha_{j_1 \ldots j_t}} \tag{11}$$

$$(LV)^{(s)}_{j_1 \ldots j_t}(W^{-t}) = \frac{W^{t(1-s)} - 1}{(1-s)W^{t(1-s)}} = -I^{(r=s)}_{j_1 \ldots j_t} \tag{12}$$

(c) The Renyi entropy measure [7]:

$$R^{(s)}_{j_1 \ldots j_t} = \lim_{r \to 1} (SM)^{(s,r)}_{j_1 \ldots j_t} = \frac{\log \alpha_{j_1 \ldots j_t}}{1-s} \tag{13}$$

$$R^{(s)}_{j_1\ldots j_t}(W^{-t}) = \frac{\log W^{t(1-s)}}{1-s} = \frac{t(1-s)\log W}{1-s} = t\log W \tag{14}$$

(d) The "nonextensive Gaussian" entropy measure [8]:

$$G^{(r)}_{j_1\ldots j_t} = \lim_{s\to 1}(SM)^{(s,r)}_{j_1\ldots j_t} = \frac{e^{(1-r)(GS)_{j_1\ldots j_t}}-1}{1-r} \tag{15}$$

$$G^{(r)}_{j_1\ldots j_t}(W^{-t}) = \frac{e^{t(1-r)\log W}-1}{1-r} \tag{16}$$

where

$$(GS)_{j_1\ldots j_t} = -\sum_{a_1,\ldots,a_t} p_{j_1\ldots j_t}(a_1,\ldots,a_t)\log p_{j_1\ldots j_t}(a_1,\ldots,a_t) \tag{17}$$

$$(GS)_{j_1\ldots j_t}(W^{-t}) = t\log W \tag{18}$$

is the Gibbs-Shannon entropy measure, which is also obtained as the convenient limit in all previous entropy measures.

$$\lim_{s\to 1}(HC)^{(s)}_{j_1\ldots j_t} = \lim_{s\to 1}(LV)^{(s)}_{j_1\ldots j_t} = \lim_{s\to 1}R^{(s)}_{j_1\ldots j_t} = \lim_{r\to 1}G^{(r)}_{j_1\ldots j_t} = (GS)_{j_1\ldots j_t} \tag{19}$$

From Eqs. (1) and (2) the Generalized Khinchin-Shannon inequalities can be written according to ref. [1] as:

$$1+(1-r)(SM)^{(s,r)}_{j_1\ldots j_t} \le \prod_{l=1}^{t}\left[1+(1-r)(SM)^{(s,r)}_{j_l}\right] \tag{20}$$

We can also then write for the information measure in [7]:

$$1+(1-r)I^{(s,r)}_{j_1\ldots j_t} \ge \prod_{l=1}^{t}\left[1+(1-r)I^{(s,r)}_{j_l}\right] \tag{21}$$

For the special cases of the Sharma-Mittal class, Eqs. (9), (11), (13), (15), and (17), we have,

$$1+(1-s)(HC)^{(s)}_{j_1\ldots j_t} \le \prod_{l=1}^{t}\left[1+(1-s)(HC)^{(s)}_{j_l}\right] \tag{22}$$

$$1 + (1 - s)(LV)^{(s)}_{j_1 \ldots j_t} \le \prod_{l=1}^{t} \left[1 + (1 - s)(LV)^{(s)}_{j_l} \right] \tag{23}$$

$$R^{(s)}_{j_1 \ldots j_t} \le \sum_{l=1}^{t} R^{(s)}_{j_l} \tag{24}$$

$$1 + (1 - r)G^{(r)}_{j_1 \ldots j_t} \le \prod_{l=1}^{t} \left[1 + (1 - r)G^{(r)}_{j_l} \right] \tag{25}$$

$$(GS)_{j_1 \ldots j_t} \le \sum_{l=1}^{t} (GS)_{j_l} \tag{26}$$

The region of the parameter space corresponding to strict concavity of the Sharma-Mittal class of entropies is usually presented in the literature as the gray region in Fig. 1 or $C = \{(s, r) | r \ge s > 0\}$. This region is the epigraph region of the half straight line $r = s > 0$, corresponding to the Havrda-Charvat entropy, Eqs. (9) and (2).

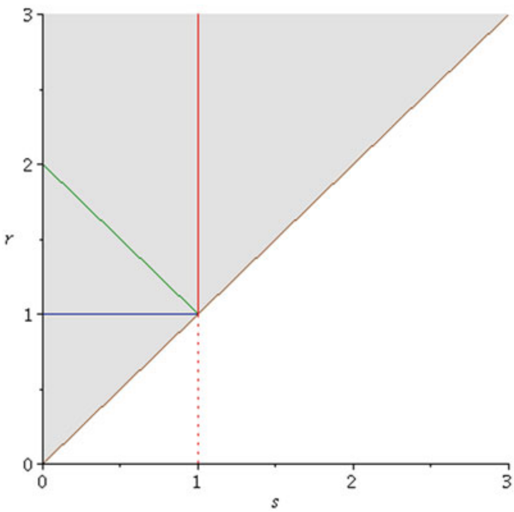


Fig. 1 The gray region is the epigraph of the brown half straight line ($r = s$) corresponding to the Havrda-Charvat entropy. This region is also assumed to be the strict concavity region in the literature. The The blue ($0 \le s < 1, r = 1$), green ($0 \le s < 1, 1 < r \le 2$) segments of straight line do correspond to Renyi and Landsberg-Vedral entropies, respectively. The red half straight line ($r > 1, s = 1$) stands for the "Gaussian" entropy which has also been defined by Sharma-Mittal [3]. The point ($r = 1, s = 1$) does correspond to the Gibbs-Shannon entropy

3 The Maximal Extension of the Strict Concavity Region in the Parameter Space of Sharma-Mittal (SM) Entropy Measures

To undertake the analysis of maximal extension of the strict concavity region for SM entropies, we shall follow the techniques of construction of the probabilistic space in Appendix 1. In the next section, we also give some examples as numerical applications of the methods introduced here.

The requirement for strict concavity of the surface representing a multivariate function is the negative definiteness of the quadratic form associated to its Hessian matrix [1, 11]. This means that the principal minors of the Hessian matrix should be negative and positive alternately (negative those of odd order and positive those of even order).

We shall now introduce the Hessian matrix of the Sharma-Mittal class of entropies, Eqs. (1), (2), and (3). Its first derivative is given by:

$$\frac{\partial (SM)_{j_1\ldots j_t}}{\partial p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})} = \frac{s}{1-s}(\alpha_{j_1\ldots j_t})^{\frac{s-r}{1-s}}\left(p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})\right)^{s-1} \tag{27}$$

A generic element of the Hessian matrix could then be written as

$$\begin{aligned} H_{q_\nu q_\xi} &= \frac{\partial^2 (SM)_{j_1\ldots j_t}}{\partial p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})\partial p_{j_1\ldots j_t}(a_1^{q_\xi},\ldots,a_t^{q_\xi})} \\ &= s(\alpha_{j_1\ldots j_t})^{\frac{s-r}{1-s}}\left(p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})\right)^{s-2} \\ &\quad \cdot\left[\frac{s(s-r)}{(1-s)^2}\frac{p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})}{p_{j_1\ldots j_t}(a_1^{q_\xi},\ldots,a_t^{q_\xi})}\hat{p}_{j_1\ldots j_t}(a_1^{q_\xi},\ldots,a_t^{q_\xi}) - \delta_{\nu\xi}\right] \end{aligned} \tag{28}$$

where $\delta_{\nu\xi}$ is the Kronecker symbol. From Eq. (28) and Appendix 1, the principal minors are then given by

$$\begin{aligned} \det H_{q_\nu q_\xi}(\nu,\xi=1,\ldots,k) &= (-1)^{k-1}s^k(\alpha_{j_1\ldots j_t})^{k\left(\frac{s-r}{1-s}\right)}\left[\prod_{\nu=1}^{k} p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})\right]^{s-2} \\ &\quad \cdot\left[\frac{s(s-r)}{(1-s)^2}\sum_{\nu=1}^{k}\hat{p}_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu}) - 1\right], \quad k=1,\ldots,M,\ 1\le M\le m, \end{aligned} \tag{29}$$

where $\hat{p}_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})$ is the escort probability associated to $p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})$ and we have,

$$\hat{p}_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu}) = \frac{\left(p_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu})\right)^s}{\sum\limits_{b_1^{q_\nu},\ldots,b_t^{q_\nu}}\left(p_{j_1\ldots j_t}(b_1^{q_\nu},\ldots,b_t^{q_\nu})\right)^s} \tag{30}$$

with $a_j^{q_\nu}; b_j^{q_\nu} = 1,\ldots,W; \nu = 1,\ldots,k; k = 1,\ldots,M.$

$$\sum_{a_1^{q_\nu},\ldots,a_t^{q_\nu}} \hat{p}_{j_1\ldots j_t}(a_1^{q_\nu},\ldots,a_t^{q_\nu}) = 1 \tag{31}$$

From Eqs. (29) and (30), and Eqs. (42)–(46) of Appendix 1, and Eqs. (64)–(68) of Appendix 2, the requirement of strict concavity could be given through the second square bracket of Eq. (29) and we can then write,

$$\left[\frac{s(s-r)}{(1-s)^2}\frac{\sum\limits_{\mu=1}^{k}\left(\frac{q_\mu}{m}\right)^s}{\sum\limits_{\mu=1}^{m}\left(\frac{q_\mu}{m}\right)^s} - 1\right] < 0, \quad k = 1,\ldots,M. \tag{32}$$

The curves $r(s)$ given by

$$\frac{s(s-r)}{(1-s)^2}\sigma_k(s) - 1 = 0, \quad k = 1,\ldots,M, \tag{33}$$

with

$$\sigma_k(s) = \frac{\sum\limits_{\mu=1}^{k}\left(\frac{q_\mu}{m}\right)^s}{\sum\limits_{\mu=1}^{m}\left(\frac{q_\mu}{m}\right)^s} \tag{34}$$

can be written as

$$r_k(s) = s - \frac{(1-s)^2}{s\sigma_k(s)}, \ k = 1,\ldots,M. \tag{35}$$

The epigraph regions of these curves can be written as

$$C \cup C_k = \{(s,r)|r \geq s > 0\} \cup \left\{(s,r)\,\middle|\, s > r \geq s - \frac{(1-s)^2}{s\sigma_k(s)}\right\}, \ k = 1,\ldots,M. \tag{36}$$

At the end of Sect. 2, we have emphasized that the epigraph region of the curve $r = s$ is $C = \{(s,r)|r \geq s > 0\}$, which is usually taken as the region of strict concavity. Here we define the extended region of strict concavity as the epigraph region of the highest curve of the set (35)

$$r_m(s) = 2 - \frac{1}{s} \tag{37}$$

which is given by the union set:

$$C_{max} = C \cup C_m = \{(s,r)|r \geq s > 0\} \cup \left\{(s,r) \,\middle|\, s > r \geq 2 - \frac{1}{s}\right\}. \tag{38}$$

This extended region is depicted in Fig. 2 as the gray region.

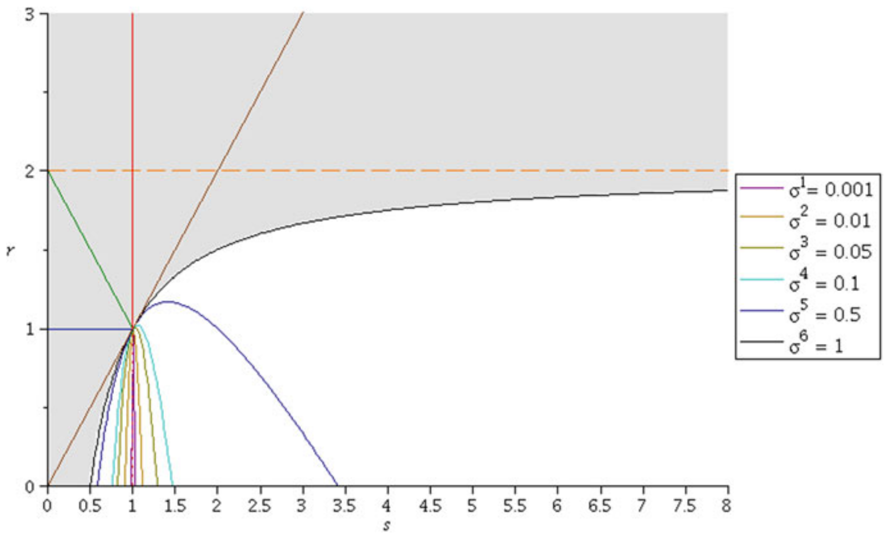


Fig. 2 The blue, green, red and brown lines do correspond to Renyi, Landsberg-Vedral, "Non-extensive" Gaussian and Havrda-Charvat entropies, respectively. The union of the regions $C = \{(s,r)|\, r \geq s > 0\}$ and $\mathbf{C}_m = \{(s,r)|\, s > r \geq 2 - 1/s\}$ is the epigraph region of the black line and corresponds to the extended region of strict concavity. Some $r_k(s)$ functions are also depicted and they correspond to $k = 1, 2, 3, 4, 5, m = 6$. We note that $r_6(0) = 0.5$ and the curve $r_6(s)$ is asymptotic to the straight line $r = 2$

$$\begin{pmatrix} A & C & Y \\ A & C & Y \\ A & C & T \\ A & T & C \\ A & Y & C \\ A & C & Y \\ T & C & A \\ Y & A & T \end{pmatrix}$$

Fig. 3 An example of a 8 × 3 array of 3-sets of amino acids

4 An Example of Systematic Derivation of $\sigma_k(s)$ Curves from Data Obtained from the Alignement of Protein Domains

In order to give an example of the construction of $\sigma_k(s)$ curves, we shall use arrays of t-amino acids which have been worked intensively on the presentation of results during the 21st BIOMAT International Symposium [10].

We shall provide an example of a 8 × 3 array of 3-sets of amino acids with 8 rows (Fig. 3). This example will be convenient for readers who intend to work with classification of amino acids distributions. According to equations of Appendices 1 and 2 there are 6 different groups on this array of equal t-sets of amino acids, $q_1, \ldots, q_6$, in the array (38). The symbol $\alpha_{j_1 j_2 j_3}$ could then be written as:

$$\begin{aligned} \alpha_{j_1 j_2 j_3} = & \Big(p_{j_1 j_2 j_3}(A^{q_1}, C^{q_1}, Y^{q_1})\Big)^s + \Big(p_{j_1 j_2 j_3}(A^{q_2}, C^{q_2}, T^{q_2})\Big)^s \\ & + \Big(p_{j_1 j_2 j_3}(A^{q_3}, T^{q_3}, C^{q_3})\Big)^s + \Big(p_{j_1 j_2 j_3}(A^{q_4}, Y^{q_4}, C^{q_4})\Big)^s \\ & + \Big(p_{j_1 j_2 j_3}(T^{q_5}, C^{q_5}, A^{q_5})\Big)^s + \Big(p_{j_1 j_2 j_3}(Y^{q_6}, A^{q_6}, T^{q_6})\Big)^s . \end{aligned} \tag{39}$$

We now refer to Eqs. (42)–(44) of Appendix 1 and we get

$$\alpha_{j_1 j_2 j_3} = \left(\frac{3}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s . \tag{40}$$

From Eqs. (34) and (42), we can also write for the $\sigma_k(s)$ functions:

$$\sigma_1(s) = \frac{\left(\frac{3}{8}\right)^s}{\alpha_{j_1 j_2 j_3}}\,;\ \ \sigma_2(s) = \frac{\left(\frac{3}{8}\right)^s + \left(\frac{1}{8}\right)^s}{\alpha_{j_1 j_2 j_3}}\,;\ \ \sigma_3(s) = \frac{\left(\frac{3}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s}{\alpha_{j_1 j_2 j_3}}\,;$$

$$\sigma_4(s) = \frac{\left(\frac{3}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s}{\alpha_{j_1 j_2 j_3}}\,;\ \ \sigma_5(s) = \frac{\left(\frac{3}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s}{\alpha_{j_1 j_2 j_3}}\,;$$

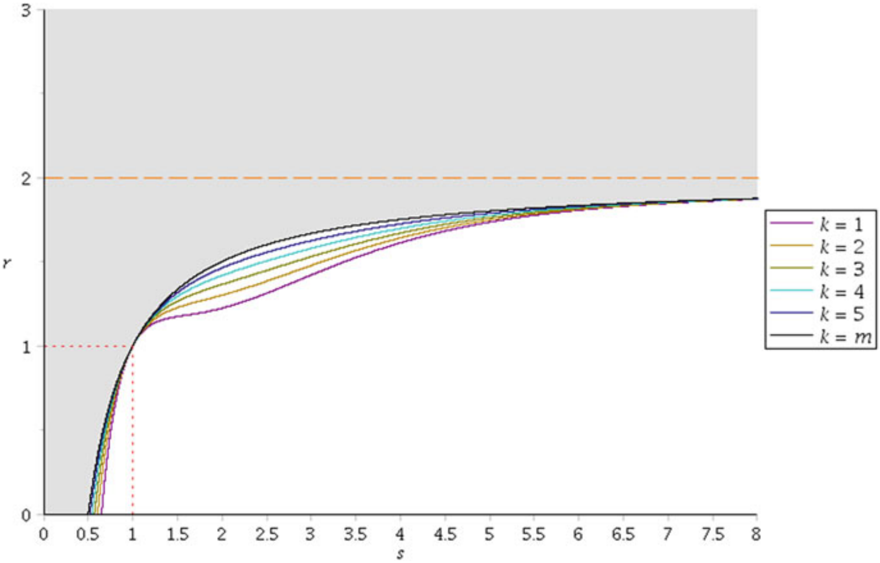


Fig. 4 The $r_k(s)$ curves and the structure of extended region of strict concavity as obtained from a 8×3 array of 3-sets of amino acids

$$\sigma_6(s) = \frac{\left(\frac{3}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s + \left(\frac{1}{8}\right)^s}{\alpha_{j_1 j_2 j_3}} = 1 \,. \tag{41}$$

In Fig. 4, the related curves $r_k(s)$, Eq. (35), are depicted. As has been emphasized at the end of Sect. 3, Sect. 3, the epigraph region of the curve corresponding to $\sigma_6(s) = 1$ and asymptotic to $r = 2$, or $r_6(s) = 2 - 1/s$, does correspond to the extended region of strict concavity.

5 Concluding Remarks

In this work we have chosen to present in detail the extensions of the region of strict concavity on the space of parameters of the Sharma-Mittal class of entropy measures. We have emphasized the structure of the parameter space and we believe that this will be very useful for working with the several special cases of entropies in models of generalized Statistical Mechanics. Some special (s-r) regions of the parameter space and the curves $r(s)$ on them could specify models of interest on the study of diseases and their interconnection from the viewpoint of their evolution in terms of entropy values [12]. A detailed study has been undertaken on the Jaccard-like Symbol and its usefulness for analysing the distributions of amino acids in protein domain families [9]. A forthcoming comprehensive review will be

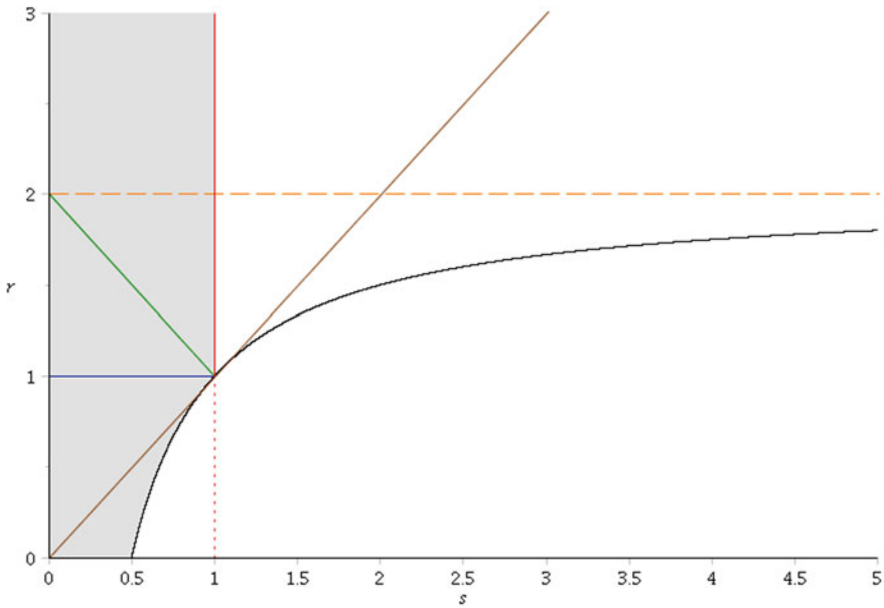


Fig. 5 The intersection of the extended region of strict concavity (Fig. 2) with the region of fully synergetic distributions of amino acids in arrays of m rows and n columns (inherited from the Hölder inequality). There are also synergetic distributions (non-Hölder specifically configurations of amino acids) on the complementary region $s > 1, r \geq 2 - 1/s$

also published with a study of the representative surfaces of entropy measures as obtained from a systematic parametrization method [9].

As has been emphasized in Appendix 2, the application of the additional criterium of fully synergetic distributions of amino acids in $m \times n$ arrays of m rows and n columns, will restrict still more the feasible region of the Sharma-Mittal entropy values associated to these arrays. This is done through the Generalized Khinchin-Shannon inequalities (Eq. (75)) and [13].

In Fig. 5, we then depict a gray region which is the intersection of the extended region of strict concavity (Fig. 2) with the region corresponding to full synergy of the probability distributions. Among all entropy measures belonging to the Sharma-Mittal entropy class and defined in Sect. 1, the "Gaussian non-extensive" entropy measure is the only one which remains for $r > 2$. This is taken as an insight to undertake the study of evolution of protein domain families and clans working with this entropy measure.

Appendix 1: The Construction and Properties of the Probabilistic Space

We fix the ideas for working with a probabilistic space by considering arrays of amino acids with m rows and n columns. We will then be able to characterize the protein domain families and the formation of several clans according the identification provided by expert biologists through alignment techniques. On some previous works [4], we have stressed that each protein domain family has as its representative at least one array of m rows and n columns. In this appendix, we summarize the usual properties of geometric objects associated to these arrays. These seem to be essential for the description of the structure of the probabilistic space and they also help to unveil some of its properties which have so far been unknown in the scientific literature.

First of all we should stress that the symbols $\alpha_{j_1\ldots j_t}$ of Eq. (2), could also be written as

$$\alpha_{j_1\ldots j_t} = \sum_{a_1^{q_\mu},\ldots,a_t^{q_\mu}} \left(p_{j_1\ldots j_t}(a_1^{q_\mu},\ldots,a_t^{q_\mu})\right)^s \leftrightarrow \sum_{\mu=1}^{m} \left(\frac{q_\mu}{m}\right)^s \; t=1,\ldots,n,\, k=1,\ldots,M,\, 1 \le M \le m. \tag{42}$$

where M is the number of μ-groups of amino acids and q_μ stands for the number of equal t-sets of the amino acids contained in the μth-group.

The significance of Eq. (42) comes from the definition of probability of occurrence:

$$p_{j_1\ldots j_t}(a_1^{q_\mu},\ldots,a_t^{q_\mu}) = \frac{n_{j_1\ldots j_t}(a_1^{q_\mu},\ldots,a_t^{q_\mu})}{m}\,, \tag{43}$$

and we have the correspondence:

$$q_\mu \leftrightarrow n_{j_1\ldots j_t}(a_1^{q_\mu},\ldots,a_t^{q_\mu}). \tag{44}$$

Since the number of groups is equal to M, this also means that there is a maximum of m different groups of t-sets or,

$$q_\mu \le m\,. \tag{45}$$

From eqs.(42) and (43), we write

$$\sum_{a_1^{q_\mu},\ldots,a_t^{q_\mu}} \frac{n_{j_1\ldots j_t}(a_1^{q_\mu},\ldots,a_t^{q_\mu})}{m} = 1 \leftrightarrow \sum_{\mu=1}^{m} \left(\frac{q_\mu}{m}\right) = 1\,. \tag{46}$$

We now pass to the probability unit vector of W components and to their generalization of geometric objects of $(W)^t$ components. From now on, in order to alleviate the notation, we do not take in consideration the super indices q_μ. For $t = 1$, $p_{j_1}(a_1)$ could be represented as a unit vector of W components:

$$p_{j_1}^{\mathsf{T}} = \left(p_{j_1}(1), \ldots, p_{j_1}(W)\right). \tag{47}$$

The escort vector associated to this vector is

$$\hat{p}_{j_1}^{\mathsf{T}} = \left(\frac{\left(p_{j_1}(1)\right)^s}{\alpha_{j_1}}, \ldots, \frac{\left(p_{j_1}(W)\right)^s}{\alpha_{j_1}}\right) \tag{48}$$

where

$$\alpha_{j_1} = \sum_{a_1} \left(p_{j_1}(a_1)\right)^s \tag{49}$$

and

$$1 = \sum_{a_1} \hat{p}_{j_1}(a_1) = \sum_{a_1} \frac{\left(p_{j_1}(a_1)\right)^s}{\alpha_{j_1}} \tag{50}$$

A geometric object of $(W)^2$ components could be also defined through a "★-product":

$$p_{j_1} \bigstar p_{j_2} = p_{j_1|j_2}\, p_{j_2}^{\mathsf{T}} \tag{51}$$

where $p_{j_1|j_2}$ will transform as a column vector.

The structure of this matrix product is given by

$$(W \times 1)(1 \times W) = (W \times W)$$

and their components could be written as:

$$p_{j_1} \bigstar p_{j_2} = \begin{pmatrix} p_{j_1 j_2}(1|1)p_{j_2}(1) & \ldots & p_{j_1 j_2}(1|W)p_{j_2}(W) \\ \vdots & \ddots & \vdots \\ p_{j_1 j_2}(W|1)p_{j_2}(1) & \ldots & p_{j_1 j_2}(W|W)p_{j_2}(W) \end{pmatrix} \tag{52}$$

where $p_{j_1 j_2}(a_1|a_2)$ are the components of the column vector of conditional probability $p_{j_1|j_2}$ of the distribution in column j_1 with a previous knowledge of the distribution in column j_2.

Since the components of the matrix 52 are joint probabilities, we then write,

$$p_{j_1} \bigstar p_{j_2} = \begin{pmatrix} p_{j_1 j_2}(1,1) & \dots & p_{j_1 j_2}(1,W) \\ \vdots & \ddots & \vdots \\ p_{j_1 j_2}(W,1) & \dots & p_{j_1 j_2}(W,W) \end{pmatrix} \tag{53}$$

where $p_{j_1 j_2}(a_1, a_2)$ are the components of the joint probability of occurrence of the 2-set (a_1, a_2) in columns j_1 and j_2.

Analogously a geometric object of $(W)^3$ components could be also defined by the $\bigstar$-product,

$$p_{j_1} \bigstar p_{j_2} \bigstar p_{j_3} = p_{j_1 j_2} \bigstar p_{j_3}^{\mathsf{T}} = p_{j_1 j_2 | j_3}\, p_{j_3}^{\mathsf{T}} = p_{j_1 j_2 j_3} \tag{54}$$

and the structure of this matrix product is

$$(W \times W \times 1)(1 \times W) = (W \times W \times W)\,.$$

The related $(W)^3$ components could be written as:

$$p_{j_1} \bigstar p_{j_2} \bigstar p_{j_3} = \begin{pmatrix} p_{j_1 j_2 j_3}(1,1,1) & \dots & p_{j_1 j_2 j_3}(1,1,W) \\ \vdots & \ddots & \vdots \\ p_{j_1 j_2 j_3}(W,1,1) & \dots & p_{j_1 j_2 j_3}(W,1,W) \\ \vdots & \ddots & \vdots \\ p_{j_1 j_2 j_3}(1,W,1) & \dots & p_{j_1 j_2 j_3}(1,W,W) \\ \vdots & \ddots & \vdots \\ p_{j_1 j_2 j_3}(W,W,1) & \dots & p_{j_1 j_2 j_3}(W,W,W) \end{pmatrix} \tag{55}$$

and so on and so forth for an object of $(W)^t$ components:

$$p_{j_1} \bigstar p_{j_2} \bigstar \dots \bigstar p_{j_t}^{\mathsf{T}} = p_{j_1 j_2 \dots j_{t-1}} \bigstar p_{j_t}^{\mathsf{T}} = p_{j_1 j_2 \dots j_{t-1} | j_t}\, p_{j_t}^{\mathsf{T}} = p_{j_1 j_2 \dots j_t} \tag{56}$$

with the structure of the matrix product given generally by

$$(W \times W \times \dots \times W \times 1)(1 \times W) = \underbrace{(W \times W \times \dots \times W)}_{t}\,.$$

The $(W)^2$, $(W)^3$ components of the associated escort geometric objects of the objects $p_{j_1} \bigstar p_{j_2}$ and $p_{j_1} \bigstar p_{j_2} \bigstar p_{j_3}$ are given by

$$\hat{p}_{j_1} \bigstar \hat{p}_{j_2} = \begin{pmatrix} \frac{\left(p_{j_1 j_2}(1,1)\right)^s}{\alpha_{j_1 j_2}} & \cdots & \frac{\left(p_{j_1 j_2}(1,W)\right)^s}{\alpha_{j_1 j_2}} \\ \vdots & \ddots & \vdots \\ \frac{\left(p_{j_1 j_2}(W,1)\right)^s}{\alpha_{j_1 j_2}} & \cdots & \frac{\left(p_{j_1 j_2}(W,W)\right)^s}{\alpha_{j_1 j_2}} \end{pmatrix} \tag{57}$$

and

$$\hat{p}_{j_1} \bigstar \hat{p}_{j_2} \bigstar \hat{p}_{j_3} = \begin{pmatrix} \frac{\left(p_{j_1 j_2 j_3}(1,1,1)\right)^s}{\alpha_{j_1 j_2 j_3}} & \cdots & \frac{\left(p_{j_1 j_2 j_3}(1,1,W)\right)^s}{\alpha_{j_1 j_2 j_3}} \\ \vdots & \ddots & \vdots \\ \frac{\left(p_{j_1 j_2 j_3}(W,1,1)\right)^s}{\alpha_{j_1 j_2 j_3}} & \cdots & \frac{\left(p_{j_1 j_2 j_3}(W,1,W)\right)^s}{\alpha_{j_1 j_2 j_3}} \\ \vdots & \ddots & \vdots \\ \frac{\left(p_{j_1 j_2 j_3}(1,W,1)\right)^s}{\alpha_{j_1 j_2 j_3}} & \cdots & \frac{\left(p_{j_1 j_2 j_3}(1,W,W)\right)^s}{\alpha_{j_1 j_2 j_3}} \\ \vdots & \ddots & \vdots \\ \frac{\left(p_{j_1 j_2 j_3}(W,W,1)\right)^s}{\alpha_{j_1 j_2 j_3}} & \cdots & \frac{\left(p_{j_1 j_2 j_3}(W,W,W)\right)^s}{\alpha_{j_1 j_2 j_3}} \end{pmatrix} \tag{58}$$

respectively.

To better understand Eq. (58), we introduce (Fig. 6).

The $(W)^t$ components of the geometric object of Eq. (56) are now written as:

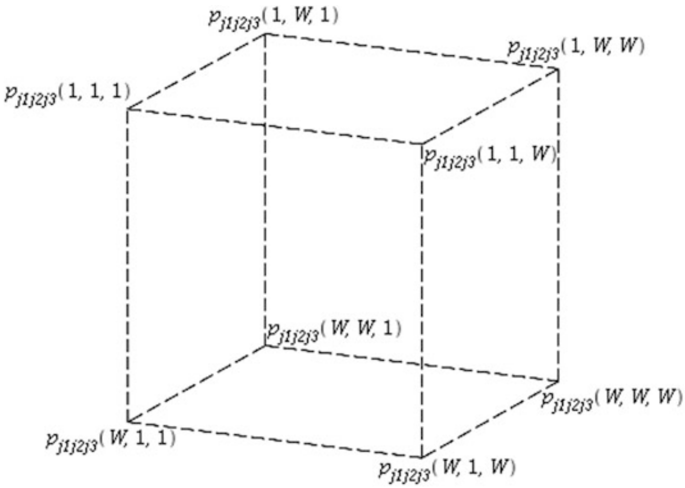


Fig. 6 A representative of $p_{j_1 j_2 j_3}$ object

$$\hat{p}_{j_1} \bigstar \hat{p}_{j_2} \bigstar \dots \bigstar \hat{p}_{j_t} = \begin{pmatrix} \frac{\left(p_{j_1\dots j_t}(1,\dots,1)\right)^s}{\alpha_{j_1\dots j_t}} & \dots & \frac{\left(p_{j_1\dots j_t}(1,\dots,1,W)\right)^s}{\alpha_{j_1\dots j_t}} \\ \vdots & \ddots & \vdots \\ \frac{\left(p_{j_1\dots j_t}(W,1,\dots,1)\right)^s}{\alpha_{j_1\dots j_t}} & \dots & \frac{\left(p_{j_1\dots j_t}(W,1,\dots,1,W)\right)^s}{\alpha_{j_1\dots j_t}} \\ \vdots & \ddots & \vdots \\ \frac{\left(p_{j_1\dots j_t}(1,W,1,\dots,1)\right)^s}{\alpha_{j_1\dots j_t}} & \dots & \frac{\left(p_{j_1\dots j_t}(1,W,1,\dots,1,W)\right)^s}{\alpha_{j_1\dots j_t}} \\ \vdots & \ddots & \vdots \\ \frac{\left(p_{j_1\dots j_t}(W,W,1,\dots,1)\right)^s}{\alpha_{j_1\dots j_t}} & \dots & \frac{\left(p_{j_1\dots j_t}(W,\dots,W)\right)^s}{\alpha_{j_1\dots j_t}} \end{pmatrix} \tag{59}$$

In order to complete this appendix and to assure its usefulness on the derivation of the results presented in Sects. 3 and 4, we now treat the case of equiprobable probabilities of occurrence.

In the case of equiprobable distributions $p_{j_1\dots j_t}(a_1,\dots,a_t) = W^{-t}$, we have from Eqs. (43) and (46),

$$1 = \sum_{\mu=1}^{m} \left(\frac{q_\mu}{m}\right) = mW^{-t} \tag{60}$$

This means that if $m \geq W^t$, we should understand this equation as

$$W^t W^{-t} + (m - W^t) \cdot 0 = 1 \tag{61}$$

We then see that for equiprobable distributions, the symbols σ_k from Sects. 3 and 4 do not depend on s and can be written as:

$$\sigma^k = \frac{\sum_{\mu=1}^{k} \left(\frac{q_\mu}{m}\right)^s}{\sum_{\mu=1}^{m} \left(\frac{q_\mu}{m}\right)^s} = \frac{k(W^{-t})^s}{m(W^{-t})^s} = \frac{k}{m} = \frac{k}{W^t}\,, \quad k = 1,\dots,W^{t-1}, W^t\,, \tag{62}$$

where we have used Eq. (60).

The corresponding values of $r(s)$ could be written from Eq. (36) of Sect. 3, as:

$$r(s) = s - \frac{(1-s)^2}{s\sigma^k} = s - \frac{(1-s)^2}{sk}\,W^t\,. \tag{63}$$

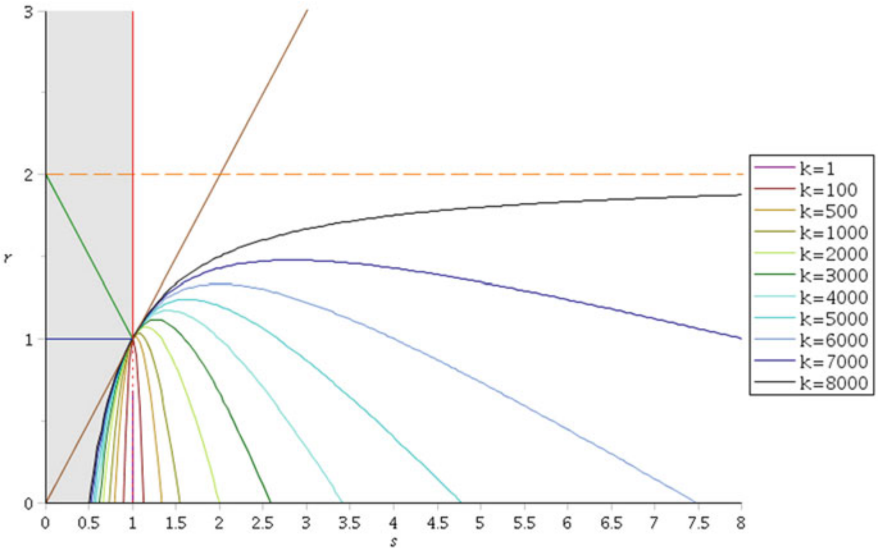


Fig. 7 The $r_k(s)$ curves and the structure of the $(s\text{-}r)$ space of parameters for some selected k-values of an equiprobable distribution of probabilities

In Sect. 3, we present a numerical application of Eq. (63), in order to continue the analysis of the structure of $(s\text{-}r)$ space of parameters.

In order to conclude this appendix, we work again with sets of 3-amino acids, with $W^3 = 8000$ for an equiprobable distribution and we choose to depict that the curves corresponding to the values: $k = 1$, 100, 500, 1000, 2000, 3000, 4000, 5000, 6000, 7000, 8000, on Fig. 7. The last curve $r_{8000}(s) = 2 - \frac{1}{s}$ was already presented in Sect. 3 on Fig. 2.

Appendix 2: The Origin of the Generalized Khinchin-Shannon Inequalities

Let us consider the definition of the conditional of the escort probability:

$$\hat{p}_{j_1\ldots j_t}(a_1, \ldots, a_{t-1}|a_t) = \frac{\hat{p}_{j_1\ldots j_t}(a_1, \ldots, a_t)}{\hat{p}_{j_t}(a_t)} \tag{64}$$

From Eq. (30) we can write, analogously:

$$\hat{p}_{j_1\ldots j_t}(a_1,\ldots,a_t) = \frac{\Big(p_{j_1\ldots j_t}(a_1,\ldots,a_t)\Big)^s}{\sum\limits_{(b_1,\ldots,b_t)} \Big(p_{j_1\ldots j_t}(b_1,\ldots,b_t)\Big)^s} \tag{65}$$

$$\hat{p}_{j_t}(a_t) = \frac{\Big(p_{j_t}(a_t)\Big)^s}{\sum\limits_{a_t} \Big(p_{j_t}(a_t)\Big)^s} \tag{66}$$

In Eqs. (65) and (66), the symbols $a_j, b_j, 1 \le j \le t$, are running over the one-letter code for the 20 amino acids

$$a_j; b_j = \text{A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y},\ 1 \le j \le t\,.$$

We then have from Eqs. (64)–(66):

$$\hat{p}_{j_1\ldots j_t}(a_1,\ldots,a_{t-1}|a_t) = \frac{\Big(p_{j_1\ldots j_t}(a_1,\ldots,a_{t-1}|a_t)\Big)^s}{\sum\limits_{(a_1,\ldots,a_t)} \hat{p}_{j_t}(a_t)\Big(p_{j_1\ldots j_t}(a_1,\ldots,a_{t-1}|a_t)\Big)^s} \tag{67}$$

We now remember the definition of the escort of the conditional probability

$$\widehat{p_{j_1\ldots j_t}(a_1,\ldots,a_{t-1}|a_t)} = \frac{\Big(p_{j_1\ldots j_t}(a_1,\ldots,a_{t-1}|a_t)\Big)^s}{\sum\limits_{(a_1,\ldots,a_{t-1})} \Big(p_{j_1\ldots j_t}(a_1,\ldots,a_{t-1}|a_t)\Big)^s} \tag{68}$$

The left hand sides of Eqs. (67) and (68) are identical if all amino acids of the t-th column are equal. For instance,

$$j_t \longrightarrow \underbrace{(A, A, A, A, \ldots, A)}_{m} \tag{69}$$

This distribution will then lead to:

$$\hat{p}^{\mathsf{T}}_{j_t} = p_{j_t} = \underbrace{1, 0, 0, 0, \ldots, 0}_{20} \tag{70}$$

For any other distributions of amino acids in the jth column, the ordering of the two denominators on the right hand sides of Eqs. (67) and (68) has to be decided after choosing a protein domain family and its related distribution of probabilities of occurrence of amino acids. In order to undertake this study, we pay special attention to some functions of probabilities already defined in ref. [1], together an additional definition, $X(a_t)$.

$$U \equiv \sum_{a_1,\dots,a_{t-1}} \left[p_{j_1\dots j_{t-1}}(a_1,\dots,a_{t-1})\right]^s = \alpha_{j_1\dots j_{t-1}} \tag{71}$$

$$J \equiv \sum_{a_1,\dots,a_{t-1}} \left[\sum_{a_t} \hat{p}_{j_t}(a_t) p_{j_1\dots j_t}(a_1,\dots,a_{t-1}|a_t)\right]^s \tag{72}$$

$$Z \equiv \sum_{a_1,\dots,a_t} \hat{p}_{j_t}(a_t)\left[p_{j_1\dots j_t}(a_1,\dots,a_{t-1}|a_t)\right]^s = \frac{\alpha_{j_1\dots j_t}}{\alpha_{j_t}} \tag{73}$$

$$X(a_t) \equiv \sum_{a_1,\dots,a_{t-1}} \left[p_{j_1\dots j_t}(a_1,\dots,a_{t-1}|a_t)\right]^s \tag{74}$$

The letters U, J, Z, X, have been chosen among those which do not codify the amino acids: B J O U X Z.

Actually, there is not any ordering between (74) and (71), (72), (73) for a generic occurrence of amino acids, as have been emphasized in ref. [1]. This assertion could be also proven "a fortiori" if the amino acid corresponding to a_t does not occur, or $X(a_t) = 0$.

It should be also stressed that the condition $J \geq Z$ i.e., the Hölder inequality [1, 12] which stands for $1 > s \geq 0$ is sufficient to guarantee the inequality $U \geq Z$, which leads to the Generalized Khinchin-Shannon inequalities to be obtained through iteration:

$$\alpha_{j_1\dots j_{t-1}} \geq \frac{\alpha_{j_1\dots j_t}}{\alpha_{j_t}}$$

$$t \to t-1 \Rightarrow \alpha_{j_1\dots j_{t-2}} \geq \frac{\alpha_{j_1\dots j_{t-1}}}{\alpha_{j_{t-1}}} \geq \frac{\alpha_{j_1\dots j_t}}{\alpha_{j_t}\cdot\alpha_{j_{t-1}}}$$

$$t \to t-2 \Rightarrow \alpha_{j_1\dots j_{t-3}} \geq \frac{\alpha_{j_1\dots j_{t-2}}}{\alpha_{j_{t-2}}} \geq \frac{\alpha_{j_1\dots j_t}}{\alpha_{j_t}\cdot\alpha_{j_{t-1}}\cdot\alpha_{j_{t-2}}}$$

$$\vdots$$

$$t \to 2 \Rightarrow \alpha_{j_1} \geq \frac{\alpha_{j_1 j_2}}{\alpha_{j_2}} \geq \frac{\alpha_{j_1\dots j_t}}{\alpha_{j_t}\cdot\ldots\cdot\alpha_{j_3}\cdot\alpha_{j_2}}$$

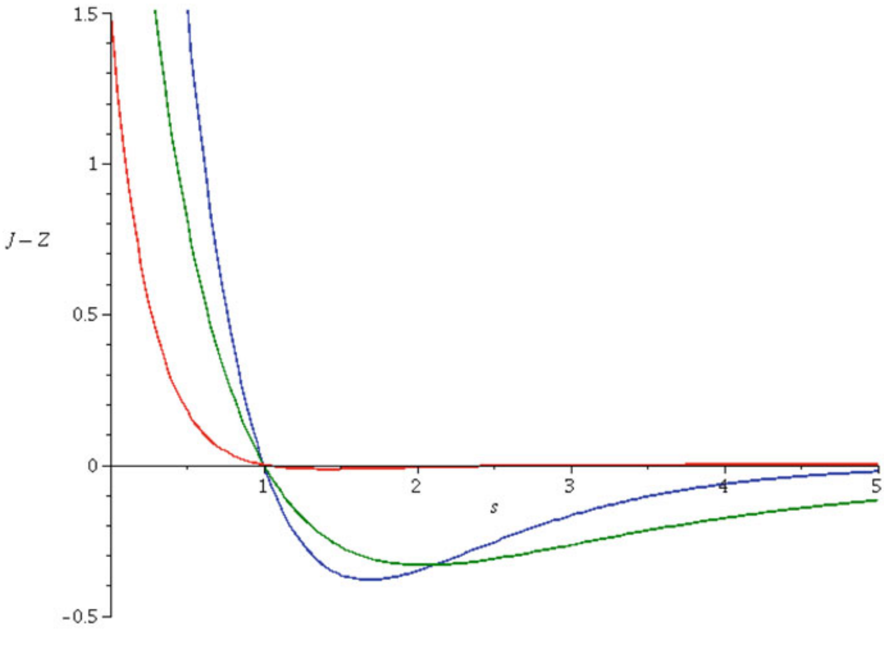
$$\Rightarrow \alpha_{j_1\dots j_t} \leq \prod_{l=1}^{t} \alpha_{j_l} \tag{75}$$

However, in Figs. 8 and 9, below, we have tried to characterize the upsurge of regions in which $J \geq Z$ for $s > 1$ by presenting the curves $U - Z$ and $J - Z$ for two 8×3 arrays obtained from the Pfam 27.0 database and a hypothetical 8×3 array which has been constructed aiming a better alignment. The results led us to conjecture that this would occur systematically on greater arrays to be obtained by working with recent versions of the database. This kind of work is now in progress and it will be published elsewhere.

$$\begin{pmatrix} K & A & Q \\ A & G & E \\ N & T & P \\ V & A & G \\ K & P & Q \\ V & P & G \\ P & K & C \\ R & P & G \end{pmatrix} \qquad \begin{pmatrix} V & I & T \\ A & I & I \\ V & I & A \\ V & I & A \\ M & V & V \\ V & L & I \\ A & I & V \\ A & L & I \end{pmatrix} \qquad \begin{pmatrix} A & A & A \\ A & C & C \\ A & C & A \\ A & C & A \\ A & C & A \\ C & A & A \\ C & C & A \\ C & C & A \end{pmatrix}$$

(a) (b) (c)

Fig. 8 8×3 arrays of amino acids: (**a**) from Pfam PF01926, rows 25–32, columns 30-32; (**b**) from Pfam PF01926, rows 3–10, columns 3–5; (**c**) a hypothetical 8×3 array aiming a good alignment



(a)

Fig. 9 The blue, green and red curves do correspond to the matrices (**a**), (**b**), and (**c**) of Fig. 8, respectively. (**a**) Study of the Hölder ($J \geq Z$) and Non-Hölder ($J < Z$) probability distributions from the 8×3 arrays of Fig. 8; (**b**) Study of the viability of Generalized Khinchin-Shannon Inequalities ($U \geq Z$) associated to Hölder probability distributions ($J \geq Z$) or $J \geq Z \Rightarrow U \geq Z$. However, there are distributions of amino acids such that $U \geq Z$ even where $J < Z$. The red curve is an example for $s > 1.4537$

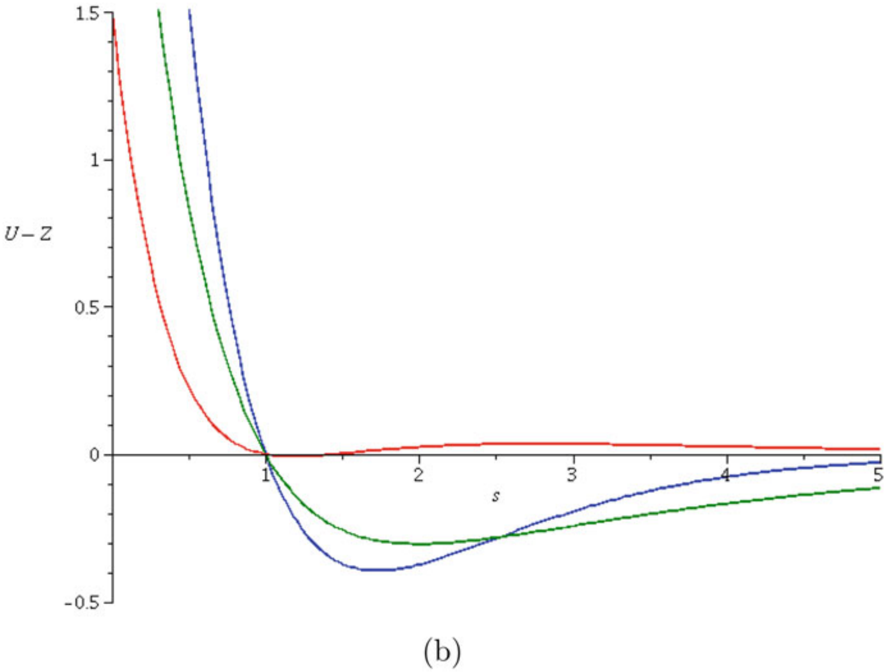


Fig. 9 (continued)

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