

Nonextensive Information Theoretic Kernels on Measures*

André F. T. Martins[†]

Noah A. Smith

Eric P. Xing

*School of Computer Science
Carnegie Mellon University
Pittsburgh, PA, USA*

AFM@CS.CMU.EDU

NASMITH@CS.CMU.EDU

EPXING@CS.CMU.EDU

Pedro M. Q. Aguiar

*Instituto de Sistemas e Robótica
Instituto Superior Técnico
Lisboa, Portugal*

AGUIAR@ISR.IST.UTL.PT

Mário A. T. Figueiredo

*Instituto de Telecomunicações
Instituto Superior Técnico
Lisboa, Portugal*

MARIO.FIGUEIREDO@LX.IT.PT

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Abstract

Positive definite kernels on probability measures have been recently applied to classification problems involving text, images, and other types of structured data. Some of these kernels are related to classic information theoretic quantities, such as (Shannon's) mutual information and the Jensen-Shannon (JS) divergence. Meanwhile, there have been recent advances in nonextensive generalizations of Shannon's information theory. This paper bridges these two trends by introducing nonextensive information theoretic kernels on probability measures, based on new JS-type divergences. These new divergences result from extending the two building blocks of the classical JS divergence: convexity and Shannon's entropy. The notion of convexity is extended to the wider concept of q -convexity, for which we prove a Jensen q -inequality. Based on this inequality, we introduce Jensen-Tsallis (JT) q -differences, a nonextensive generalization of the JS divergence, and define a k -th order JT q -difference between stochastic processes. We then define a new family of nonextensive mutual information kernels, which allow weights to be assigned to their arguments, and which includes the Boolean, JS, and linear kernels as particular cases. Nonextensive string kernels are also defined that generalize the p -spectrum kernel. We illustrate the performance of these kernels on text categorization tasks, in which documents are modeled both as bags of words and as sequences of characters.

Keywords: positive definite kernels, nonextensive information theory, Tsallis entropy, Jensen-Shannon divergence, string kernels

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†. Also at Instituto de Telecomunicações, Instituto Superior Técnico, Lisboa, Portugal.

1. Introduction

In kernel-based machine learning (Schölkopf and Smola, 2002; Shawe-Taylor and Cristianini, 2004), there has been recent interest in defining kernels on probability distributions to tackle several problems involving structured data (Desobry et al., 2007; Moreno et al., 2004; Jebara et al., 2004; Hein and Bousquet, 2005; Lafferty and Lebanon, 2005; Cuturi et al., 2005). By defining a parametric family S containing the distributions from which the data points (in the input space X) are assumed to have been generated, and defining a map from X from S (e.g., via maximum likelihood estimation), a distribution in S may be fitted to each datum. Therefore, a kernel that is defined on $S \times S$ automatically induces a kernel on $X \times X$, through map composition. In text categorization, this framework appears as an alternative to the Euclidean geometry inherent to the usual bag-of-words representations. In fact, approaches that map data to statistical manifolds, equipped with well-motivated non-Euclidean metrics (Lafferty and Lebanon, 2005), often outperform support vector machine (SVM) classifiers with linear kernels (Joachims, 2002). Some of these kernels have a natural information theoretic interpretation, establishing a bridge between kernel methods and information theory (Cuturi et al., 2005; Hein and Bousquet, 2005).

The main goal of this paper is to widen that bridge; we do that by introducing a new class of kernels rooted in *nonextensive* information theory, which contains previous information theoretic kernels as particular elements. The Shannon and Rényi entropies (Shannon, 1948; Rényi, 1961) share the *extensivity* property: the joint entropy of a pair of independent random variables equals the sum of the individual entropies. Abandoning this property yields the so-called nonextensive entropies (Havrda and Charvát, 1967; Lindhard, 1974; Lindhard and Nielsen, 1971; Tsallis, 1988), which have raised great interest among physicists in modeling phenomena such as long-range interactions and multifractals, and in constructing nonextensive generalizations of Boltzmann-Gibbs statistical mechanics (Abe, 2006). Nonextensive entropies have also been recently used in signal/image processing (Li et al., 2006) and other areas (Gell-Mann and Tsallis, 2004). The so-called *Tsallis entropies* (Havrda and Charvát, 1967; Tsallis, 1988) form a parametric family of nonextensive entropies that includes the Shannon-Boltzmann-Gibbs entropy as a particular case. Nonextensive generalizations of information theory have been proposed (Furuichi, 2006).

Convexity and Jensen's inequality are key concepts underlying several central results of information theory, for example, the non-negativity of the *Kullback-Leibler (KL) divergence* (or *relative entropy*) (Kullback and Leibler, 1951). Jensen's inequality (Jensen, 1906) also underlies the *Jensen-Shannon (JS) divergence*, a symmetrized and smoothed version of the KL divergence (Lin and Wong, 1990; Lin, 1991), often used in statistics, machine learning, signal/image processing, and physics.

In this paper, we introduce new extensions of JS-type divergences by generalizing its two pillars: *convexity* and *Shannon's entropy*. These divergences are then used to define new information-theoretic kernels between probability distributions. More specifically, our main contributions are:

- The concept of *q-convexity*, generalizing that of convexity, for which we prove a *Jensen q-inequality*. The related concept of *Jensen q-differences*, which generalize Jensen differences, is also proposed. Based on these concepts, we introduce the *Jensen-Tsallis (JT) q-difference*, a nonextensive generalization of the JS divergence, which is also a “mutual information” in the sense of Furuichi (2006).
- Characterization of the JT *q-difference*, with respect to convexity and extrema, extending work by Burbea and Rao (1982) and by Lin (1991) for the JS divergence.

- Definition of k -th order joint and conditional JT q -differences for families of stochastic processes, and derivation of a chain rule.
- A broad family of (nonextensive information theoretic) positive definite kernels, interpretable as nonextensive mutual information kernels, ranging from the Boolean to the linear kernels, and including the JS kernel proposed by Hein and Bousquet (2005).
- A family of (nonextensive information theoretic) positive definite kernels between stochastic processes, subsuming well-known string kernels (e.g., the p -spectrum kernel) (Leslie et al., 2002).
- Extensions of results of Hein and Bousquet (2005) proving positive definiteness of kernels based on the unbalanced JS divergence. A connection between these new kernels and those studied by Fuglede (2005) and Hein and Bousquet (2005) is also established. In passing, we show that the parametrix approximation of the multinomial diffusion kernel introduced by Lafferty and Lebanon (2005) is *not* positive definite in general.

The paper is organized as follows. Section 2 reviews nonextensive entropies, with emphasis on the Tsallis case. Section 3 discusses Jensen differences and divergences. The concepts of q -differences and q -convexity are introduced in Section 4, where they are used to define and characterize some new divergence-type quantities. In Section 5, we define the Jensen-Tsallis q -difference and derive some of its properties; in that section, we also define k -th order Jensen-Tsallis q -differences for families of stochastic processes. The new family of entropic kernels is introduced and characterized in Section 6, which also introduces nonextensive kernels between stochastic processes. Experiments on text categorization are reported in Section 7. Section 8 concludes the paper and discusses future research.

2. Nonextensive Entropies and Tsallis Statistics

In this section, we start with a brief overview of nonextensive entropies. We then introduce the family of Tsallis entropies, and extend their domain to unnormalized measures.

2.1 Nonextensivity

In what follows, \mathbb{R}_+ denotes the nonnegative reals, \mathbb{R}_{++} denotes the strictly positive reals, and

$$\Delta^{n-1} \triangleq \left\{ (x_1, \dots, x_n) \in \mathbb{R}^n \mid \sum_{i=1}^n x_i = 1, \forall i x_i \geq 0 \right\}$$

denotes the $(n - 1)$ -dimensional simplex.

Inspired by the axiomatic formulation of Shannon’s entropy (Khinchin, 1957; Shannon and Weaver, 1949), Suyari (2004) proposed an axiomatic framework for nonextensive entropies and a uniqueness theorem. Let $q \geq 0$ be a fixed scalar, called the *entropic index*. Suyari’s axioms (Appendix A) determine a function $S_{q,\phi} : \Delta^{n-1} \rightarrow \mathbb{R}$ of the form

$$S_{q,\phi}(p_1, \dots, p_n) = \begin{cases} \frac{k}{\phi(q)} (1 - \sum_{i=1}^n p_i^q) & \text{if } q \neq 1 \\ -k \sum_{i=1}^n p_i \ln p_i & \text{if } q = 1, \end{cases} \quad (1)$$

where k is a positive constant, and $\phi : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a continuous function that satisfies the following three conditions: (i) $\phi(q)$ has the same sign as $q-1$; (ii) $\phi(q)$ vanishes if and only if $q = 1$; (iii) ϕ is differentiable in a neighborhood of 1 and $\phi'(1) = 1$.

Note that $S_{1,\phi} = \lim_{q \rightarrow 1} S_{q,\phi}$, thus $S_{q,\phi}(p_1, \dots, p_n)$, seen as a function of q , is continuous at $q = 1$. For any ϕ satisfying these conditions, $S_{q,\phi}$ has the *pseudoadditivity* property: for any two independent random variables A and B , with probability mass functions $p_A \in \Delta^{n_A-1}$ and $p_B \in \Delta^{n_B-1}$, respectively, consider the new random variable $A \otimes B$ defined by the joint distribution $p_A \otimes p_B \in \Delta^{n_A n_B-1}$; then,

$$S_{q,\phi}(A \otimes B) = S_{q,\phi}(A) + S_{q,\phi}(B) - \frac{\phi(q)}{k} S_{q,\phi}(A) S_{q,\phi}(B),$$

where we denote (as usual) $S_{q,\phi}(A) \triangleq S_{q,\phi}(p_A)$.

For $q = 1$, Suyari's axioms recover the Shannon-Boltzmann-Gibbs (SBG) entropy,

$$S_{1,\phi}(p_1, \dots, p_n) = H(p_1, \dots, p_n) = -k \sum_{i=1}^n p_i \ln p_i,$$

and pseudoadditivity turns into *additivity*, that is, $H(A \otimes B) = H(A) + H(B)$ holds.

Several proposals for ϕ have appeared in the literature (Havrda and Charvát, 1967; Daróczy, 1970; Tsallis, 1988). In this article, unless stated otherwise, we set $\phi(q) = q - 1$, which yields the *Tsallis entropy*:

$$S_q(p_1, \dots, p_n) = \frac{k}{q-1} \left(1 - \sum_{i=1}^n p_i^q \right). \tag{2}$$

To simplify, we let $k = 1$ and write the Tsallis entropy as

$$S_q(X) \triangleq S_q(p_1, \dots, p_n) = - \sum_{x \in X} p(x)^q \ln_q p(x), \tag{3}$$

where $\ln_q(x) \triangleq (x^{1-q} - 1)/(1 - q)$ is the *q-logarithm function*, which satisfies $\ln_q(xy) = \ln_q(x) + x^{1-q} \ln_q(y)$ and $\ln_q(1/x) = -x^{q-1} \ln_q(x)$. This notation was introduced by Tsallis (1988).

2.2 Tsallis Entropies

Furuichi (2006) derived some information theoretic properties of Tsallis entropies. Tsallis *joint* and *conditional entropies* are defined, respectively, as

$$S_q(X, Y) \triangleq - \sum_{x,y} p(x,y)^q \ln_q p(x,y)$$

and

$$S_q(X|Y) \triangleq - \sum_{x,y} p(x,y)^q \ln_q p(x|y) = \sum_y p(y)^q S_q(X|y), \tag{4}$$

and the chain rule $S_q(X, Y) = S_q(X) + S_q(Y|X)$ holds.

For two probability mass functions $p_X, p_Y \in \Delta^n$, the *Tsallis relative entropy*, generalizing the KL divergence, is defined as

$$D_q(p_X || p_Y) \triangleq - \sum_x p_X(x) \ln_q \frac{p_Y(x)}{p_X(x)}. \tag{5}$$

Finally, the *Tsallis mutual entropy* is defined as

$$I_q(X;Y) \triangleq S_q(X) - S_q(X|Y) = S_q(Y) - S_q(Y|X), \quad (6)$$

generalizing (for $q > 1$) Shannon's mutual information (Furuichi, 2006). In Section 5, we establish a relationship between Tsallis mutual entropy and a quantity called *Jensen-Tsallis q -difference*, generalizing the one between mutual information and the JS divergence (shown, e.g., by Grosse et al. 2002, and recalled below, in Section 3.2).

Furuichi (2006) also mentions an alternative generalization of Shannon's mutual information, defined as

$$\tilde{I}_q(X;Y) \triangleq D_q(p_{X,Y} \| p_X \otimes p_Y), \quad (7)$$

where $p_{X,Y}$ is the true joint probability mass function of (X,Y) and $p_X \otimes p_Y$ denotes their joint probability if they were independent. This alternative definition of a "Tsallis mutual entropy" has also been used by Lamberti and Majtey (2003); notice that $I_q(X;Y) \neq \tilde{I}_q(X;Y)$ in general, the case $q = 1$ being a notable exception. In Section 5, we show that this alternative definition also leads to a nonextensive analogue of the JS divergence.

2.3 Entropies of Measures and Denormalization Formulae

Throughout this paper, we consider functionals that extend the domain of the Shannon-Boltzmann-Gibbs and Tsallis entropies to include unnormalized measures. Although, as shown below, these functionals are completely characterized by their restriction to the normalized probability distributions, the denormalization expressions will play an important role in Section 6 to derive novel positive definite kernels inspired by mutual informations.

In order to keep generality, whenever possible we do not restrict to finite or countable sample spaces. Instead, we consider a measure space (X, \mathcal{M}, ν) where X is Hausdorff and ν is a σ -finite Radon measure. We denote by $M_+(X)$ the set of *finite* Radon ν -absolutely continuous measures on X , and by $M_+^1(X)$ the subset of those which are probability measures. For simplicity, we often identify each measure in $M_+(X)$ or $M_+^1(X)$ with its corresponding nonnegative density; this is legitimated by the Radon-Nikodym theorem, which guarantees the existence and uniqueness (up to equivalence within measure zero) of a density function $f : X \rightarrow \mathbb{R}_+$. In the sequel, Lebesgue-Stieltjes integrals of the form $\int_{\mathcal{A}} f(x) d\nu(x)$ are often written as $\int_{\mathcal{A}} f$, or simply $\int f$, if $\mathcal{A} = X$. Unless otherwise stated, ν is the Lebesgue-Borel measure, if $X \subseteq \mathbb{R}^n$ and $\text{int}X \neq \emptyset$, or the counting measure, if X is countable. In the latter case integrals can be seen as finite sums or infinite series.

Define $\overline{\mathbb{R}} \triangleq \mathbb{R} \cup \{-\infty, +\infty\}$. For some functional $G : M_+(X) \rightarrow \overline{\mathbb{R}}$, let the set $M_+^G(X) \triangleq \{f \in M_+(X) : |G(f)| < \infty\}$ be its effective domain, and $M_+^{1,G}(X) \triangleq M_+^G(X) \cap M_+^1(X)$ be its subdomain of probability measures.

The following functional (Cuturi and Vert, 2005), extends the Shannon-Boltzmann-Gibbs entropy from $M_+^{1,H}(X)$ to the unnormalized measures in $M_+^H(X)$:

$$H(f) = -k \int f \ln f = \int \phi_H \circ f, \quad (8)$$

where $k > 0$ is a constant, the function $\phi_H : \mathbb{R}_+ \rightarrow \mathbb{R}$ is defined as

$$\phi_H(y) = -k y \ln y,$$

and, as usual, $0 \ln 0 \triangleq 0$.

The generalized form of the KL divergence, often called *generalized I-divergence* (Csiszar, 1975), is a directed divergence between two measures $\mu_f, \mu_g \in M_+^H(X)$, such that μ_f is μ_g -absolutely continuous (denoted $\mu_f \ll \mu_g$). Let f and g be the densities associated with μ_f and μ_g , respectively. In terms of densities, this generalized KL divergence is

$$D(f, g) = k \int \left(g - f + f \ln \frac{f}{g} \right). \tag{9}$$

Let us now proceed similarly with the nonextensive entropies. For $q \geq 0$, let $M_+^{S_q}(X) = \{f \in M_+(X) : f^q \in M_+(X)\}$ for $q \neq 1$, and $M_+^{S_q}(X) = M_+^H(X)$ for $q = 1$. The nonextensive counterpart of (8), defined on $M_+^{S_q}(X)$, is

$$S_q(f) = \int \varphi_q \circ f, \tag{10}$$

where $\varphi_q : \mathbb{R}_+ \rightarrow \mathbb{R}$ is given by

$$\varphi_q(y) = \begin{cases} \varphi_H(y) & \text{if } q = 1, \\ \frac{k}{\phi(q)} (y - y^q) & \text{if } q \neq 1, \end{cases} \tag{11}$$

and $\phi : \mathbb{R}_+ \rightarrow \mathbb{R}$ satisfies conditions (i)-(iii) stated following Equation (1). The Tsallis entropy is obtained for $\phi(q) = q - 1$,

$$S_q(f) = -k \int f^q \ln_q f. \tag{12}$$

Similarly, a nonextensive generalization of the generalized KL divergence (9) is

$$D_q(f, g) = -\frac{k}{\phi(q)} \int (qf + (1 - q)g - f^q g^{1-q}),$$

for $q \neq 1$, and $D_1(f, g) \triangleq \lim_{q \rightarrow 1} D_q(f, g) = D(f, g)$.

Define $|f| \triangleq \int f = \mu_f(X)$. For $|f| = |g| = 1$, several particular cases are recovered: if $\phi(q) = 1 - 2^{1-q}$, then $D_q(f, g)$ is the Havrda-Charvát relative entropy (Havrda and Charvát, 1967; Daróczy, 1970); if $\phi(q) = q - 1$, then $D_q(f, g)$ is the Tsallis relative entropy (5); finally, if $\phi(q) = q(q - 1)$, then $D_q(f, g)$ is the canonical α -divergence defined by Amari and Nagaoka (2001) in the realm of information geometry (with the reparameterization $\alpha = 2q - 1$ and assuming $q > 0$ so that $\phi(q) = q(q - 1)$ conforms with the axioms).

Remark 1 Both functionals S_q and D_q are completely determined by their restriction to the normalized measures. Indeed, the following equalities hold for any $c \in \mathbb{R}_{++}$ and $f, g \in M_+^{S_q}(X)$, with $\mu_f \ll \mu_g$:

$$\begin{aligned} S_q(cf) &= c^q S_q(f) + |f| \varphi_q(c), \\ D_q(cf, cg) &= c D_q(f, g), \\ D_q(cf, g) &= c^q D_q(f, g) - q \varphi_q(c) |f| + \frac{k}{\phi(q)} (q - 1) (1 - c^q) |g|. \end{aligned} \tag{13}$$

For any $f \in M_+^{S_q}(\mathcal{X})$ and $g \in M_+^{S_q}(\mathcal{Y})$,

$$S_q(f \otimes g) = |g|S_q(f) + |f|S_q(g) - \frac{\phi(q)}{k}S_q(f)S_q(g).$$

If $|f| = |g| = 1$, we recover the pseudo-additivity property of nonextensive entropies:

$$S_q(f \otimes g) = S_q(f) + S_q(g) - \frac{\phi(q)}{k}S_q(f)S_q(g).$$

For $\phi(q) = q - 1$, D_q is the Tsallis relative entropy and (13) reduces to

$$D_q(cf, g) = c^q D_q(f, g) - q\phi_q(c)|f| + k(1 - c^q)|g|.$$

By taking the limit $q \rightarrow 1$, we obtain the following formulae for H and D :

$$\begin{aligned} H(cf) &= cH(f) + |f|\phi_H(c), \\ D(cf, cg) &= cD(f, g), \\ D(cf, g) &= cD(f, g) - |f|\phi_H(c) + k(1 - c)|g|. \end{aligned}$$

Consider $f \in M_+^H(\mathcal{X})$ and $g \in M_+^H(\mathcal{Y})$, and define $f \otimes g \in M_+^H(\mathcal{X} \times \mathcal{Y})$ as $(f \otimes g)(x, y) \triangleq f(x)g(y)$. Then,

$$H(f \otimes g) = |g|H(f) + |f|H(g).$$

If $|f| = |g| = 1$, we recover the additivity property of the Shannon-Boltzmann-Gibbs entropy, $H(f \otimes g) = H(f) + H(g)$.

3. Jensen Differences and Divergences

In this section, we review the concept of Jensen difference. We then discuss three particular cases: the Jensen-Shannon, Jensen-Rényi, and Jensen-Tsallis divergences.

3.1 The Jensen Difference

Jensen's inequality (Jensen, 1906) is at the heart of many important results in information theory. Let $E[\cdot]$ denote the expectation operator. Jensen's inequality states that if Z is an integrable random variable taking values in a set \mathcal{Z} , and f is a measurable convex function defined on the convex hull of \mathcal{Z} , then

$$f(E[Z]) \leq E[f(Z)].$$

Burbea and Rao (1982) considered the scenario where \mathcal{Z} is finite, and took $f \triangleq -H_\phi$, where $H_\phi : [a, b]^n \rightarrow \mathbb{R}$ is a concave function, called a ϕ -entropy, defined as

$$H_\phi(z) \triangleq - \sum_{i=1}^n \phi(z_i), \tag{14}$$

where $\phi : [a, b] \rightarrow \mathbb{R}$ is convex. They studied the Jensen difference

$$J_\phi^\pi(y_1, \dots, y_m) \triangleq H_\phi\left(\sum_{t=1}^m \pi_t y_t\right) - \sum_{t=1}^m \pi_t H_\phi(y_t),$$

where $\pi \triangleq (\pi_1, \dots, \pi_m) \in \Delta^{m-1}$, and each $y_1, \dots, y_m \in [a, b]^n$.

We consider here a more general scenario, involving two measure sets (X, \mathcal{M}, ν) and $(\mathcal{T}, \mathcal{T}, \tau)$, where the second is used to index the first.

Definition 2 Let $\mu \triangleq (\mu_t)_{t \in \mathcal{T}} \in [M_+(\mathcal{X})]^\mathcal{T}$ be a family of finite Radon measures on X , indexed by \mathcal{T} , and let $\omega \in M_+(\mathcal{T})$ be a finite Radon measure on \mathcal{T} . Define:

$$J_\Psi^\omega(\mu) \triangleq \Psi \left(\int_{\mathcal{T}} \omega(t) \mu_t d\tau(t) \right) - \int_{\mathcal{T}} \omega(t) \Psi(\mu_t) d\tau(t) \tag{15}$$

where:

- (i) Ψ is a concave functional such that $\text{dom } \Psi \subseteq M_+(\mathcal{X})$;
- (ii) $\omega(t)\mu_t(x)$ is τ -integrable, for all $x \in X$;
- (iii) $\int_{\mathcal{T}} \omega(t)\mu_t d\tau(t) \in \text{dom } \Psi$;
- (iv) $\mu_t \in \text{dom } \Psi$, for all $t \in \mathcal{T}$;
- (v) $\omega(t)\Psi(\mu_t)$ is τ -integrable.

If $\omega \in M_+^1(\mathcal{T})$, we still call (15) a Jensen difference.

In the following subsections, we consider several instances of Definition 2, leading to several Jensen-type divergences.

3.2 The Jensen-Shannon Divergence

Let p be a random probability distribution taking values in $\{p_t\}_{t \in \mathcal{T}}$ according to a distribution $\pi \in M_+^1(\mathcal{T})$. (In classification/estimation theory parlance, π is called the prior distribution and $p_t \triangleq p(\cdot|t)$ the likelihood function.) Then, (15) becomes

$$J_\Psi^\pi(p) = \Psi(E[p]) - E[\Psi(p)], \tag{16}$$

where the expectations are with respect to π .

Let now $\Psi = H$, the Shannon-Boltzmann-Gibbs entropy. Consider the random variables T and X , taking values respectively in \mathcal{T} and X , with densities $\pi(t)$ and $p(x) \triangleq \int_{\mathcal{T}} p(x|t)\pi(t)$. Using standard notation of information theory (Cover and Thomas, 1991),

$$\begin{aligned} J^\pi(p) \triangleq J_H^\pi(p) &= H \left(\int_{\mathcal{T}} \pi(t) p_t \right) - \int_{\mathcal{T}} \pi(t) H(p_t) \\ &= H(X) - \int_{\mathcal{T}} \pi(t) H(X|T=t) \\ &= H(X) - H(X|T) \\ &= I(X;T), \end{aligned} \tag{17}$$

where $I(X;T)$ is the mutual information between X and T . (This relationship between JS divergence and mutual information was pointed out by Grosse et al. 2002.) Since $I(X;T)$ is also equal to the

KL divergence between the joint distribution and the product of the marginals (Cover and Thomas, 1991), we have

$$J^\pi(p) = H(E[p]) - E[H(p)] = E[D(p||E[p])]. \tag{18}$$

When \mathcal{X} and \mathcal{T} are finite with $|\mathcal{T}| = m$, $J_H^\pi(p_1, \dots, p_m)$ is called the *Jensen-Shannon (JS) divergence* of p_1, \dots, p_m , with weights π_1, \dots, π_m (Burbea and Rao, 1982; Lin, 1991). Equality (18) allows two interpretations of the JS divergence:

- the Jensen difference of the Shannon entropy of p ;
- the expected KL divergence from p to the expectation of p .

A remarkable fact is that $J^\pi(p) = \min_r E[D(p||r)]$, that is, $r^* = E[p]$ is a minimizer of $E[D(p||r)]$ with respect to r . It has been shown that this property together with Equality (18) characterize the so-called *Bregman divergences*: they hold not only for $\Psi = H$, but for any concave Ψ and the corresponding Bregman divergence, in which case J_Ψ^π is the *Bregman information* (Banerjee et al., 2005).

When $|\mathcal{T}| = 2$ and $\pi = (1/2, 1/2)$, p may be seen as a random distribution whose value on $\{p_1, p_2\}$ is chosen by tossing a fair coin. In this case, $J^{(1/2, 1/2)}(p) = JS(p_1, p_2)$, where

$$\begin{aligned} JS(p_1, p_2) &\triangleq H\left(\frac{p_1 + p_2}{2}\right) - \frac{H(p_1) + H(p_2)}{2} \\ &= \frac{1}{2}D\left(p_1 \parallel \frac{p_1 + p_2}{2}\right) + \frac{1}{2}D\left(p_2 \parallel \frac{p_1 + p_2}{2}\right), \end{aligned}$$

as introduced by Lin (1991). It has been shown that \sqrt{JS} satisfies the triangle inequality (hence being a metric) and that, moreover, it is a Hilbertian metric¹ (Endres and Schindelin, 2003; Topsøe, 2000), which has motivated its use in kernel-based machine learning (Cuturi et al., 2005; Hein and Bousquet, 2005) (see Section 6).

3.3 The Jensen-Rényi Divergence

Consider again the scenario above (Section 3.2), with the Rényi q -entropy

$$R_q(p) = \frac{1}{1-q} \ln \int p^q$$

replacing the Shannon-Boltzmann-Gibbs entropy. It is worth noting that the Rényi and Tsallis q -entropies are monotonically related through $R_q(p) = \ln\left([1 + (1-q)S_q(p)]^{\frac{1}{1-q}}\right)$, or, using the q -logarithm function,

$$S_q(p) = \ln_q \exp R_q(p).$$

The Rényi q -entropy is concave for $q \in [0, 1)$ and has the Shannon-Boltzmann-Gibbs entropy as the limit when $q \rightarrow 1$. Letting $\Psi = R_q$, (16) becomes

$$J_{R_q}^\pi(p) = R_q(E[p]) - E[R_q(p)]. \tag{19}$$

1. A metric $d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is Hilbertian if there is some Hilbert space \mathcal{H} and an isometry $f : \mathcal{X} \rightarrow \mathcal{H}$ such that $d^2(x, y) = \langle f(x) - f(y), f(x) - f(y) \rangle_{\mathcal{H}}$ holds for any $x, y \in \mathcal{X}$ (Hein and Bousquet, 2005).

Unlike in the JS divergence case, there is no counterpart of equality (18) based on the Rényi q -divergence

$$D_{R_q}(p_1 \| p_2) = \frac{1}{q-1} \ln \int p_1^q p_2^{1-q}.$$

When \mathcal{X} and \mathcal{T} are finite, we call $J_{R_q}^\pi$ in (19) the *Jensen-Rényi (JR) divergence*. Furthermore, when $|\mathcal{T}| = 2$ and $\pi = (1/2, 1/2)$, we write $J_{R_q}^\pi(p) = JR_q(p_1, p_2)$, where

$$JR_q(p_1, p_2) = R_q\left(\frac{p_1 + p_2}{2}\right) - \frac{R_q(p_1) + R_q(p_2)}{2}.$$

The JR divergence has been used in several signal/image processing applications, such as registration, segmentation, denoising, and classification (Ben-Hamza and Krim, 2003; He et al., 2003; Karakos et al., 2007). In Section 6, we show that the JR divergence is (like the JS divergence) a Hilbertian metric, which is relevant for its use in kernel-based machine learning.

3.4 The Jensen-Tsallis Divergence

Burbea and Rao (1982) have defined Jensen-type divergences of the form (16) based on the Tsallis q -entropy S_q , defined in (12). Like the Shannon-Boltzmann-Gibbs entropy, but unlike the Rényi entropies, the Tsallis q -entropy, for finite \mathcal{T} , is an instance of a ϕ -entropy (see Equation 14). Letting $\Psi = S_q$, (16) becomes

$$J_{S_q}^\pi(p) = S_q(E[p]) - E[S_q(p)]. \tag{20}$$

Again, as in Section 3.3, if we consider the Tsallis q -divergence,

$$D_q(p_1 \| p_2) = \frac{1}{1-q} \left(1 - \int p_1^q p_2^{1-q}\right),$$

there is no counterpart of the Equality (18).

When \mathcal{X} and \mathcal{T} are finite, $J_{S_q}^\pi$ in (20) is called the *Jensen-Tsallis (JT) divergence* and it has also been applied in image processing (Ben-Hamza, 2006). Unlike the JS divergence, the JT divergence lacks an interpretation as a mutual information. Despite this, for $q \in [1, 2]$, it exhibits joint convexity (Burbea and Rao, 1982). In the next section, we propose an alternative to the JT divergence which, among other features, is interpretable as a nonextensive mutual information (in the sense of Furuichi 2006) and is jointly convex, for $q \in [0, 1]$.

4. q -Convexity and q -Differences

This section introduces a novel class of functions, termed *Jensen q -differences*, which generalize Jensen differences. Later (in Section 5), we will use these functions to define the *Jensen-Tsallis q -difference*, which we will propose as an alternative nonextensive generalization of the JS divergence, instead of the JT divergence discussed in Section 3.4. We begin by recalling the concept of q -expectation (Tsallis, 1988).

Definition 3 *The unnormalized q -expectation of a random variable X , with probability density p , is*

$$E_q[X] \triangleq \int x p(x)^q.$$

Of course, $q = 1$ corresponds to the standard notion of expectation. For $q \neq 1$, the q -expectation does not match the intuitive meaning of average/expectation (e.g., $E_q[1] \neq 1$, in general). The q -expectation is a convenient concept in nonextensive information theory; for example, it yields a very compact form for the Tsallis entropy: $S_q(X) = -E_q[\ln_q p(X)]$.

4.1 q -Convexity

We now introduce the novel concept of q -convexity and use it to derive a set of results, namely the *Jensen q -inequality*.

Definition 4 Let $q \in \mathbb{R}$ and X be a convex set. A function $f : X \rightarrow \mathbb{R}$ is q -convex if for any $x, y \in X$ and $\lambda \in [0, 1]$,

$$f(\lambda x + (1 - \lambda)y) \leq \lambda^q f(x) + (1 - \lambda)^q f(y). \tag{21}$$

If $-f$ is q -convex, f is said to be q -concave.

Of course, 1-convexity is the usual notion of convexity. Many properties of 1-convex functions do not have q -analogues. For example, for $q \neq 1$, any q -convex function must be either nonnegative (if $q < 1$) or nonpositive (if $q > 1$); this simple fact can be shown through *reductio ad absurdum* by setting $x = y$ in (21). However, other properties remain: the next proposition states the Jensen q -inequality.

Proposition 5 If $f : X \rightarrow \mathbb{R}$ is q -convex, then for any $n \in \mathbb{N}$, $x_1, \dots, x_n \in X$ and $\pi = (\pi_1, \dots, \pi_n) \in \Delta^{n-1}$,

$$f\left(\sum_{i=1}^n \pi_i x_i\right) \leq \sum_{i=1}^n \pi_i^q f(x_i).$$

Moreover, if f is continuous, the above still holds for countably many points $(x_i)_{i \in \mathbb{N}}$.

Proof In the finite case, the proof can be carried out by induction, as in the proof of the standard Jensen inequality (Cover and Thomas, 1991). Assuming that the inequality holds for $n \in \mathbb{N}$, then, from the definition of q -convexity, it will also hold for $n + 1$:

$$\begin{aligned} f\left(\sum_{i=1}^{n+1} \pi_i x_i\right) &= f\left(\sum_{i=1}^n \pi_i x_i + \pi_{n+1} x_{n+1}\right) \\ &= f\left((1 - \pi_{n+1}) \sum_{i=1}^n \pi'_i x_i + \pi_{n+1} x_{n+1}\right) \\ &\leq (1 - \pi_{n+1})^q f\left(\sum_{i=1}^n \pi'_i x_i\right) + \pi_{n+1}^q f(x_{n+1}) \\ &\leq \sum_{i=1}^n \pi_i^q f(x_i) + \pi_{n+1}^q f(x_{n+1}) = \sum_{i=1}^{n+1} \pi_i^q f(x_i), \end{aligned}$$

where we used the fact that $\pi_{n+1} = 1 - \sum_{i=1}^n \pi_i$, and we defined $\pi'_i \triangleq \pi_i / (1 - \pi_{n+1})$ (note that $\sum_{i=1}^n \pi'_i = 1$.) Furthermore, if f is continuous, it commutes with taking limits, thus

$$f\left(\sum_{i=1}^{\infty} \pi_i x_i\right) = f\left(\lim_{n \rightarrow \infty} \sum_{i=1}^n \pi_i x_i\right) = \lim_{n \rightarrow \infty} f\left(\sum_{i=1}^n \pi_i x_i\right) \leq \lim_{n \rightarrow \infty} \sum_{i=1}^n \pi_i^q f(x_i) = \sum_{i=1}^{\infty} \pi_i^q f(x_i).$$

■

Proposition 6 *Let $f \geq 0$ and $q \geq r \geq 0$; then,*

$$f \text{ is } q\text{-convex} \quad \Rightarrow \quad f \text{ is } r\text{-convex} \tag{22}$$

$$f \text{ is } r\text{-concave} \quad \Rightarrow \quad f \text{ is } q\text{-concave}. \tag{23}$$

Proof Implication (22) results from

$$f(\lambda x + (1 - \lambda)y) \leq \lambda^q f(x) + (1 - \lambda)^q f(y) \leq \lambda^r f(x) + (1 - \lambda)^r f(y),$$

where the first inequality states the q -convexity of f and the second one is valid because $f(x), f(y) \geq 0$ and $t^r \geq t^q \geq 0$, for any $t \in [0, 1]$ and $q \geq r$. The proof of (23) is similar. ■

4.2 Jensen q -Differences

We now generalize Jensen differences, formalized in Definition 2, by introducing the concept of Jensen q -differences.

Definition 7 *Let $\mu \triangleq (\mu_t)_{t \in \mathcal{T}} \in [M_+(\mathcal{X})]^{\mathcal{T}}$ be a family of finite Radon measures on \mathcal{X} , indexed by \mathcal{T} , and let $\omega \in M_+(\mathcal{T})$ be a finite Radon measure on \mathcal{T} . For $q \geq 0$, define*

$$T_{q,\Psi}^{\omega}(\mu) \triangleq \Psi\left(\int_{\mathcal{T}} \omega(t) \mu_t d\tau(t)\right) - \int_{\mathcal{T}} \omega(t)^q \Psi(\mu_t) d\tau(t), \tag{24}$$

where:

- (i) Ψ is a concave functional such that $\text{dom } \Psi \subseteq M_+(\mathcal{X})$;
- (ii) $\omega(t)\mu_t(x)$ is τ -integrable for all $x \in \mathcal{X}$;
- (iii) $\int_{\mathcal{T}} \omega(t)\mu_t d\tau(t) \in \text{dom } \Psi$;
- (iv) $\mu_t \in \text{dom } \Psi$, for all $t \in \mathcal{T}$;
- (v) $\omega(t)^q \Psi(\mu_t)$ is τ -integrable.

If $\omega \in M_+^1(\mathcal{T})$, we call the function defined in (24) a Jensen q -difference.

Burbea and Rao (1982) established necessary and sufficient conditions on ϕ for the Jensen difference of a ϕ -entropy (see Equation 14) to be convex. The following proposition generalizes that result, extending it to Jensen q -differences.

Proposition 8 *Let \mathcal{T} and \mathcal{X} be finite sets, with $|\mathcal{T}| = m$ and $|\mathcal{X}| = n$, and let $\pi \in M_+^1(\mathcal{T})$. Let $\phi : [0, 1] \rightarrow \mathbb{R}$ be a function of class C^2 and consider the (ϕ -entropy, Burbea and Rao, 1982) function $\Psi : [0, 1]^n \rightarrow \mathbb{R}$ defined as $\Psi(z) \triangleq -\sum_{i=1}^n \phi(z_i)$. Then, the q -difference $T_{q,\Psi}^{\pi} : [0, 1]^{nm} \rightarrow \mathbb{R}$ is convex if and only if ϕ is convex and $-1/\phi''$ is $(2 - q)$ -convex.*

The proof is rather long, thus it is relegated to Appendix B.

5. The Jensen-Tsallis q -Difference

This section introduces the Jensen-Tsallis q -difference, a nonextensive generalization of the Jensen-Shannon divergence. After deriving some properties concerning the convexity and extrema of these functionals, we introduce the notion of joint and conditional Jensen-Tsallis q -difference, a contrast measure between stochastic processes. We end the section with a brief asymptotic analysis for the extensive case.

5.1 Definition

As in Section 3.2, let p be a random probability distribution taking values in $\{p_t\}_{t \in \mathcal{T}}$ according to a distribution $\pi \in M_+^1(\mathcal{T})$. Then, we may write

$$T_{q,\Psi}^\pi(p) = \Psi(E[p]) - E_q[\Psi(p)],$$

where the expectations are with respect to π . Hence Jensen q -differences may be seen as deformations of the standard Jensen differences (16), in which the second expectation is replaced by a q -expectation.

Let $\Psi = S_q$, the nonextensive Tsallis q -entropy. Introducing the random variables T and X , with values respectively in \mathcal{T} and \mathcal{X} , with densities $\pi(t)$ and $p(x) \triangleq \int_{\mathcal{T}} p(x|t)\pi(t)$, we have (writing T_{q,S_q}^π simply as T_q^π)

$$\begin{aligned} T_q^\pi(p) &= S_q(E[p]) - E_q[S_q(p)] \\ &= S_q(X) - \int_{\mathcal{T}} \pi(t)^q S_q(X|T=t) \\ &= S_q(X) - S_q(X|T) \\ &= I_q(X;T), \end{aligned} \tag{25}$$

where $S_q(X|T)$ is the Tsallis conditional entropy (4), and $I_q(X;T)$ is the Tsallis mutual information (6), as defined by Furuichi (2006). Observe that (25) is a nonextensive analogue of (17). Since, in general, $I_q \neq \tilde{I}_q$ (see Equation 7), unless $q = 1$ (in that case, $I_1 = \tilde{I}_1 = I$), there is no counterpart of (18) in terms of q -differences. Nevertheless, Lamberti and Majtey (2003) have proposed a non-logarithmic version of the JS divergence, which corresponds to using \tilde{I}_q for the Tsallis mutual q -entropy (although this interpretation is not explicitly mentioned).

When \mathcal{X} and \mathcal{T} are finite with $|\mathcal{T}| = m$, we call the quantity $T_q^\pi(p_1, \dots, p_m)$ the *Jensen-Tsallis (JT) q -difference* of p_1, \dots, p_m with weights π_1, \dots, π_m . Although the JT q -difference is a generalization of the JS divergence, for $q \neq 1$, the term “divergence” would be misleading in this case, since T_q^π may take negative values (if $q < 1$) and does not vanish in general if p is deterministic.

When $|\mathcal{T}| = 2$ and $\pi = (1/2, 1/2)$, define $T_q \triangleq T_q^{1/2, 1/2}$,

$$T_q(p_1, p_2) = S_q\left(\frac{p_1 + p_2}{2}\right) - \frac{S_q(p_1) + S_q(p_2)}{2^q}.$$

Notable cases arise for particular values of q :

- For $q = 0$, $S_0(p) = -1 + \nu(\text{supp}(p))$, where $\nu(\text{supp}(p))$ denotes the measure of the support of p (recall that p is defined on the measure space $(\mathcal{X}, \mathcal{M}, \nu)$). For example, if \mathcal{X} is finite and

ν is the counting measure, $\nu(\text{supp}(p)) = \|p\|_0$ is the so-called *0-norm* (although it is not a norm) of vector p , that is, its number of nonzero components. The Jensen-Tsallis 0-difference is thus

$$\begin{aligned} T_0(p_1, p_2) &= -1 + \nu\left(\text{supp}\left(\frac{p_1 + p_2}{2}\right)\right) + 1 - \nu(\text{supp}(p_1)) + 1 - \nu(\text{supp}(p_2)) \\ &= 1 + \nu(\text{supp}(p_1) \cup \text{supp}(p_2)) - \nu(\text{supp}(p_1)) - \nu(\text{supp}(p_2)) \\ &= 1 - \nu(\text{supp}(p_1) \cap \text{supp}(p_2)); \end{aligned} \tag{26}$$

if \mathcal{X} is finite and ν is the counting measure, this becomes

$$T_0(p_1, p_2) = 1 - \|p_1 \odot p_2\|_0,$$

where \odot denotes the Hadamard-Schur (i.e., elementwise) product. We call T_0 the *Boolean difference*.

- For $q = 1$, since $S_1(p) = H(p)$, T_1 is the JS divergence,

$$T_1(p_1, p_2) = JS(p_1, p_2).$$

- For $q = 2$, $S_2(p) = 1 - \langle p, p \rangle$, where $\langle a, b \rangle = \int_{\mathcal{X}} a(x)b(x) d\nu(x)$ is the inner product between a and b (which reduces to $\langle a, b \rangle = \sum_i a_i b_i$ if \mathcal{X} is finite and ν is the counting measure). Consequently, the Tsallis 2-difference is

$$T_2(p_1, p_2) = \frac{1}{2} - \frac{1}{2} \langle p_1, p_2 \rangle,$$

which we call the *linear difference*.

5.2 Properties of the JT q -Difference

This subsection presents results regarding convexity and extrema of the JT q -difference, for certain values of q , extending known properties of the JS divergence ($q = 1$). Some properties of the JS divergence are lost in the transition to nonextensivity; for example, while the former is nonnegative and vanishes if and only if all the distributions are identical, this is not true in general with the JT q -difference. Nonnegativity of the JT q -difference is only guaranteed if $q \geq 1$, which explains why some authors (e.g., Furuichi 2006) only consider values of $q \geq 1$, when looking for nonextensive analogues of Shannon’s information theory. Moreover, unless $q = 1$, it is not generally true that $T_q^\pi(p, \dots, p) = 0$ or even that $T_q^\pi(p, \dots, p, p') \geq T_q^\pi(p, \dots, p, p)$. For example, the solution of the optimization problem

$$\min_{p_1 \in \Delta^n} T_q(p_1, p_2), \tag{27}$$

is, in general, different from p_2 , unless $q = 1$. Instead, this minimizer is closer to the uniform distribution if $q \in [0, 1)$, and closer to a degenerate distribution for $q \in (1, 2]$ (see Fig. 1). This is not so surprising: recall that $T_2(p_1, p_2) = \frac{1}{2} - \frac{1}{2} \langle p_1, p_2 \rangle$; in this case, (27) becomes a linear program, and the solution is not $p_1^* = p_2$, but $p_1^* = \delta_j$, where $j = \arg \max_i p_{2i}$.

At this point, we should also remark that, when \mathcal{X} is a finite set, the uniform distribution maximizes the Tsallis entropy for any $q \geq 0$, which is in fact one of the Suyari axioms underlying the Tsallis entropy (see Axiom A2 in Appendix A).

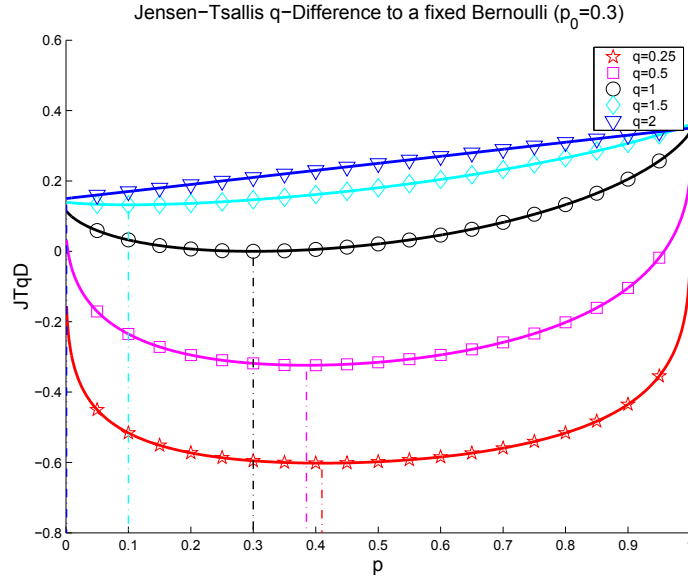


Figure 1: Jensen-Tsallis q -difference between two Bernoulli distributions, $p_1 = (0.3, 0.7)$ and $p_2 = (p, 1 - p)$, for several values of the entropic index q . Observe that, for $q \in [0, 1)$, the minimizer of the JT q -difference approaches the uniform distribution $(0.5, 0.5)$ as q approaches 0; for $q \in (1, 2]$, this minimizer approaches the degenerate distribution, as $q \rightarrow 2$.

We start with the following corollary of Proposition 8, which establishes the joint convexity of the JT q -difference, for $q \in [0, 1]$. (Interestingly, this “complements” the joint convexity of the JT divergence (20), for $q \in [1, 2]$, proved by Burbea and Rao 1982.)

Corollary 9 *Let \mathcal{T} and \mathcal{X} be finite sets with cardinalities m and n , respectively. For $q \in [0, 1]$, the JT q -difference is a jointly convex function on $M_+^{1, S_q}(\mathcal{X})$. Formally, let $\{p_t^{(i)}\}_{t \in \mathcal{T}}$, and $i = 1, \dots, l$, be a collection of l sets of probability distributions on \mathcal{X} ; then, for any $(\lambda_1, \dots, \lambda_l) \in \Delta^{l-1}$,*

$$T_q^\pi \left(\sum_{i=1}^l \lambda_i p_1^{(i)}, \dots, \sum_{i=1}^l \lambda_i p_m^{(i)} \right) \leq \sum_{i=1}^l \lambda_i T_q^\pi(p_1^{(i)}, \dots, p_m^{(i)}).$$

Proof Observe that the Tsallis entropy (3) of a probability distribution $p_t = \{p_{t1}, \dots, p_{tn}\}$ can be written as

$$S_q(p_t) = - \sum_{i=1}^n \varphi(p_{ti}), \quad \text{where } \varphi_q(x) = \frac{x - x^q}{1 - q};$$

thus, from Proposition 8, T_q^π is convex if and only if φ_q is convex and $-1/\varphi_q''$ is $(2 - q)$ -convex. Since $\varphi_q''(x) = qx^{q-2}$, φ_q is convex for $x \geq 0$ and $q \geq 0$. To show the $(2 - q)$ -convexity of $-1/\varphi_q''(x) = -(1/q)x^{2-q}$, for $x_t \geq 0$, and $q \in [0, 1]$, we use a version of the power mean inequality (Steele, 2006),

$$- \left(\sum_{i=1}^l \lambda_i x_i \right)^{2-q} \leq - \sum_{i=1}^l (\lambda_i x_i)^{2-q} = - \sum_{i=1}^l \lambda_i^{2-q} x_i^{2-q},$$

thus concluding that $-1/\phi_q''$ is in fact $(2 - q)$ -convex. ■

A consequence of Corollary 9 is that, for finite \mathcal{X} and any $q \in [0, 1]$, the JT q -difference is upper bounded, namely $T_q^\pi(p_1, \dots, p_m) \leq S_q(\pi)$. Indeed, since T_q^π is convex and its domain is the Cartesian product of m simplices (a convex polytope), its maximum must occur on a vertex, that is, when each argument p_t is a degenerate distribution at x_t , denoted δ_{x_t} . In particular, if $|\mathcal{X}| \geq |\mathcal{T}|$, this maximum occurs at a vertex corresponding to disjoint degenerate distributions, that is, such that $x_i \neq x_j$ if $i \neq j$. At this maximum,

$$\begin{aligned} T_q^\pi(\delta_{x_1}, \dots, \delta_{x_m}) &= S_q\left(\sum_{t=1}^m \pi_t \delta_{x_t}\right) - \sum_{t=1}^m \pi_t S_q(\delta_{x_t}) \\ &= S_q\left(\sum_{t=1}^m \pi_t \delta_{x_t}\right) \\ &= S_q(\pi) \end{aligned} \tag{28}$$

where the equality in (28) results from $S_q(\delta_{x_t}) = 0$. (Notice that this maximum may not be achieved if $|\mathcal{X}| < |\mathcal{T}|$.) The next proposition provides a stronger result: it establishes upper and lower bounds for the JT q -difference to any non-negative q and to countable \mathcal{X} and \mathcal{T} .

Proposition 10 *Let \mathcal{T} and \mathcal{X} be countable sets. For $q \geq 0$,*

$$T_q^\pi((p_t)_{t \in \mathcal{T}}) \leq S_q(\pi), \tag{29}$$

and, if $|\mathcal{X}| \geq |\mathcal{T}|$, the maximum of T_q^π is reached for a set of disjoint degenerate distributions. This maximum may not be attained if $|\mathcal{X}| < |\mathcal{T}|$.

For $q \geq 1$,

$$T_q^\pi((p_t)_{t \in \mathcal{T}}) \geq 0,$$

and the minimum of T_q^π is attained in the purely deterministic case, that is, when all distributions are equal to the same degenerate distribution.

For $q \in [0, 1]$ and \mathcal{X} a finite set with $|\mathcal{X}| = n$,

$$T_q^\pi((p_t)_{t \in \mathcal{T}}) \geq S_q(\pi)[1 - n^{1-q}]. \tag{30}$$

This lower bound (which is zero or negative) is attained when all distributions are uniform.

Proof The proof is given in Appendix C. ■

Finally, the next proposition characterizes the convexity/concavity of the JT q -difference on each argument.

Proposition 11 *Let \mathcal{T} and \mathcal{X} be countable sets. The JT q -difference is convex in each argument, for $q \in [0, 2]$, and concave in each argument, for $q \geq 2$.*

Proof Notice that the JT q -difference can be written as $T_q^\pi(p_1, \dots, p_m) = \sum_j \Psi(p_{1j}, \dots, p_{mj})$, with

$$\Psi(y_1, \dots, y_m) = \frac{1}{q-1} \left[\sum_i (\pi_i - \pi_i^q) y_i + \sum_i \pi_i^q y_i^q - \left(\sum_i \pi_i y_i \right)^q \right].$$

It suffices to consider the second derivative of Ψ with respect to y_1 . Introducing $z = \sum_{i=2}^m \pi_i y_i$,

$$\begin{aligned} \frac{\partial^2 \Psi}{\partial y_1^2} &= q \left[\pi_1^q y_1^{q-2} - \pi_1^2 (\pi_1 y_1 + z)^{q-2} \right] \\ &= q \pi_1^2 \left[(\pi_1 y_1)^{q-2} - (\pi_1 y_1 + z)^{q-2} \right]. \end{aligned} \quad (31)$$

Since $\pi_1 y_1 \leq (\pi_1 y_1 + z) \leq 1$, the quantity in (31) is nonnegative for $q \in [0, 2]$ and non-positive for $q \geq 2$. \blacksquare

5.3 Joint and Conditional JT q -Differences and a Chain Rule

This subsection introduces joint and conditional JT q -differences, which will later be used as a contrast measure between stochastic processes. A chain rule is derived that relates conditional and joint JT q -differences.

Definition 12 Let \mathcal{X} , \mathcal{Y} and \mathcal{T} be measure spaces. Let $(p_t)_{t \in \mathcal{T}} \in [M_+^1(\mathcal{X} \times \mathcal{Y})]^{\mathcal{T}}$ be a family of measures in $M_+^1(\mathcal{X} \times \mathcal{Y})$ indexed by \mathcal{T} , and let p be a random probability distribution taking values in $\{p_t\}_{t \in \mathcal{T}}$ according to a distribution $\pi \in M_+^1(\mathcal{T})$. Consider also:

- for each $t \in \mathcal{T}$, the marginals $p_t(Y) \in M_+^1(\mathcal{Y})$,
- for each $t \in \mathcal{T}$ and $y \in \mathcal{Y}$, the conditionals $p_t(X|Y=y) \in M_+^1(\mathcal{X})$,
- the mixture $r(X, Y) \triangleq \int_{\mathcal{T}} \pi(t) p_t(X, Y) \in M_+^1(\mathcal{X} \times \mathcal{Y})$,
- the marginal $r(Y) \in M_+^1(\mathcal{Y})$,
- for each $y \in \mathcal{Y}$, the conditionals $r(X|Y=y) \in M_+^1(\mathcal{X})$.

For notational convenience, we also append a subscript to p to emphasize its joint or conditional dependency of the random variables X and Y , that is, $p_{XY} \triangleq p$, and $p_{X|Y}$ denotes a random conditional probability distribution taking values in $\{p_t(\cdot|Y)\}_{t \in \mathcal{T}}$ according to the distribution π .

For $q \geq 0$, we refer to the joint JT q -difference of p_{XY} by

$$T_q^\pi(p_{XY}) \triangleq T_q^\pi(p) = S_q(r) - E_{q, \mathcal{T} \sim \pi(\mathcal{T})} [S_q(p_t)]$$

and to the conditional JT q -difference of $p_{X|Y}$ by

$$T_q^\pi(p_{X|Y}) \triangleq E_{q, Y \sim r(Y)} [S_q(r(\cdot|Y=y))] - E_{q, \mathcal{T} \sim \pi(\mathcal{T})} [E_{q, Y \sim p_t(Y)} [S_q(p_t(\cdot|Y=y))]], \quad (32)$$

where we appended the random variables being used in each q -expectation, for the sake of clarity.

Note that the joint JT q -difference is just the usual JT q -difference of the joint random variable $X \times Y$, which equals (cf. 25)

$$T_q^\pi(p_{XY}) = S_q(X, Y) - S_q(X, Y|T) = I_q(X \times Y; T), \quad (33)$$

and the conditional JT q -difference is simply the usual JT q -difference with all entropies replaced by conditional entropies (conditioned on Y). Indeed, expression (32) can be rewritten as:

$$T_q^\pi(p_{X|Y}) = S_q(X|Y) - S_q(X|T, Y) = I_q(X; T | Y), \quad (34)$$

that is, the conditional JT q -difference may also interpreted as a Tsallis mutual information, as in (25), but now *conditioned* on the random variable Y .

Note also that, for the extensive case $q = 1$, (32) may also be rewritten in terms of the conditional KL divergences,

$$\begin{aligned} J^\pi(p_{X|Y}) \triangleq T_1^\pi(p_{X|Y}) &= E_{Y \sim r(Y)} [H(r(\cdot|Y = y))] - E_{T \sim \pi(T)} [E_{Y \sim p_t(Y)} [H(p_t(\cdot|Y = y))]] \\ &= E_{T \sim \pi(T)} [E_{Y \sim r(Y)} [D(p_t(\cdot|Y = y) || r(\cdot|Y = y))]]. \end{aligned}$$

Proposition 13 *The following chain rule holds:*

$$T_q^\pi(p_{XY}) = T_q^\pi(p_{X|Y}) + T_q^\pi(p_Y)$$

Proof Writing the joint/conditional JT q -differences as joint/conditional mutual informations (33–34) and invoking the chain rule provided by (4), we have that

$$\begin{aligned} I_q(X; T|Y) + I_q(Y; T) &= S_q(X|T, Y) - S_q(X|Y) + S_q(Y|T) - S_q(Y) \\ &= S_q(X, Y|T) - S_q(X, Y), \end{aligned}$$

which is the joint JT q -difference associated with the random variable $X \times Y$. ■

Let us now turn our attention to the case where $Y = X^k$ for some $k \in \mathbb{N}$. In the following, the notation $(A_n)_{n \in \mathbb{N}}$ denotes a stationary ergodic process with values on some finite alphabet \mathcal{A} .

Definition 14 *Let X and \mathcal{T} be measure spaces, with X finite, and let $\mathcal{F} = [(X_n)_{n \in \mathbb{N}}]^{\mathcal{T}}$ be a family of stochastic processes (taking values on the alphabet X) indexed by \mathcal{T} . The k -th order JT q -difference of \mathcal{F} is defined, for $k = 1, \dots, n$, as*

$$T_{q,k}^{\text{joint},\pi}(\mathcal{F}) \triangleq T_q^\pi(p_{X^k})$$

and the k -th order conditional JT q -difference of \mathcal{F} is defined, for $k = 1, \dots, n$, as

$$T_{q,k}^{\text{cond},\pi}(\mathcal{F}) \triangleq T_q^\pi(p_{X|X^k}),$$

and, for $k = 0$, as $T_{q,0}^{\text{cond},\pi}(\mathcal{F}) \triangleq T_{q,1}^{\text{joint},\pi}(\mathcal{F}) = T_q^\pi(p_X)$.

Proposition 15 *The joint and conditional k -th order JT q -differences are related through:*

$$T_{q,k}^{\text{joint},\pi}(\mathcal{F}) = \sum_{i=0}^{k-1} T_{q,i}^{\text{cond},\pi}(\mathcal{F}) \quad (35)$$

Proof Use Proposition 13 and induction. ■

5.4 Asymptotic Analysis in the Extensive Case

We now focus on the extensive case ($q = 1$) for a brief asymptotic analysis of the k -th order joint and conditional JT 1-differences (or *conditional Jensen-Shannon divergences*) when k goes to infinity.

The conditional Jensen-Shannon divergence was introduced by El-Yaniv et al. (1998) to address the *two-sample problem* for strings emitted by Markovian sources. Given two strings s and t , the goal is to decide whether they were emitted by the same source or by different sources. Under some fair assumptions, the most likely k -th order Markovian joint source of s and t is governed by a distribution \hat{r} given by

$$\hat{r} = \arg \min_r \lambda D(\hat{p}_s \| r) + (1 - \lambda) D(\hat{p}_t \| r). \quad (36)$$

where $D(\cdot \| \cdot)$ are conditional KL divergences, \hat{p}_s and \hat{p}_t are the empirical $(k - 1)$ -th order conditionals associated with s and t , respectively, and $\lambda = |s| / (|s| + |t|)$ is the length ratio. The solution of the optimization problem is

$$\hat{r}(a|c) = \frac{\lambda \hat{p}_s(c)}{\lambda \hat{p}_s(c) + (1 - \lambda) \hat{p}_t(c)} \hat{p}_s(a|c) + \frac{(1 - \lambda) \hat{p}_t(c)}{\lambda \hat{p}_s(c) + (1 - \lambda) \hat{p}_t(c)} \hat{p}_t(a|c),$$

where $a \in \mathcal{A}$ is a symbol and $c \in \mathcal{A}^{k-1}$ is a context; this can be rewritten as $\hat{r}(a, c) = \lambda \hat{p}_s(a, c) + (1 - \lambda) \hat{p}_t(a, c)$; that is, the optimum in (36) is a mixture of \hat{p}_s and \hat{p}_t weighted by the string lengths. Notice that, at the minimum, we have

$$\lambda D(\hat{p}_s \| \hat{r}) + (1 - \lambda) D(\hat{p}_t \| \hat{r}) = JS_k^{\text{cond}, (\lambda, 1-\lambda)}(\hat{p}_s, \hat{p}_t).$$

It is tempting to investigate the asymptotic behavior of the conditional and joint JS divergences when $k \rightarrow \infty$; however, unlike other asymptotic information theoretic quantities, like the entropy or cross entropy rates, this behavior fails to characterize the sources s and t . Intuitively, this is justified by the fact that observing more and more symbols drawn from the mixture of the two sources rapidly decreases the uncertainty about which source generated the sample. Indeed, from the asymptotic equipartition property of stationary ergodic sources (Cover and Thomas, 1991), we have that $\lim_{k \rightarrow \infty} \frac{1}{k} H(p_{X_k}) = \lim_{k \rightarrow \infty} H(p_{X|X_k})$, which implies

$$\lim_{k \rightarrow \infty} JS_k^{\text{cond}, \pi} = \lim_{k \rightarrow \infty} \frac{1}{k} JS_k^{\text{joint}, \pi} \leq \lim_{k \rightarrow \infty} \frac{1}{k} H(\pi) = 0,$$

where we used the fact that the JS divergence is upper-bounded by the entropy of the mixture $H(\pi)$ (see Proposition 10). Since the conditional JS divergence must be non-negative, we therefore conclude that $\lim_{k \rightarrow \infty} JS_k^{\text{cond}, \pi} = 0$, pointwise.

6. Nonextensive Mutual Information Kernels

In this section we consider the application of extensive and nonextensive entropies to define kernels on measures; since kernels involve pairs of measures, throughout this section $|\mathcal{T}| = 2$. Based on the denormalization formulae presented in Section 2.3, we devise novel kernels related to the JS divergence and the JT q -difference; these kernels allow setting a weight for each argument, thus will be called *weighted Jensen-Tsallis kernels*. We also introduce kernels related to the JR divergence (Section 3.3) and the JT divergence (Section 3.4), and establish a connection between the Tsallis kernels and a family of kernels investigated by Hein et al. (2004) and Fuglede (2005), placing

those kernels under a new information-theoretic light. After that, we give a brief overview of string kernels, and using the results of Section 5.3, we devise k -th order Jensen-Tsallis kernels between stochastic processes that subsume the well-known p -spectrum kernel of Leslie et al. (2002).

6.1 Positive and Negative Definite Kernels

We start by recalling basic concepts from kernel theory (Schölkopf and Smola, 2002); in the following, \mathcal{X} denotes a nonempty set.

Definition 16 Let $\varphi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a symmetric function, that is, a function satisfying $\varphi(y, x) = \varphi(x, y)$, for all $x, y \in \mathcal{X}$. φ is called a positive definite (pd) kernel if and only if

$$\sum_{i=1}^n \sum_{j=1}^n c_i c_j \varphi(x_i, x_j) \geq 0$$

for all $n \in \mathbb{N}$, $x_1, \dots, x_n \in \mathcal{X}$ and $c_1, \dots, c_n \in \mathbb{R}$.

Definition 17 Let $\psi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be symmetric. ψ is called a negative definite (nd) kernel if and only if

$$\sum_{i=1}^n \sum_{j=1}^n c_i c_j \psi(x_i, x_j) \leq 0$$

for all $n \in \mathbb{N}$, $x_1, \dots, x_n \in \mathcal{X}$ and $c_1, \dots, c_n \in \mathbb{R}$, satisfying the additional constraint $c_1 + \dots + c_n = 0$. In this case, $-\psi$ is called conditionally pd; obviously, positive definiteness implies conditional positive definiteness.

The sets of pd and nd kernels are both closed under pointwise sums/integrations, the former being also closed under pointwise products; moreover, both sets are closed under pointwise convergence. While pd kernels “correspond” to inner products via embedding in a Hilbert space, nd kernels that vanish on the diagonal and are positive anywhere else, “correspond” to squared Hilbertian distances. These facts, and the following propositions and lemmas, are shown in Berg et al. (1984).

Proposition 18 Let $\psi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a symmetric function, and $x_0 \in \mathcal{X}$. Let $\varphi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be given by

$$\varphi(x, y) = \psi(x, x_0) + \psi(y, x_0) - \psi(x, y) - \psi(x_0, x_0).$$

Then, φ is pd if and only if ψ is nd.

Proposition 19 The function $\psi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a nd kernel if and only if $\exp(-t\psi)$ is pd for all $t > 0$.

Proposition 20 The function $\psi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$ is a nd kernel if and only if $(t + \psi)^{-1}$ is pd for all $t > 0$.

Lemma 21 If ψ is nd and nonnegative on the diagonal, that is, $\psi(x, x) \geq 0$ for all $x \in \mathcal{X}$, then ψ^α , for $\alpha \in [0, 1]$, and $\ln(1 + \psi)$, are also nd.

Lemma 22 *If $f : X \rightarrow \mathbb{R}$ satisfies $f \geq 0$, then, for $\alpha \in [1, 2]$, the function $\psi_\alpha(x, y) = -(f(x) + f(y))^\alpha$ is a nd kernel.*

The following definition (Berg et al., 1984) has been used in a machine learning context by Cuturi and Vert (2005).

Definition 23 *Let (X, \oplus) be a semigroup.² A function $\phi : X \rightarrow \mathbb{R}$ is called pd (in the semigroup sense) if $k : X \times X \rightarrow \mathbb{R}$, defined as $k(x, y) = \phi(x \oplus y)$, is a pd kernel. Likewise, ϕ is called nd if k is a nd kernel. Accordingly, these are called semigroup kernels.*

6.2 Jensen-Shannon and Tsallis Kernels

The basic result that allows deriving pd kernels based on the JS divergence and, more generally, on the JT q -difference, is the fact that the denormalized Tsallis q -entropies (10) are nd functions on $(M_+^{S_q}(X), +)$, for $q \in [0, 2]$. Of course, this includes the denormalized Shannon-Boltzmann-Gibbs entropy (8) as a particular case, corresponding to $q = 1$. Although part of the proof was given by Berg et al. (1984) (and by Topsøe 2000 and Cuturi and Vert 2005 for the Shannon entropy case), we present a complete proof here.

Proposition 24 *For $q \in [0, 2]$, the denormalized Tsallis q -entropy S_q is a nd function on $(M_+^{S_q}(X), +)$.*

Proof Since nd kernels are closed under pointwise integration, it suffices to prove that ϕ_q (see Equation 11) is nd on $(\mathbb{R}_+, +)$. For $q \neq 1$, $\phi_q(y) = (q - 1)^{-1}(y - y^q)$. Let us consider two cases separately: if $q \in [0, 1)$, $\phi_q(y)$ equals a positive constant times $-\iota + \iota^q$, where $\iota(y) = y$ is the identity map defined on \mathbb{R}_+ . Since the set of nd functions is closed under sums, we only need to show that both $-\iota$ and ι^q are nd. Both ι and $-\iota$ are nd, as can easily be seen from the definition; besides, since ι is nd and nonnegative, Lemma 21 guarantees that ι^q is also nd. For the second case, where $q \in (1, 2]$, $\phi_q(y)$ equals a positive constant times $\iota - \iota^q$. It only remains to show that $-\iota^q$ is nd for $q \in (1, 2]$: Lemma 22 guarantees that the kernel $k(x, y) = -(x + y)^q$ is nd; therefore $-\iota^q$ is a nd function.

For $q = 1$, we use the fact that,

$$\phi_1(x) = \phi_H(x) = -x \ln x = \lim_{q \rightarrow 1} \frac{x - x^q}{q - 1} = \lim_{q \rightarrow 1} \phi_q(x),$$

where the limit is obtained by L'Hôpital's rule; since the set of nd functions is closed under limits, $\phi_1(x)$ is nd. ■

The following lemma, proved in Berg et al. (1984), will also be needed below.

Lemma 25 *The function $\zeta_q : \mathbb{R}_{++} \rightarrow \mathbb{R}$, defined as $\zeta_q(y) = y^{-q}$ is pd, for $q \in [0, 1]$.*

We are now in a position to present the main contribution of this section, which is a family of *weighted Jensen-Tsallis kernels*, generalizing the JS-based (and other) kernels in two ways: (i) they allow using unnormalized measures; equivalently, they allow using different weights for each of the two arguments; (ii) they extend the mutual information feature of the JS kernel to the nonextensive scenario.

2. Recall that (X, \oplus) is a *semigroup* if \oplus is a binary operation in X that is associative and has an identity element.

Definition 26 (weighted Jensen-Tsallis kernels) *The kernel $\tilde{k}_q : M_+^{S_q}(\mathcal{X}) \times M_+^{S_q}(\mathcal{X}) \rightarrow \mathbb{R}$ is defined as*

$$\begin{aligned} \tilde{k}_q(\mu_1, \mu_2) &\triangleq \tilde{k}_q(\omega_1 p_1, \omega_2 p_2) \\ &= (S_q(\pi) - T_q^\pi(p_1, p_2)) (\omega_1 + \omega_2)^q, \end{aligned}$$

where $p_1 = \mu_1/\omega_1$ and $p_2 = \mu_2/\omega_2$ are the normalized counterparts of μ_1 and μ_2 , with corresponding masses $\omega_1, \omega_2 \in \mathbb{R}_+$, and $\pi = (\omega_1/(\omega_1 + \omega_2), \omega_2/(\omega_1 + \omega_2))$.

The kernel $k_q : (M_+^{S_q}(\mathcal{X}) \setminus \{0\})^2 \rightarrow \mathbb{R}$ is defined as

$$k_q(\mu_1, \mu_2) \triangleq k_q(\omega_1 p_1, \omega_2 p_2) = S_q(\pi) - T_q^\pi(p_1, p_2).$$

Recalling (25), notice that $S_q(\pi) - T_q^\pi(p_1, p_2) = S_q(T) - I_q(X; T) = S_q(T|X)$ can be interpreted as the *Tsallis posterior conditional entropy*. Hence, k_q can be seen (in Bayesian classification terms) as a nonextensive expected measure of uncertainty in correctly identifying the class, given the prior $\pi = (\pi_1, \pi_2)$, and a sample from the mixture $\pi_1 p_1 + \pi_2 p_2$. The more similar the two distributions are, the greater this uncertainty.

Proposition 27 *The kernel \tilde{k}_q is pd, for $q \in [0, 2]$. The kernel k_q is pd, for $q \in [0, 1]$.*

Proof With $\mu_1 = \omega_1 p_1$ and $\mu_2 = \omega_2 p_2$ and using the denormalization formula of Remark 1, we obtain $\tilde{k}_q(\mu_1, \mu_2) = -S_q(\mu_1 + \mu_2) + S_q(\mu_1) + S_q(\mu_2)$. Now invoke Proposition 18 with $\psi = S_q$ (which is nd by Proposition 24), $x = \mu_1$, $y = \mu_2$, and $x_0 = 0$ (the null measure). Observe now that $k_q(\mu_1, \mu_2) = \tilde{k}_q(\mu_1, \mu_2)(\omega_1 + \omega_2)^{-q}$. Since the product of two pd kernels is a pd kernel and (Proposition 25) $(\omega_1 + \omega_2)^{-q}$ is a pd kernel, for $q \in [0, 1]$, we conclude that k_q is pd. ■

As we can see, the weighted Jensen-Tsallis kernels have two inherent properties: they are parameterized by the entropic index q and they allow their arguments to be unbalanced, that is, to have different weights ω_i . We now mention some instances of kernels where each of these degrees of freedom is suppressed. We start with the following subfamily of kernels, obtained by setting $q = 1$.

Definition 28 (weighted Jensen-Shannon kernels) *The kernel $\tilde{k}_{WJS} : (M_+^H(\mathcal{X}))^2 \rightarrow \mathbb{R}$ is defined as $\tilde{k}_{WJS} \triangleq \tilde{k}_1$, that is,*

$$\begin{aligned} \tilde{k}_{WJS}(\mu_1, \mu_2) &= \tilde{k}_{WJS}(\omega_1 p_1, \omega_2 p_2) \\ &= (H(\pi) - J^\pi(p_1, p_2)) (\omega_1 + \omega_2), \end{aligned}$$

where $p_1 = \mu_1/\omega_1$ and $p_2 = \mu_2/\omega_2$ are the normalized counterpart of μ_1 and μ_2 , and $\pi = (\omega_1/(\omega_1 + \omega_2), \omega_2/(\omega_1 + \omega_2))$.

Analogously, the kernel $k_{WJS} : (M_+^H(\mathcal{X}) \setminus \{0\})^2 \rightarrow \mathbb{R}$ is simply $k_{WJS} \triangleq k_1$, that is,

$$k_{WJS}(\mu_1, \mu_2) = k_{WJS}(\omega_1 p_1, \omega_2 p_2) = H(\pi) - J^\pi(p_1, p_2).$$

Corollary 29 *The weighted Jensen-Shannon kernels \tilde{k}_{WJS} and k_{WJS} are pd.*

Proof Invoke Proposition 27 with $q = 1$. ■

The following family of *weighted exponentiated JS kernels*, generalize the so-called *exponentiated JS kernel*, that has been used, and shown to be pd, by Cuturi and Vert (2005).

Definition 30 (Exponentiated JS kernel) *The kernel $k_{EJS} : M_+^1(\mathcal{X}) \times M_+^1(\mathcal{X}) \rightarrow \mathbb{R}$ is defined, for $t > 0$, as*

$$k_{EJS}(p_1, p_2) = \exp[-t JS(p_1, p_2)].$$

Definition 31 (Weighted exponentiated JS kernels) *The kernel $k_{WEJS} : M_+^H(\mathcal{X}) \times M_+^H(\mathcal{X}) \rightarrow \mathbb{R}$ is defined, for $t > 0$, as*

$$\begin{aligned} k_{WEJS}(\mu_1, \mu_2) &= \exp[t k_{WJS}(\mu_1, \mu_2)] \\ &= \exp(t H(\pi)) \exp[-t J^\pi(p_1, p_2)]. \end{aligned} \tag{37}$$

Corollary 32 *The kernels k_{WEJS} are pd. In particular, k_{EJS} is pd.*

Proof Results from Proposition 19 and Corollary 29. Notice that although k_{WEJS} is pd, none of its two exponential factors in (37) is pd. ■

We now keep $q \in [0, 2]$ but consider the weighted JT kernel family restricted to normalized measures, $k_q|_{(M_+^1(\mathcal{X}))^2}$. This corresponds to setting uniform weights ($\omega_1 = \omega_2 = 1/2$); note that in this case \tilde{k}_q and k_q collapse into the same kernel,

$$\tilde{k}_q(p_1, p_2) = k_q(p_1, p_2) = \ln_q(2) - T_q(p_1, p_2).$$

Proposition 27 guarantees that these kernels are pd for $q \in [0, 2]$. Remarkably, we recover three well-known particular cases for $q \in \{0, 1, 2\}$. We start with the Jensen-Shannon kernel, introduced and shown to be pd by Hein et al. (2004); it is a particular case of a weighted Jensen-Shannon kernel in Definition 28.

Definition 33 (Jensen-Shannon kernel) *The kernel $k_{JS} : M_+^1(\mathcal{X}) \times M_+^1(\mathcal{X}) \rightarrow \mathbb{R}$ is defined as*

$$k_{JS}(p_1, p_2) = \ln 2 - JS(p_1, p_2).$$

Corollary 34 *The kernel k_{JS} is pd.*

Proof k_{JS} is the restriction of k_{WJS} to $M_+^1(\mathcal{X}) \times M_+^1(\mathcal{X})$. ■

Finally, we study two other particular cases of the family of Tsallis kernels: the Boolean and linear kernels.

Definition 35 (Boolean kernel) *Let the kernel $k_{\text{Bool}} : M_+^{S_0,1}(\mathcal{X}) \times M_+^{S_0,1}(\mathcal{X}) \rightarrow \mathbb{R}$ be defined as $k_{\text{Bool}} = k_0$, that is,*

$$k_{\text{Bool}}(p_1, p_2) = \mathfrak{v}(\text{supp}(p_1) \cap \text{supp}(p_2)),$$

that is, $k_{\text{Bool}}(p_1, p_2)$ equals the measure of the intersection of the supports (cf. Equation 26). In particular, if \mathcal{X} is finite and \mathfrak{v} is the counting measure, the above may be written as

$$k_{\text{Bool}}(p_1, p_2) = \|p_1 \odot p_2\|_0.$$

Definition 36 (Linear kernel) *Let the kernel $k_{\text{lin}} : M_+^{S_2,1}(\mathcal{X}) \times M_+^{S_2,1}(\mathcal{X}) \rightarrow \mathbb{R}$ be defined as*

$$k_{\text{lin}}(p_1, p_2) = \frac{1}{2} \langle p_1, p_2 \rangle.$$

Corollary 37 *The kernels k_{Bool} and k_{lin} are pd.*

Proof Invoke Proposition 27 with $q = 0$ and $q = 2$. Notice that, for $q = 2$, we just recover the well-known property of the inner product kernel (Schölkopf and Smola, 2002), which is equal to k_{lin} up to a scalar. ■

In conclusion, the Boolean kernel, the Jensen-Shannon kernel, and the linear kernel are simply particular elements of the much wider family of Jensen-Tsallis kernels, continuously parameterized by $q \in [0, 2]$. Furthermore, the Jensen-Tsallis kernels are a particular subfamily of the even wider set of weighted Jensen-Tsallis kernels.

One of the key features of our generalization is that the kernels are defined on unnormalized measures, with arbitrary mass. This is relevant, for example, in applications of kernels on empirical measures (e.g., word counts, pixel intensity histograms); instead of the usual step of normalization Hein et al. 2004, we may leave these empirical measures unnormalized, thus allowing objects of different size (e.g., total number of words in a document, total number of image pixels) to be weighted differently. Another possibility opened by our generalization is the explicit inclusion of weights: given two normalized measures, they can be multiplied by arbitrary (positive) weights before being fed to the kernel function.

6.3 Other Kernels Based on Jensen Differences and q -Differences

It is worthwhile to note that the Jensen-Rényi and the Jensen-Tsallis divergences also yield positive definite kernels, albeit there are not any obvious “weighted generalizations” like the ones presented above for the Tsallis kernels.

Proposition 38 (Jensen-Rényi and Jensen-Tsallis kernels) *For any $q \in [0, 2]$, the kernel*

$$(p_1, p_2) \mapsto S_q \left(\frac{p_1 + p_2}{2} \right)$$

and the (unweighted) Jensen-Tsallis divergence J_{S_q} (20) are nd kernels on $M_+^1(\mathcal{X}) \times M_+^1(\mathcal{X})$.

Also, for any $q \in [0, 1]$, the kernel

$$(p_1, p_2) \mapsto R_q \left(\frac{p_1 + p_2}{2} \right)$$

and the (unweighted) Jensen-Rényi divergence J_{R_q} (19) are nd kernels on $M_+^1(\mathcal{X}) \times M_+^1(\mathcal{X})$.

Proof The fact that $(p_1, p_2) \mapsto S_q \left(\frac{p_1 + p_2}{2} \right)$ is nd results from the embedding $x \mapsto x/2$ and Proposition 24. Since $(p_1, p_2) \mapsto \frac{S_q(p_1) + S_q(p_2)}{2}$ is trivially nd, we have that J_{S_q} is a sum of nd functions, which turns it nd. To prove the negative definiteness of the kernel $(p_1, p_2) \mapsto R_q \left(\frac{p_1 + p_2}{2} \right)$, notice first that the kernel $(x, y) \mapsto (x + y)/2$ is clearly nd. From Lemma 21 and integrating,

we have that $(p_1, p_2) \mapsto \int \left(\frac{p_1+p_2}{2}\right)^q$ is nd for $q \in [0, 1]$. From the same lemma we have that $(p_1, p_2) \mapsto \ln\left(t + \int \left(\frac{p_1+p_2}{2}\right)^q\right)$ is nd for any $t > 0$. Since $\int \left(\frac{p_1+p_2}{2}\right)^q > 0$, the nonnegativity of $(p_1, p_2) \mapsto R_q\left(\frac{p_1+p_2}{2}\right)$ follows by taking the limit $t \rightarrow 0$. By the same argument as above, we conclude that J_{R_q} is nd. ■

As a consequence, we have from Lemma 19 that the following kernels are pd for any $q \in [0, 1]$ and $t > 0$:

$$\tilde{k}_{\text{EJR}}(p_1, p_2) = \exp\left(-tR_q\left(\frac{p_1+p_2}{2}\right)\right) = \left(\int \left(\frac{p_1+p_2}{2}\right)^q\right)^{-\frac{t}{1-q}},$$

and its “normalized” counterpart,

$$k_{\text{EJR}}(p_1, p_2) = \exp(-tJ_{R_q}(p_1, p_2)) = \left(\frac{\int \left(\frac{p_1+p_2}{2}\right)^q}{\sqrt{\int p_1^q \int p_2^q}}\right)^{-\frac{t}{1-q}}.$$

Although we could have derived its positive definiteness without ever referring to the Rényi entropy, the latter has in fact a suggestive interpretation: it corresponds to an exponentiation of the Jensen-Rényi divergence; it generalizes the case $q = 1$ which corresponds to the exponentiated Jensen-Shannon kernel.

Finally, we point out a relationship between the Jensen-Tsallis divergences (Section 3.4) and a family of difference kernels introduced by Fuglede (2005),

$$\Psi_{\alpha,\beta}(x, y) = \left(\frac{x^\alpha + y^\alpha}{2}\right)^{1/\alpha} - \left(\frac{x^\beta + y^\beta}{2}\right)^{1/\beta}.$$

Fuglede (2005) derived the negative definiteness of the above family of kernels provided $1 \leq \alpha \leq \infty$ and $1/2 \leq \beta \leq \alpha$; he went further by providing representations for these kernels. Hein et al. (2004) used the fact that the integral $\int \Psi_{\alpha,\beta}(x(t), y(t))d\tau(t)$ is also nd to derive a family of pd kernels for probability measures that included the Jensen-Shannon kernel (see Def. 33).

We start by noting the following property of the extended Tsallis entropy, which is very easy to establish:

$$S_q(\mu) = q^{-1}S_{1/q}(\mu^q)$$

As a consequence, by making the substitutions $r \triangleq q^{-1}$, $x_1 \triangleq y_1^q$ and $x_2 \triangleq y_2^q$, we have that

$$\begin{aligned} J_{S_q}(y_1, y_2) &= S_q\left(\frac{y_1+y_2}{2}\right) - \left(\frac{S_q(y_1) + S_q(y_2)}{2}\right) \\ &= r \left[S_r\left(\left(\frac{x_1^r + x_2^r}{2}\right)^{1/r}\right) - \frac{S_r(x_1) + S_r(x_2)}{2} \right] \\ &\triangleq r\tilde{J}_{S_r}(x_1, x_2) \end{aligned}$$

where we introduced

$$\begin{aligned}\tilde{J}_{S_r}(x_1, x_2) &= S_r \left(\left(\frac{x_1^r + x_2^r}{2} \right)^{1/r} \right) - \frac{S_r(x_1) + S_r(x_2)}{2} \\ &= (r-1)^{-1} \int \left[\left(\frac{x_1^r + x_2^r}{2} \right)^{1/r} - \frac{x_1 + x_2}{2} \right].\end{aligned}\quad (38)$$

Since J_{S_q} is nd for $q \in [0, 2]$, we have that \tilde{J}_{S_r} is nd for $r \in [1/2, \infty]$.

Notice that while J_{S_q} may be interpreted as “the difference between the Tsallis q -entropy of the mean and the mean of the Tsallis q -entropies,” \tilde{J}_{S_q} may be interpreted as “the difference between the Tsallis q -entropy of the q -power mean and the mean of the Tsallis q -entropies.”

From (38) we have that

$$\int \Psi_{\alpha, \beta}(x, y) = (\alpha - 1)\tilde{J}_{S_\alpha}(x, y) - (\beta - 1)\tilde{J}_{S_\beta}(x, y),$$

so the family of probabilistic kernels studied in Hein et al. (2004) can be written in terms of Jensen-Tsallis divergences.

6.4 k -th Order Jensen-Tsallis String Kernels

This subsection introduces a new class of string kernels inspired by the k -th order JT q -difference introduced in Section 5.3. Although we refer to them as “string kernels,” they are more generally kernels between stochastic processes.

Several string kernels (i.e., kernels operating on the space of strings) have been proposed in the literature (Haussler, 1999; Lodhi et al., 2002; Leslie et al., 2002; Vishwanathan and Smola, 2003; Shawe-Taylor and Cristianini, 2004; Cortes et al., 2004). These are kernels defined on $\mathcal{A}^* \times \mathcal{A}^*$, where \mathcal{A}^* is the Kleene closure of a finite alphabet \mathcal{A} (i.e., the set of all finite strings formed by characters in \mathcal{A} together with the empty string ϵ). The p -spectrum kernel (Leslie et al., 2002) is associated with a feature space indexed by \mathcal{A}^p (the set of length- p strings). The feature representation of a string s , $\Phi^p(s) \triangleq (\phi_u^p(s))_{u \in \mathcal{A}^p}$, counts the number of times each $u \in \mathcal{A}^p$ occurs as a substring of s ,

$$\phi_u^p(s) = |\{(v_1, v_2) : s = v_1 u v_2\}|.$$

The p -spectrum kernel is then defined as the standard inner product in $\mathbb{R}^{|\mathcal{A}^p|}$

$$k_{\text{SK}}^p(s, t) = \langle \Phi^p(s), \Phi^p(t) \rangle. \quad (39)$$

A more general kernel is the *weighted all-substrings kernel* (Vishwanathan and Smola, 2003), which takes into account the contribution of all the substrings weighted by their length. This kernel can be viewed as a conic combination of p -spectrum kernels and can be written as

$$k_{\text{WASK}}(s, t) = \sum_{p=1}^{\infty} \alpha_p k_{\text{SK}}^p(s, t), \quad (40)$$

where α_p is often chosen to decay exponentially with p and truncated; for example, $\alpha_p = \lambda^p$, if $p_{\min} \leq p \leq p_{\max}$, and $\alpha_p = 0$, otherwise, where $0 < \lambda < 1$ is the decaying factor.

Both k_{SK}^p and k_{WASK} are trivially positive definite, the former by construction and the latter because it is a conic combination of positive definite kernels. A remarkable fact is that both kernels may be computed in $O(|s| + |t|)$ time (i.e., with cost that is linear in the length of the strings), as shown by Vishwanathan and Smola (2003), by using data structures such as suffix trees or suffix arrays (Gusfield, 1997). Moreover, with s fixed, any kernel $k(s, t)$ may be computed in time $O(|t|)$, which is particularly useful for classification applications.

We will now see how Jensen-Tsallis kernels may be used as string kernels. In Section 5.3, we have introduced the concept of *joint* and *conditional* JT q -differences. We have seen that joint JT q -differences are just JT q -differences in a product space of the form $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2$; for k -th order joint JT q -differences this product space is of the form $\mathcal{A}^k = \mathcal{A} \times \mathcal{A}^{k-1}$. Therefore, they still yield positive definite kernels as those introduced in Definition 26, where $\mathcal{X} = \mathcal{A}^k$. The next definition and proposition summarize these statements.

Definition 39 (k -th order weighted JT kernels) Let $\mathcal{S}(\mathcal{A})$ be the set of stationary and ergodic stochastic processes that take values on the alphabet \mathcal{A} . For $k \in \mathbb{N}$ and $q \in [0, 2]$, let the kernel $\tilde{k}_{q,k} : (\mathbb{R}_+ \times \mathcal{S}(\mathcal{A}))^2 \rightarrow \mathbb{R}$ be defined as

$$\begin{aligned} \tilde{k}_{q,k}((\omega_1, s_1), (\omega_2, s_2)) &\triangleq \tilde{k}_q(\omega_1 p_{s_1,k}, \omega_2 p_{s_2,k}) \\ &= \left(S_q(\boldsymbol{\pi}) - T_{q,k}^{\text{joint},\boldsymbol{\pi}}(s_1, s_2) \right) (\omega_1 + \omega_2)^q, \end{aligned} \quad (41)$$

where $p_{s_1,k}$ and $p_{s_2,k}$ are the k -th order joint probability functions associated with the stochastic sources s_1 and s_2 , and $\boldsymbol{\pi} = (\omega_1/(\omega_1 + \omega_2), \omega_2/(\omega_1 + \omega_2))$.

Let the kernel $k_{q,k} : (\mathbb{R}_{++} \times \mathcal{S}(\mathcal{A}))^2 \rightarrow \mathbb{R}$ be defined as

$$\begin{aligned} k_{q,k}((\omega_1, s_1), (\omega_2, s_2)) &\triangleq k_q(\omega_1 p_{s_1,k}, \omega_2 p_{s_2,k}) \\ &= \left(S_q(\boldsymbol{\pi}) - T_{q,k}^{\text{joint},\boldsymbol{\pi}}(s_1, s_2) \right), \end{aligned} \quad (42)$$

Proposition 40 The kernel $\tilde{k}_{q,k}$ is pd, for $q \in [0, 2]$. The kernel $k_{q,k}$ is pd, for $q \in [0, 1]$.

Proof Define the map $g : \mathbb{R}_+ \times \mathcal{S}(\mathcal{A}) \rightarrow \mathbb{R}_+ \times M_+^{1,S_q}(\mathcal{A}^k)$ as $(\omega, s) \mapsto g(\omega, s) = (\omega, p_{s,k})$. From Proposition 27, the kernel $\tilde{k}_q(g(\omega_1, s_1), g(\omega_2, s_2))$ is pd and therefore so is $\tilde{k}_{q,k}((\omega_1, s_1), (\omega_2, s_2))$; proceed analogously for $k_{q,k}$. \blacksquare

At this point, one might wonder whether the “ k -th order conditional JT kernel” $\tilde{k}_{q,k}^{\text{cond}}$ that would be obtained by replacing $T_{q,k}^{\text{joint},\boldsymbol{\pi}}$ with $T_{q,k}^{\text{cond},\boldsymbol{\pi}}$ in (41–42) is also pd. Formula (35) shows that such “conditional JT kernel” is a difference between two joint JT kernels, which is inconclusive. The following proposition shows that $\tilde{k}_{q,k}^{\text{cond}}$ and $k_{q,k}^{\text{cond}}$ are not pd in general. The proof, which is in Appendix D, proceeds by building a counterexample.

Proposition 41 Let $\tilde{k}_{q,k}^{\text{cond}}$ be defined as $\tilde{k}_{q,k}^{\text{cond}}(s_1, s_2) \triangleq \left(S_q(\boldsymbol{\pi}) - T_{q,k}^{\text{cond},\boldsymbol{\pi}}(s_1, s_2) \right) (\omega_1 + \omega_2)^q$; and $k_{q,k}^{\text{cond}}$ be defined as $k_{q,k}^{\text{cond}}(s_1, s_2) \triangleq \left(S_q(\boldsymbol{\pi}) - T_{q,k}^{\text{cond},\boldsymbol{\pi}}(s_1, s_2) \right)$. It holds that $\tilde{k}_{q,k}^{\text{cond}}$ and $k_{q,k}^{\text{cond}}$ are not pd in general.

Despite the negative result in Proposition 41, the chain rule in Proposition 15 still allows us to define pd kernels by combining conditional JT q -differences.

Proposition 42 *Let $(\beta_k)_{k \in \mathbb{N}}$ be a non-increasing infinitesimal sequence, that is, satisfying*

$$\beta_0 \geq \beta_1 \geq \dots \geq \beta_n \rightarrow 0$$

Any kernel of the form

$$\sum_{k=0}^{\infty} \beta_k \tilde{k}_{q,k}^{\text{cond}} \tag{43}$$

is pd for $q \in [0, 2]$; and any kernel of the form

$$\sum_{k=0}^{\infty} \beta_k k_{q,k}^{\text{cond}}$$

is pd for $q \in [0, 1]$, provided both series above converge pointwise.

Proof From the chain rule, we have that (defining the 0-th order joint JT q -difference as $\tilde{k}_{q,0} \triangleq 0$)

$$\sum_{k=0}^{\infty} \beta_k \tilde{k}_{q,k}^{\text{cond}} = \sum_{k=0}^{\infty} \beta_k (\tilde{k}_{q,k+1} - \tilde{k}_{q,k}) = \lim_{n \rightarrow \infty} \sum_{k=1}^n \alpha_k \tilde{k}_{q,k} + \beta_n \tilde{k}_{q,n+1} = \sum_{k=1}^{\infty} \alpha_k \tilde{k}_{q,k} \tag{44}$$

with $\alpha_k = \beta_{k-1} - \beta_k$ (the term $\lim \beta_n \tilde{k}_{q,n+1}$ was dropped because $\beta_n \rightarrow 0$ and $\tilde{k}_{q,n+1}$ is bounded). Since $(\beta_k)_{k \in \mathbb{N}}$ is non-increasing, we have that $(\alpha_k)_{k \in \mathbb{N} \setminus \{0\}}$ is non-negative, which makes (44) the pointwise limit of a conic combination of pd kernels, and therefore a pd kernel. The proof for $\sum_{k=0}^{\infty} \beta_k k_{q,k}^{\text{cond}}$ is analogous. ■

Notice that if we set $\beta_0 = \dots = \beta_{k-1} = 1$ and $\beta_j = 0, \forall j \geq k$, in the above proposition, we recover the k -th order joint JT q -difference.

Finally, notice that, in the same way that the linear kernel is a special case of a JT kernel when $q = 2$ (see Cor. 37), the p -spectrum kernel (39) is a particular case of a p -th order joint JT kernel, and the weighted all substrings kernel (40) is a particular case of a combination of joint JT kernels in the form (43), both obtained when we set $q = 2$ and the weights ω_1 and ω_2 equal to the length of the strings. Therefore, we conclude that the JT string kernels introduced in this section subsume these two well-known string kernels.

7. Experiments

We illustrate the performance of the proposed nonextensive information theoretic kernels, in comparison with common kernels, for SVM-based text classification. We performed experiments with two standard data sets: *Reuters-21578*³ and *WebKB*.⁴ Since our objective was to evaluate the kernels, we considered a simple binary classification task that tries to discriminate among the two largest categories of each data set; this led us to the *earn-vs-acq* classification task for the first data set, and *stud-vs-fac* (students' vs. faculty webpages) in the second data set. Two different frameworks were considered: modeling documents as bags of words, and modeling them as strings of characters. Therefore, both bags of words kernels and string kernels were employed for each task.

3. Available at www.daviddlewis.com/resources/testcollections.

4. Available at www.cs.cmu.edu/afs/cs.cmu.edu/project/theo-20/www/data.

7.1 Documents as Bags of Words

For the bags of words framework, after the usual preprocessing steps of stemming and stop-word removal, we mapped text documents into probability distributions over words using the bag-of-words model and maximum likelihood estimation; this corresponds to normalizing the *term frequencies* (tf) using the ℓ_1 -norm, and is referred to as *tf* (Joachims, 2002; Baeza-Yates and Ribeiro-Neto, 1999). We also used the *tf-idf* (term frequency-inverse document frequency) representation, which penalizes terms that occur in many documents (Joachims, 2002; Baeza-Yates and Ribeiro-Neto, 1999). To weight the documents for the Tsallis kernels, we tried four strategies: uniform weighting, word counts, square root of the word counts, and one plus the logarithm of the word counts; however, for both tasks, uniform weighting revealed the best strategy, which may be due to the fact that documents in both collections are usually short and do not differ much in size.

As baselines, we used the linear kernel with ℓ_2 normalization, commonly used for this task (Joachims, 2002), and the heat kernel approximation introduced by Lafferty and Lebanon (2005):

$$k_{\text{heat}}(p_1, p_2) = (4\pi t)^{-\frac{n}{2}} \exp\left(-\frac{1}{4t} d_g^2(p_1, p_2)\right),$$

where $t > 0$ and $d_g(p_1, p_2) = 2 \arccos(\sum_i \sqrt{p_{1i} p_{2i}})$. Although Lafferty and Lebanon (2005) provide empirical evidence that the heat kernel outperforms the linear kernel, it is not guaranteed to be pd for an arbitrary choice of t , as we show in Appendix E. This parameter and the SVM C parameter were tuned by cross-validation over the training set. The SVM-Light package (available at <http://svmlight.joachims.org/>) was used to solve the SVM quadratic optimization problem.

Figures 2–3 summarize the results. We report the performance of the Tsallis kernels as a function of the entropic index q . For comparison, we also plot the performance of an instance of a Tsallis kernel with q tuned by cross-validation. For the first task, this kernel and the two baselines exhibit similar performance for both the *tf* and the *tf-idf* representations; differences are not statistically significant. In the second task, the Tsallis kernel outperformed the ℓ_2 -normalized linear kernel for both representations, and the heat kernel for *tf-idf*; the differences are statistically significant (using the unpaired t test at the 0.05 level). Regarding the influence of the entropic index, we observe that in both tasks, the optimal value of q is usually higher for *tf-idf* than for *tf*.

The results on these two problems are representative of the typical relative performance of the kernels considered: in almost all tested cases, both the heat kernel and the Tsallis kernels (for a suitable value of q) outperform the ℓ_2 -normalized linear kernel; the Tsallis kernels are competitive with the heat kernel.

7.2 Documents as Strings

In the second set of experiments, each document is mapped into a probability distribution over character p -grams, using maximum likelihood estimation; we did experiments for $p = 3, 4, 5$. To weight the documents for the p -th order joint Jensen-Tsallis kernels, four strategies were attempted: uniform weighting, document lengths (in characters), square root of the document lengths, and one plus the logarithm of the document lengths. For the *earn-vs-acq* task, all strategies performed similarly, with a slight advantage for the square root and logarithm of the document lengths; for the *stud-vs-fac* task, uniform weighting revealed the best strategy. For simplicity, all experiments reported here use uniform weighting.

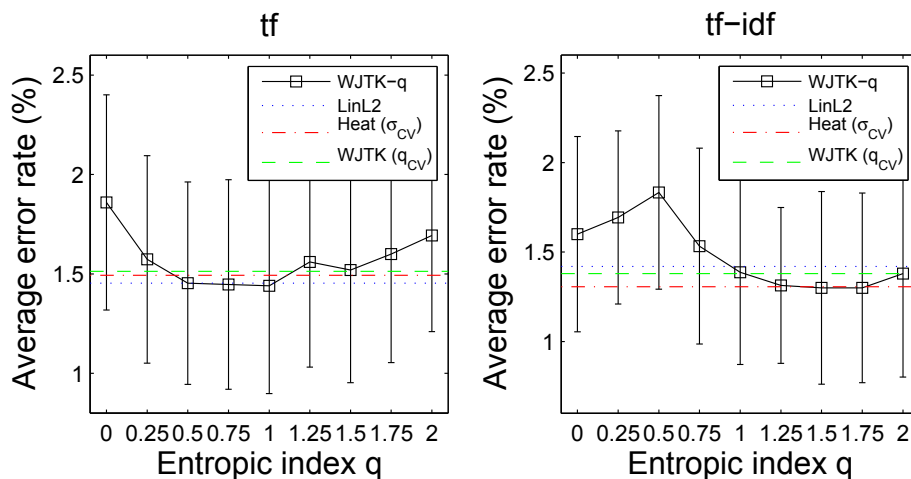


Figure 2: Results for *earn-vs-acq* using *tf* and *tf-idf* representations. The error bars represent ± 1 standard deviation on 30 runs. Training (resp. testing) with 200 (resp. 250) samples per class.

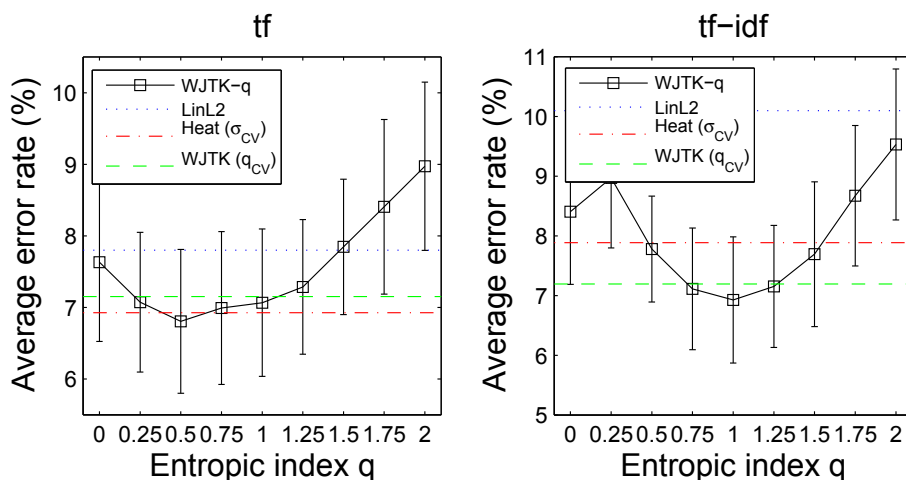


Figure 3: Results for *stud-vs-fac* using *tf* and *tf-idf* representations. The error bars represent ± 1 standard deviation on 30 runs. Training (resp. testing) with 200 (resp. 250) samples per class.

As baselines, we used the p -spectrum kernel (PSK, see 39) for the values of p referred above, and the weighted all substrings kernel (WASK, see 40) with decaying factor tuned to $\lambda = 0.75$ (which yielded the best results), with $p_{\min} = p$ set to the values above, and $p_{\max} = \infty$. The SVM C parameter was tuned by cross-validation over the training set.

Figures 4–5 summarize the results.

For the first task, the JT string kernel and the WASK outperformed the PSK (with statistical significance for $p = 3$), all kernels performed similarly for $p = 4$, and the JT string kernel outperformed the WASK for $p = 5$; all other differences are not statistically significant. In the second task, the JT string kernel outperformed both the WASK and the PSK (and the WASK outperformed the PSK), with statistical significance for $p = 3, 4, 5$. Furthermore, by comparing Figures 3 and 5, we

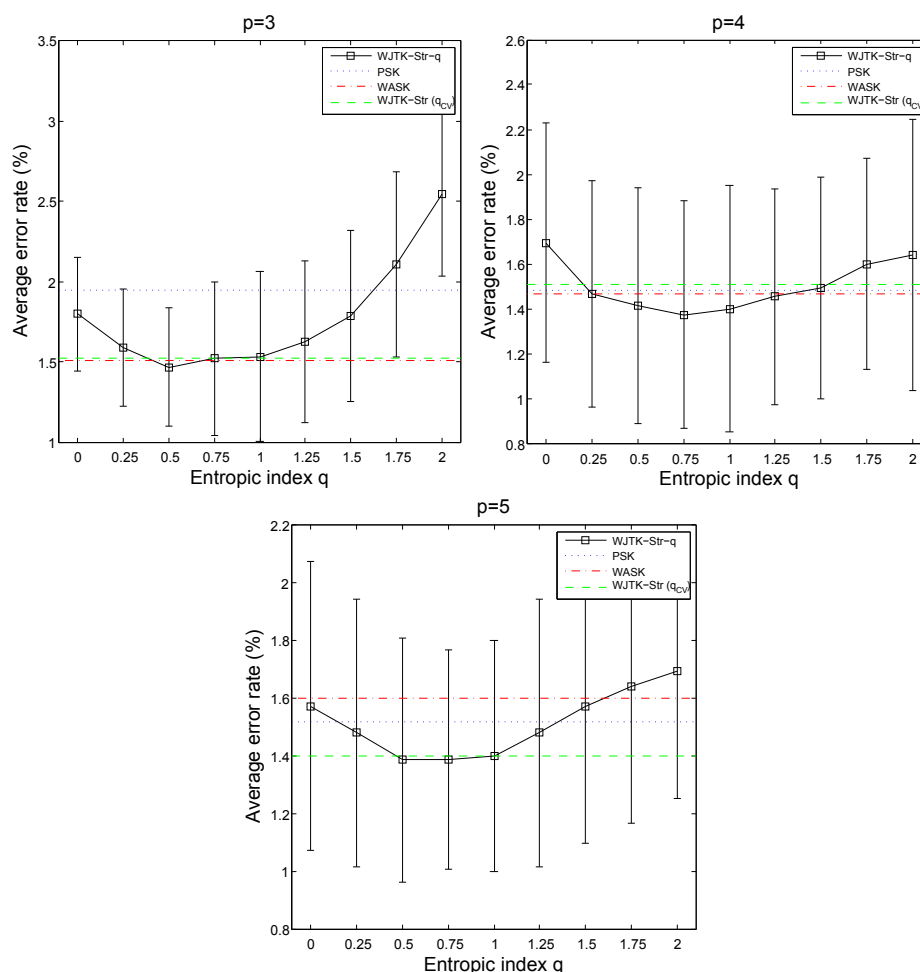


Figure 4: Results for *earn-vs-acq* using string kernels and $p = 3, 4, 5$. The error bars represent ± 1 standard deviation on 15 runs. Training (resp. testing) with 200 (resp. 250) samples per class.

also observe that the 5-th order JT string kernel remarkably outperforms all bags of words kernels for the *stud-vs-fac* task, even though it does not use or build any sort of language model at the word level.

8. Conclusions

In this paper we have introduced a new family of positive definite kernels between measures, which includes previous information-theoretic kernels on probability measures as particular cases. One of the key features of the new kernels is that they are defined on unnormalized measures (not necessarily normalized probabilities). This is relevant, for example, for kernels on empirical measures (such as word counts, pixel intensity histograms); instead of the usual step of normalization (Hein et al., 2004), we may leave these empirical measures unnormalized, thus allowing objects of different sizes (e.g., documents of different lengths, images with different sizes) to be weighted differently. Another possibility is the explicit inclusion of weights: given two normalized measures, they can

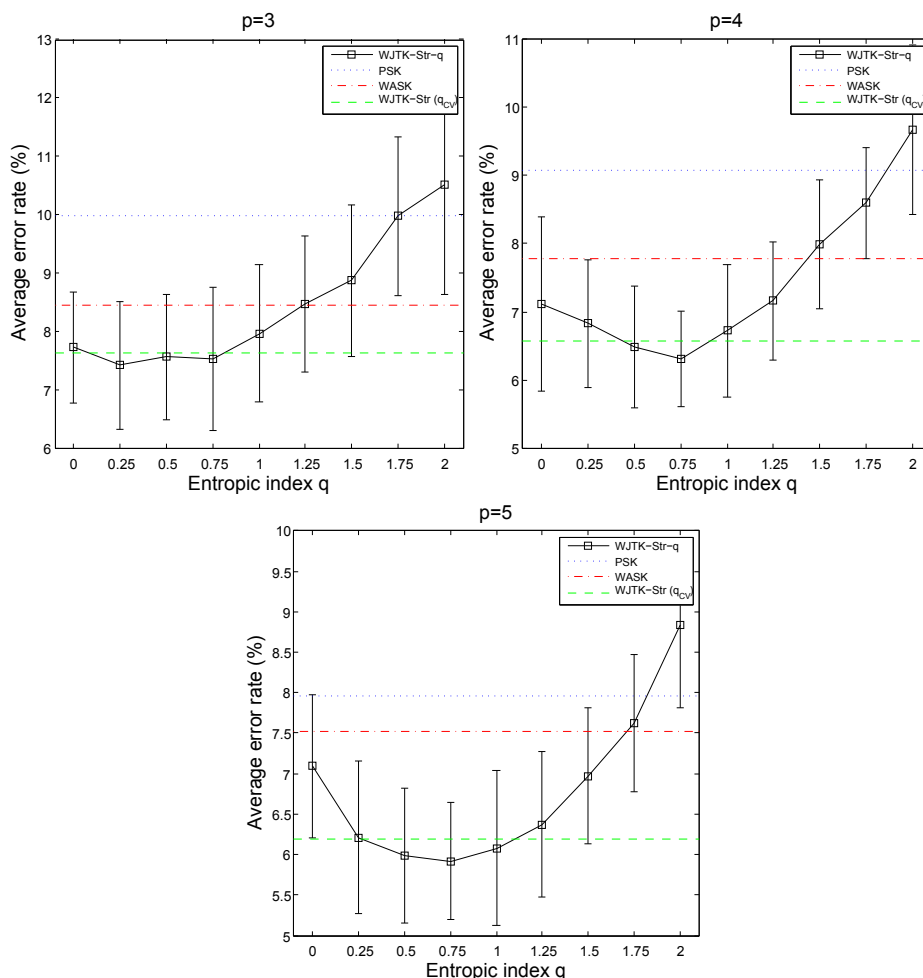


Figure 5: Results for *stud-vs-fac* using string kernels and $p = 3, 4, 5$. The error bars represent ± 1 standard deviation on 15 runs. Training (resp. testing) with 200 (resp. 250) samples per class.

be multiplied by arbitrary (positive) weights before being fed to the kernel function. In addition, we define positive definite kernels between stochastic processes that subsume well-known string kernels.

The new kernels and the proofs of positive definiteness rely on other main contributions of this paper: the new concept of q -convexity, for which we proved a *Jensen q -inequality*; the concept of *Jensen-Tsallis q -difference*, a nonextensive generalization of the Jensen-Shannon divergence; denormalization formulae for several entropies and divergences.

We have reported experiments in which these new kernels were used in support vector machines for text classification tasks. Although the reported experiments do not lead to strong conclusions, they show that the new kernels are competitive with the state-of-the-art, in some cases yielding a significant performance improvement.

Future research will concern applying Jensen-Tsallis q -differences to other learning problems, like clustering, possibly exploiting the fact that they accept more than two arguments.

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Appendix A. Suyari’s Axioms for Nonextensive Entropies

Suyari (2004) proposed the following set of axioms (above referred as Suyari’s axioms) that determine nonextensive entropies of the form stated in (1). Below, $q \geq 0$ is any fixed scalar and f_q is a function defined on $\cup_{n=1}^{\infty} \Delta^{n-1}$.

(A1) *Continuity*: $f_q|_{\Delta^{n-1}}$ is continuous, for any $n \in \mathbb{N}$;

(A2) *Maximality*: For any $n \in \mathbb{N}$ and $(p_1, \dots, p_n) \in \Delta^{n-1}$,

$$f_q(p_1, \dots, p_n) \leq S_q(1/n, \dots, 1/n);$$

(A3) *Generalized additivity*: For $i = 1, \dots, n$, $j = 1, \dots, m_i$, $p_{ij} \geq 0$, and $p_i = \sum_{j=1}^{m_i} p_{ij}$,

$$f_q(p_{11}, \dots, p_{nm_n}) = f_q(p_1, \dots, p_n) + \sum_{i=1}^n p_i^q f_q\left(\frac{p_{i1}}{p_i}, \dots, \frac{p_{im_i}}{p_i}\right);$$

(A4) *Expandability*: $f_q(p_1, \dots, p_n, 0) = f_q(p_1, \dots, p_n)$.

Appendix B. Proof of Proposition 8

Proof The case $q = 1$ corresponds to the Jensen difference and was proved by Burbea and Rao (1982) (Theorem 1). Our proof extends that to $q \neq 1$. Let $y = (y_1, \dots, y_m)$, where $y_t = (y_{t1}, \dots, y_{tm})$. Thus

$$\begin{aligned} T_{q,\Psi}^{\pi}(y) &= \Psi\left(\sum_{t=1}^m \pi_t y_t\right) - \sum_{t=1}^m \pi_t^q \Psi(y_t) \\ &= \sum_{i=1}^n \left[\sum_{t=1}^m \pi_t^q \varphi(y_{ti}) - \varphi\left(\sum_{t=1}^m \pi_t y_{ti}\right) \right], \end{aligned}$$

showing that it suffices to consider $n = 1$, where each $y_t \in [0, 1]$, that is,

$$T_{q,\Psi}^{\pi}(y_1, \dots, y_m) = \sum_{t=1}^m \pi_t^q \varphi(y_t) - \varphi\left(\sum_{t=1}^m \pi_t y_t\right);$$

this function is convex on $[0, 1]^m$ if and only if, for every fixed $a_1, \dots, a_m \in [0, 1]$, and $b_1, \dots, b_m \in \mathbb{R}$, the function

$$f(x) = T_{q,\Psi}^\pi(a_1 + b_1x, \dots, a_m + b_mx)$$

is convex in $\{x \in \mathbb{R} : a_t + b_tx \in [0, 1], t = 1, \dots, m\}$. Since f is C^2 , it is convex if and only if $f''(t) \geq 0$.

We first show that convexity of f (equivalently of $T_{q,\Psi}^\pi$) implies convexity of φ . Letting $c_t = a_t + b_tx$,

$$f''(x) = \sum_{t=1}^m \pi_t^q b_t^2 \varphi''(c_t) - \left(\sum_{t=1}^m \pi_t b_t \right)^2 \varphi'' \left(\sum_{t=1}^m \pi_t c_t \right). \tag{45}$$

By choosing $x = 0$, $a_t = a \in [0, 1]$, for $t = 1, \dots, m$, and b_1, \dots, b_m satisfying $\sum_t \pi_t b_t = 0$ in (45), we get

$$f''(0) = \varphi''(a) \sum_{t=1}^m \pi_t^q b_t^2,$$

hence, if f is convex, $\varphi''(a) \geq 0$ thus φ is convex.

Next, we show that convexity of f also implies $(2 - q)$ -convexity of $-1/\varphi''$. By choosing $x = 0$ (thus $c_t = a_t$) and $b_t = \pi_t^{1-q}(\varphi''(a_t))^{-1}$, we get

$$\begin{aligned} f''(0) &= \sum_{t=1}^m \frac{\pi_t^{2-q}}{\varphi''(a_t)} - \left(\sum_{t=1}^m \frac{\pi_t^{2-q}}{\varphi''(a_t)} \right)^2 \varphi'' \left(\sum_{t=1}^m \pi_t a_t \right) \\ &= \left[\frac{1}{\varphi''(\sum_{t=1}^m \pi_t a_t)} - \sum_{t=1}^m \frac{\pi_t^{2-q}}{\varphi''(a_t)} \right] \left(\sum_{t=1}^m \frac{\pi_t^{2-q}}{\varphi''(a_t)} \right) \varphi'' \left(\sum_{t=1}^m \pi_t a_t \right), \end{aligned}$$

where the expression inside the square brackets is the Jensen $(2 - q)$ -difference of $1/\varphi''$ (see Definition 7). Since $\varphi''(x) \geq 0$, the factor outside the square brackets is non-negative, thus the Jensen $(2 - q)$ -difference of $1/\varphi''$ is also nonnegative and $-1/\varphi''$ is $(2 - q)$ -convex.

Finally, we show that if φ is convex and $-1/\varphi''$ is $(2 - q)$ -convex, then $f'' \geq 0$, thus $T_{q,\Psi}^\pi$ is convex. Let $r_t = (q\pi_t^{2-q}/\varphi''(c_t))^{1/2}$ and $s_t = b_t(\pi_t^q \varphi''(c_t)/q)^{1/2}$; then, non-negativity of f'' results from the following chain of inequalities/equalities:

$$0 \leq \left(\sum_{t=1}^m r_t^2 \right) \left(\sum_{t=1}^m s_t^2 \right) - \left(\sum_{t=1}^m r_t s_t \right)^2 \tag{46}$$

$$= \sum_{t=1}^m \frac{\pi_t^{2-q}}{\varphi''(c_t)} \sum_{t=1}^m b_t^2 \pi_t^q \varphi''(c_t) - \left(\sum_{t=1}^m b_t \pi_t \right)^2 \tag{47}$$

$$\leq \frac{1}{\varphi''(\sum_{t=1}^m \pi_t c_t)} \sum_{t=1}^m b_t^2 \pi_t^q \varphi''(c_t) - \left(\sum_{t=1}^m b_t \pi_t \right)^2 \tag{48}$$

$$= \frac{1}{\varphi''(\sum_{t=1}^m \pi_t c_t)} \cdot f''(t), \tag{49}$$

where: (46) is the Cauchy-Schwarz inequality; Equality (47) results from the definitions of r_t and s_t and from the fact that $r_t s_t = b_t \pi_t$; Inequality (48) states the $(2 - q)$ -convexity of $-1/\varphi''$; equality (49) results from (45). ■

Appendix C. Proof of Proposition 10

Proof The proof of (29), for $q \geq 0$, results from

$$\begin{aligned} T_q^\pi(p_1, \dots, p_m) &= \frac{1}{q-1} \left[1 - \sum_{j=1}^n \left(\sum_{t=1}^m \pi_t p_{tj} \right)^q - \sum_{t=1}^m \pi_t^q \left(1 - \sum_{j=1}^n p_{tj}^q \right) \right] \\ &= S_q(\pi) + \frac{1}{q-1} \sum_{j=1}^n \left[\sum_{t=1}^m (\pi_t p_{tj})^q - \left(\sum_{t=1}^m \pi_t p_{tj} \right)^q \right] \\ &\leq S_q(\pi), \end{aligned}$$

where the inequality holds since, for $y_i \geq 0$: if $q \geq 1$, then $\sum_i y_i^q \leq (\sum_i y_i)^q$; if $q \in [0, 1]$, then $\sum_i y_i^q \geq (\sum_i y_i)^q$.

The proof that $T_q^\pi \geq 0$ for $q \geq 1$, uses the notion of q -convexity. Since \mathcal{X} is countable, the Tsallis entropy is as in (2), thus $S_q \geq 0$. Since $-S_q$ is 1-convex, then, by Proposition 6, it is also q -convex for $q \geq 1$. Consequently, from the q -Jensen inequality (Proposition 5), for finite \mathcal{T} , with $|\mathcal{T}| = m$,

$$T_q^\pi(p_1, \dots, p_m) = S_q \left(\sum_{t=1}^m \pi_t p_t \right) - \sum_{t=1}^m \pi_t^q S_q(p_t) \geq 0.$$

Since S_q is continuous, so is T_q^π , thus the inequality is valid in the limit as $m \rightarrow \infty$, which proves the assertion for \mathcal{T} countable. Finally, $T_q^\pi(\delta_1, \dots, \delta_1, \dots) = 0$, where δ_1 is some degenerate distribution.

Finally, to prove (30), for $q \in [0, 1]$ and \mathcal{X} finite,

$$\begin{aligned} T_q^\pi(p_1, \dots, p_m) &= S_q \left(\sum_{t=1}^m \pi_t p_t \right) - \sum_{t=1}^m \pi_t^q S_q(p_t) \\ &\geq \sum_{t=1}^m \pi_t S_q(p_t) - \sum_{t=1}^m \pi_t^q S_q(p_t) \tag{50} \\ &= \sum_{t=1}^m (\pi_t - \pi_t^q) S_q(p_t) \\ &\geq S_q(U) \sum_{t=1}^m (\pi_t - \pi_t^q) \tag{51} \\ &= S_q(\pi) [1 - n^{1-q}]. \end{aligned}$$

where the Inequality (50) results from S_q being concave, and the Inequality (51) holds since $\pi_t - \pi_t^q \leq 0$, for $q \in [0, 1]$, and the uniform distribution U maximizes S_q , with $S_q(U) = (1 - n^{1-q}) / (q - 1)$. ■

Appendix D. Proof of Proposition 41

Proof We show a counterexample with $q = 1$ (the extensive case), $\pi = (1/2, 1/2)$ and $k = 1$, that discards both cases. It suffices to show that $\sqrt{JS_1^{\text{cond}}} \triangleq \sqrt{T_{1,1}^{\text{cond},(1/2,1/2)}}$ violates the triangle inequality for some choice of stochastic processes s_1, s_2, s_3 and therefore is not a squared distance;

this in turn implies that $\sqrt{JS_1^{\text{cond}}}$ is not nd and, from Proposition 18, that the above two kernels are not pd. We define s_1, s_2, s_3 to be stationary first order Markov processes in a binary alphabet $\mathcal{A} = \{0, 1\}$ defined by the following transition matrices, respectively:

$$S_1 = \lim_{\varepsilon \rightarrow 0} \begin{bmatrix} 1 - \varepsilon & \varepsilon \\ 1/4 & 3/4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1/4 & 3/4 \end{bmatrix},$$

$$S_2 = \lim_{\varepsilon \rightarrow 0} \begin{bmatrix} 3/4 & 1/4 \\ \varepsilon & 1 - \varepsilon \end{bmatrix} = \begin{bmatrix} 3/4 & 1/4 \\ 0 & 1 \end{bmatrix},$$

and

$$S_3 = \lim_{\varepsilon \rightarrow 0} \begin{bmatrix} \varepsilon & 1 - \varepsilon \\ 1/4 & 3/4 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1/4 & 3/4 \end{bmatrix},$$

whose stationary distributions are

$$\sigma_1 = \lim_{\varepsilon \rightarrow 0} \frac{1}{1 + 4\varepsilon} \begin{bmatrix} 1 \\ 4\varepsilon \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

$$\sigma_2 = \lim_{\varepsilon \rightarrow 0} \frac{1}{1 + 4\varepsilon} \begin{bmatrix} 4\varepsilon \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

and

$$\sigma_3 = \lim_{\varepsilon \rightarrow 0} \frac{1}{5 - 4\varepsilon} \begin{bmatrix} 1 \\ 4 - 4\varepsilon \end{bmatrix} = \begin{bmatrix} 1/5 \\ 4/5 \end{bmatrix}.$$

The matrix of first order conditional JT 1-differences (or first order conditional Jensen-Shannon divergences) is

$$\begin{bmatrix} 0 & 0 & \frac{3}{5}H(\frac{5}{6}) \\ * & 0 & \frac{9}{10}H(\frac{8}{9}) - \frac{2}{5}H(\frac{1}{4}) \\ * & * & 0 \end{bmatrix} \approx \begin{bmatrix} 0 & 0 & 0.390 \\ * & 0 & 0.128 \\ * & * & 0 \end{bmatrix}, \tag{52}$$

which fails to be negative definite, since

$$\sqrt{JS_1^{\text{cond}}(s_1, s_2)} + \sqrt{JS_1^{\text{cond}}(s_2, s_3)} < \sqrt{JS_1^{\text{cond}}(s_1, s_3)},$$

which violates the triangle inequality required for $\sqrt{JS_1^{\text{cond}}}$ to be a metric.

Interestingly, the 0-th order conditional Jensen-Shannon divergence matrix (this one ensured to be negative definite because it equals a standard Jensen-Shannon divergence matrix) is

$$\begin{bmatrix} 0 & 1 & H(\frac{2}{5}) - \frac{1}{2}H(\frac{1}{5}) \\ * & 0 & H(\frac{1}{10}) - \frac{1}{2}H(\frac{1}{5}) \\ * & * & 0 \end{bmatrix} \approx \begin{bmatrix} 0 & 1 & 0.610 \\ * & 0 & 0.108 \\ * & * & 0 \end{bmatrix}. \tag{53}$$

From the chain rule (35), we have that the sum of the matrices (52) and (53) is the second order joint Jensen-Shannon divergence, and therefore is also guaranteed to be negative definite. ■

Appendix E. The Heat Kernel Approximation

The diffusion kernel for statistical manifolds, recently proposed by Lafferty and Lebanon (2005), is grounded in information geometry (Amari and Nagaoka, 2001). It models the diffusion of “information” over a statistical manifold according to the heat equation. Since in the case of the multinomial manifold (the relative interior of Δ^n), the diffusion kernel has no closed form, the authors adopt the so-called “first-order parametrix expansion,” which resembles the Gaussian kernel replacing the Euclidean distance by the geodesic distance that is induced when the manifold is endowed with a Riemannian structure given by the Fisher information (we refer to Lafferty and Lebanon 2005 for further details). The resulting heat kernel approximation is

$$k_{\text{heat}}(p_1, p_2) = (4\pi t)^{-\frac{n}{2}} \exp\left(-\frac{1}{4t} d_g^2(p_1, p_2)\right),$$

where $t > 0$ and $d_g(p_1, p_2) = 2 \arccos(\sum_i \sqrt{p_{1i} p_{2i}})$. Whether k_{heat} is pd has been an open problem (Hein et al., 2004; Zhang et al., 2005). Let \mathbb{S}_+^n be the positive orthant of the n -dimensional sphere, that is,

$$\mathbb{S}_+^n = \left\{ (x_1, \dots, x_{n+1}) \in \mathbb{R}^{n+1} \mid \sum_{i=1}^{n+1} x_i^2 = 1, \forall i x_i \geq 0 \right\}.$$

The problem can be restated as follows: is there an isometric embedding from \mathbb{S}_+^n to some Hilbert space? In this section we answer that question in the negative.

Proposition 43 *Let $n \geq 2$. For sufficiently large t , the kernel k_{heat} is not pd.*

Proof From Proposition 19, k_{heat} is pd, for all $t > 0$, if and only if d_g^2 is nd. We provide a counterexample, using the following four points in Δ^2 : $p_1 = (1, 0, 0)$, $p_2 = (0, 1, 0)$, $p_3 = (0, 0, 1)$ and $p_4 = (1/2, 1/2, 0)$. The squared distance matrix $[D_{ij}] = [d_g^2(p_i, p_j)]$ is

$$D = \frac{\pi^2}{4} \cdot \begin{bmatrix} 0 & 4 & 4 & 1 \\ 4 & 0 & 4 & 1 \\ 4 & 4 & 0 & 4 \\ 1 & 1 & 4 & 0 \end{bmatrix}.$$

Taking $c = (-4, -4, 1, 7)$ we have $c^T D c = 2\pi^2 > 0$, showing that D is not nd. Although p_1, p_2, p_3, p_4 lie on the boundary of Δ^2 , continuity of d_g^2 implies that it is not nd on the relative interior of Δ^2 . The case $n > 2$ follows easily, by appending zeros to the four vectors above. ■

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