

## TOPOLOGICAL DATA ANALYSIS IN INFORMATION SPACE\*

Herbert Edelsbrunner,<sup>†</sup> Žiga Virk,<sup>‡</sup> and Hubert Wagner\*

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ABSTRACT. Various kinds of data are routinely represented as discrete probability distributions. Examples include text documents summarized by histograms of word occurrences and images represented as histograms of oriented gradients. Viewing a discrete probability distribution as a point in the standard simplex of the appropriate dimension, we can understand collections of such objects in geometric and topological terms. Importantly, instead of using the standard Euclidean distance, we look into dissimilarity measures with information-theoretic justification, and we develop the theory needed for applying topological data analysis in this setting. In doing so, we emphasize constructions that enable the usage of existing computational topology software in this context.

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### 1 Introduction

The field of *computational topology* has a very short history, at least if compared with standard subfields of mathematics [15]. Starting as a broadening of the geometric tool-set to answer low-dimensional topology questions, it soon extended its scope to include topological problems in high-dimensional data analysis, giving rise to the subfield of *topological data analysis* (TDA) [11]. At the very foundation of topology is the notion of neighborhood, which in practice is often constructed from the Euclidean metric in real space. One reason for its popularity is the extensive tool-set associated with this metric, but there is evidence that this choice is often suboptimal [22]. Other popular options are the Hamming distance and discrete distances, which are preferred for their simplicity.

While the choice of distance is important, there is a paucity in our understanding of the consequences. We contribute to the study by connecting distances with information-theoretic foundations [14] to the tool-set of topological data analysis. These distances include the *Fisher information metric* [2], and the *relative entropy*, also known as *Kullback–Leibler divergence* [25]. The former is obtained by integrating the square root of the relative entropy along shortest paths. Restricting the points to the standard simplex, we get a metric between discrete probability distributions, which has information-theoretic significance. While the latter is not a distance in the strict sense, it plays an important role in many application areas as preferred measurement between probability distributions. The

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<sup>†</sup>IST Austria (Institute of Science and Technology Austria), Am Campus 1, 3400 Klosterneuburg, Austria, edels@ist.ac.at, hub.wag@gmail.com

<sup>‡</sup>Faculty of Computer and Information Science, University of Ljubljana, Vecna pot 113, 1000 Ljubljana, Slovenia, ziga.virk@fri.uni-lj.si

Kullback–Leibler divergence is also an example of the broader class of Bregman divergences [10], which have been studied from a geometric point of view in [8, 29]. To clearly distinguish the spaces equipped with dissimilarity measures based on information-theoretic notions from the standard Euclidean setting, we call them *information spaces*.

Our interest in information-theoretic distances complements the common theme of incorporating statistical tools into the topological data analysis pipeline. Like-minded efforts advocate that results obtained with topological methods need calibration through statistics, and that new developments in both fields will be needed to achieve this [1]. The goal of this paper is more modest: the import of concepts from information theory into the inner workings of the topological tools. This can be compared with the *persistent entropy* introduced by Rucco and collaborators [27] to sharpen the sensitivity of persistent homology in the assessment of network organization. Unrelated to this thought but important to our effort is the work of Antonelli and collaborators [4] on the isometry between Fisher information space and Euclidean space, which we recast in Section 3. We follow up with a list of concrete contributions the reader finds in this paper:

- In Section 2, we prove that relative entropy balls are convex. In contrast, the balls based on the Burg entropy, which is popular in speech recognition, are convex only for small radii, as elaborated in Appendix A.
- In Section 3, we give an explicit description of the Fisher information metric derived from the relative entropy and of Antonelli’s isometry, prove that Fisher information balls are convex, and generalize the Antonelli isometry to decomposable Bregman divergences.
- In Section 4, we prove tight bounds relating the Jensen–Shannon divergence with the Fisher information metric, recalling that the square root of the former is a metric [19].

In a final technical section, we tie things together by explaining how these notions of distance are used to compute the persistence diagrams of data in this space. We compare the results for the three notions of distance studied in this paper: the *relative entropy*, the *Fisher information metric*, and the *Jensen–Shannon divergence*. In the Appendix, we expand these considerations to the case of Burg entropy.

**Scope of the paper.** Apart from reporting the above technical results, our aim is to provide a self-contained reference for researchers interested in the theoretical and applied side of information theory in the context of computational topology. To this end, we provide intuitive explanations of basic topological objects measured with information-theoretic distances.

**Overview.** To put our results in perspective, we mention that this paper is third in a series. The entry point is [18], where Bregman divergences are shown to be compatible with basic topological tools. In subsequent work [20], we studied properties of Bregman balls, in particular bounding the location of first intersection of such balls. Our previous work was concerned with shared properties of Bregman divergences; in this work, we focus on information-theoretic distances based on Shannon’s entropy.

While working directly with the Kullback–Leibler divergence is ideal from a purely

information-theoretic viewpoint, its lack of symmetry and the triangle inequality prohibits its use with existing computational geometry and topology tools. This prompts the study of metrics derived from Bregman divergences in general, and from Kullback–Leibler divergence specifically. The latter include the Fisher metric and the Jensen–Shannon metric. Studying properties of these metrics is the main focus of this paper, which is structured as follows: Section 2 presents the background on Shannon entropy and relative entropy. Section 3 relates the Fisher information metric to the relative entropy and to the Euclidean metric. Section 4 proves inequalities relating the Jensen–Shannon divergence with the Fisher information metric. Section 5 uses persistent homology to compare these notions of distance if applied to data. Section 6 concludes this paper. In addition, Appendices A, B, C consider distance measures based on the Burg entropy.

## 2 Entropy and Relative Entropy

Starting with the Shannon entropy, we define the relative entropy of an ordered pair of points, and provide an intuitive explanation of this measurement. Considering the ball consisting of all points for which the relative entropy from the center does not exceed a given threshold, we prove that it is convex, in the original coordinate system and in all dimensions.

**Convex function and divergence.** We write  $\mathbb{R}_+$  for the set of positive real numbers,  $\mathbb{R}_+^n$  for the positive orthant in  $n$  dimensions, and  $x = (x_1, x_2, \dots, x_n) \in \mathbb{R}_+^n$  for a point in the orthant. Its components satisfy  $x_i > 0$  for  $1 \leq i \leq n$ . The (negative, extended) *Shannon entropy* is the function  $E: \mathbb{R}_+^n \rightarrow \mathbb{R}$  defined by mapping  $x$  to

$$E(x) = \sum_{i=1}^n [x_i \ln x_i - x_i]. \quad (1)$$

It is strictly convex and infinitely often differentiable; see Figure 1 for the graph of the function in one dimension. The *relative entropy* from  $x$  to  $y$  is the difference between  $E$  and the best linear approximation of  $E$  at  $y$ , both evaluated at  $x$ :

$$D_E(x||y) = E(x) - [E(y) + \langle \nabla E(y), x - y \rangle] \quad (2)$$

$$= \sum_{i=1}^n [x_i \ln \frac{x_i}{y_i} - x_i + y_i]. \quad (3)$$

The relative entropy is also known as the *Kullback–Leibler divergence*; see [3, page 57]. The construction of the relative entropy is illustrated in Figure 1, making it obvious that  $D_E(x||y)$  is neither symmetric in its two arguments, nor does it satisfy the triangle inequality. Notwithstanding, the primary interpretation of the relative entropy is as a measure of distance. Intuitively, the relative entropy from a distribution  $x$  to another distribution  $y$  measures the average *surprisal* when we expect items according to  $y$  but observe items according to  $x$ . More technically, this surprisal is expressed as the loss of coding efficiency, namely the expected number of extra bits needed to encode the messages from  $x$  using a code optimized for  $y$ . In practice, it quantifies how well  $y$  approximates  $x$ , and later we use this interpretation to understand the meaning of relative-entropy balls and their intersections.

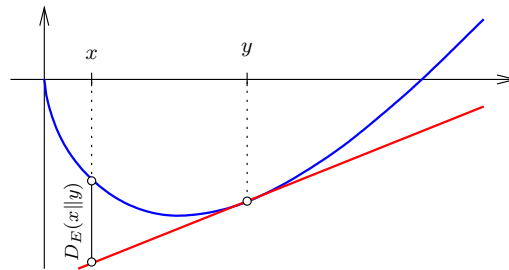


Figure 1: The graph of the Shannon entropy, the graph of its best linear approximation at  $y$ , and the relative entropy from  $x$  to  $y$ .

REMARK 1: The definition of the relative entropy is an example of a more general construction. Letting  $\Omega \subseteq \mathbb{R}^n$  be open and convex, a function  $F: \Omega \rightarrow \mathbb{R}$  is of *Legendre type* if it is strictly convex, differentiable, and the gradient diverges when we approach the boundary of  $\Omega$ . Clearly, the Shannon entropy is of Legendre type. Named after Lev Bregman [10], the corresponding *Bregman divergence* is defined by substituting  $F$  for  $E$  in (2).

REMARK 2: If we restrict a Legendre type function to an affine subspace, we get another Legendre type function and therefore another divergence. An important example is the *standard  $(n-1)$ -simplex*,  $\Delta = \Delta^{n-1}$ , which is the intersection of  $\mathbb{R}_+^n$  with the  $(n-1)$ -plane defined by  $\sum_{i=1}^n x_i = 1$ . Since  $\mathbb{R}_+^n$  is open so is  $\Delta$ . Every point of  $\Delta$  can be interpreted as a discrete probability distribution for  $n$  elements. The Shannon entropy and the relative entropy are defined as in (1) and (3), except for a smaller domain.

**Decomposability and convexity.** We note that a function  $F: \Omega \rightarrow \mathbb{R}$  whose restrictions obtained by fixing coordinates are convex is not necessarily convex. An example is the function  $F(x) = \prod_{i=1}^n x_i$ . On the other hand, if  $F$  is *decomposable*:  $F(x) = \sum_{i=1}^n F_i(x_i)$ , then the convexity of the components implies the convexity of  $F$ .

**Lemma 1** (Composable Convexity). *Let  $\Omega \subseteq \mathbb{R}^n$  be convex and  $F: \Omega \rightarrow \mathbb{R}$  a decomposable function. The components of  $F$  are convex if and only if  $F$  is convex.*

PROOF. It is clear that the convexity of  $F$  implies the convexity of its components. We thus limit ourselves to proving the other implication. Let  $x, y \in \Omega$ , let  $0 \leq \lambda \leq 1$ , and let  $u = (1 - \lambda)x + \lambda y$  be the corresponding convex combination. Since the components of  $F$  are convex, by assumption, we have  $F_i(u_i) \leq (1 - \lambda)F_i(x_i) + \lambda F_i(y_i)$  for every  $1 \leq i \leq n$ . Taking sums on the left and on the right, we get  $F(u) \leq (1 - \lambda)F(x) + \lambda F(y)$ ; that is:  $F$  is convex as claimed.  $\square$

REMARK 3: While nonconvex components imply a nonconvex function, they do not imply nonconvex sublevel sets. This stronger implication is valid for *strongly decomposable* functions  $F$ , by which we mean that all components are the same:  $F_i = F_j$  for all  $1 \leq i, j \leq n$ . To see this, let the component  $f$  of  $F$  be nonconvex, assume  $f$  is nonnegative, and let  $a < b$  such that  $f(\frac{a+b}{2}) > \frac{1}{2}f(a) + \frac{1}{2}f(b)$ . Supposing 1 is in the domain of  $f$ , we set

$x = (a, b, 1, \dots, 1)$  and  $y = (b, a, 1, \dots, 1)$  and note that  $\frac{x+y}{2} = (\frac{a+b}{2}, \frac{a+b}{2}, 1, \dots, 1)$ . Hence,

$$F(\frac{x+y}{2}) = 2f(\frac{a+b}{2}) + (n-2)f(1) > f(a) + f(b) + (n-2)f(1) = \frac{1}{2}[F(x) + F(y)]. \quad (4)$$

Setting  $r^2 = F(x) = F(y)$ , we see that  $F^{-1}[0, r^2]$  is a nonconvex subset of  $\mathbb{R}^n$ .

**Convexity of entropy balls.** To study the local behavior of a divergence, we fix a point  $x \in \Omega$  and call  $D_x: \Omega \rightarrow \mathbb{R}$  defined by  $D_x(y) = D_F(x||y)$  the *divergence function* of  $x$ . Its sublevel sets are balls of points whose divergence from  $x$  is bounded by a non-negative threshold:

$$B_r(x) = D_x^{-1}[0, r^2] = \{y \in \Omega \mid D_F(x||y) \leq r^2\}. \quad (5)$$

Assuming  $F$  is the Shannon entropy, we call  $B_r(x)$  an *entropy ball*. Observe that such a ball is the set of all probability distributions that approximate the center distribution,  $x$ , with a loss of at most  $r^2$  bits. We recall that in practice each distribution characterizes an object, perhaps an image or a text document. In this case, it is clear that a ball represents a collection of similar objects, for a chosen similarity threshold  $r^2$ .

For general Legendre type functions, the balls are not necessarily convex, and we will encounter nonconvex balls shortly. However, entropy balls are necessarily convex.

**Theorem 1** (Convexity of Entropy Balls). *Let  $E: \mathbb{R}_+^n \rightarrow \mathbb{R}$  be the Shannon entropy. Then the entropy ball  $B_r(x)$  is convex for every  $x \in \mathbb{R}_+^n$  and every  $r^2 \geq 0$ .*

PROOF. Since the Shannon entropy is strongly decomposable, so is the divergence function of every point  $x \in \mathbb{R}_+^n$ :  $D_x(y) = E(x) - E(y) - \langle \nabla E(y), x - y \rangle = \sum_{i=1}^n [x_i \ln x_i - x_i \ln y_i - x_i + y_i]$ , in which the  $y_i$  are variables and the  $x_i$  are constants. Each component is convex because  $-\ln t$  is convex. By Lemma 1, this implies that  $D_x$  is convex, so all of its sublevel sets are convex.  $\square$

### 3 Fisher Information Metric

Like any other twice differentiable Legendre type function, the Shannon entropy induces a metric that integrates infinitesimal steps along shortest paths. This metric has an isometry to Euclidean space, which facilitates topological methods applied to data in information space. Analogous study based on the Burg entropy can be found in Appendix B.

**From divergence to distance.** Recall that the Shannon entropy is twice differentiable, so the *Hessian matrix* of second derivatives at any point  $y \in \mathbb{R}_+^n$  is well defined:

$$H_E(y) = \left[ \frac{\partial^2 E}{\partial x_i \partial x_j}(y) \right]_{1 \leq i, j \leq n}. \quad (6)$$

This symmetric square matrix defines a scalar product at  $y$  by mapping two vectors  $u, v \in \mathbb{R}^n$  to  $\langle u, v \rangle_y = \frac{1}{2} u^T H_E(y) v$ . The corresponding Riemannian metric is called the *Fisher*

*information metric:*  $d_E: \mathbb{R}_+^n \times \mathbb{R}_+^n \rightarrow \mathbb{R}$ . Given points  $x, y \in \mathbb{R}_+^n$ , the distance is the length of the shortest path  $\gamma: [0, 1] \rightarrow \mathbb{R}_+^n$  with  $\gamma(0) = x$  and  $\gamma(1) = y$ , in which the length is

$$\text{Length}(\gamma) = \int_{t=0}^1 \sqrt{\langle \dot{\gamma}(t), \dot{\gamma}(t) \rangle_{\gamma(t)}} dt = \int_{t=0}^1 \sqrt{\frac{1}{2} \dot{\gamma}(t)^T H_E(\gamma(t)) \dot{\gamma}(t)} dt. \quad (7)$$

Since the Shannon entropy is decomposable, the only non-zero entries in the Hessian matrix are the second derivatives of the component functions in the diagonal:

$$H_E(y) = \begin{bmatrix} 1/y_1 & 0 & \dots & 0 \\ 0 & 1/y_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1/y_n \end{bmatrix}. \quad (8)$$

Accordingly, the formula for the length of a smooth path simplifies to

$$\text{Length}(\gamma) = \int_{t=0}^1 \sqrt{\frac{1}{2} \sum_{i=1}^n \frac{\dot{\gamma}_i(t)^2}{\gamma_i(t)}} dt, \quad (9)$$

in which  $\gamma_i(t)$  and  $\dot{\gamma}_i(t)$  are the  $i$ -th components of the curve and its velocity vector at  $t$ .

REMARK 4: The construction of the metric can be restricted to any smooth submanifold of the domain. Since this limits the set of available paths, the distance between two points cannot be less than without the restriction. For example, we may restrict the Fisher information metric in  $\mathbb{R}_+^n$  to the standard simplex:  $d_{E|\Delta}: \Delta \times \Delta \rightarrow \mathbb{R}$ . While the relative entropy in  $\Delta$  is the restriction of the relative entropy in  $\mathbb{R}_+^n$ , this is not the case for the Fisher information metric.

**Euclidean isometries.** As discovered by Antonelli [4], there is a simple diffeomorphism that maps  $\mathbb{R}_+^n$  equipped with the Fisher information metric to  $\mathbb{R}_+^n$  equipped with the Euclidean metric. Such an isometry exists for every length metric defined by a twice differentiable decomposable Legendre type function. We explain its construction in this more general setting. Suppose  $\varphi: \Omega \rightarrow \Omega_2$  is a diffeomorphism between open convex subsets of  $\mathbb{R}_+^n$ . Given a metric  $d_2: \Omega_2 \times \Omega_2 \rightarrow \mathbb{R}$ , we get an *induced metric*,  $d_\varphi: \Omega \times \Omega \rightarrow \mathbb{R}$ , defined by  $d_\varphi(x, y) = d_2(\varphi(x), \varphi(y))$ . By construction,  $\varphi$  is an isometry between the two metric spaces. We are interested in the case in which  $d_2$  is the Euclidean metric.

**Lemma 2** (Euclidean Isometry). *Let  $\Omega$  be an open convex subset of  $\mathbb{R}^n$  and  $F: \Omega \rightarrow \mathbb{R}$  a twice differentiable decomposable Legendre type function. Then there exists a decomposable isometry  $\varphi: \Omega \rightarrow \Omega_2 \subseteq \mathbb{R}^n$  connecting the length metric defined by  $F$  in  $\Omega$  with the Euclidean metric in  $\Omega_2$ .*

PROOF. We construct a decomposable diffeomorphism  $\varphi: \Omega \rightarrow \Omega_2$  such that the length metric  $d_F$  is induced by  $\varphi$  and the Euclidean metric on  $\Omega_2$ . Write  $\varphi_i(x_i)$  for the components of the diffeomorphism and  $\sum_{i=1}^n (du_i)^2$  for the differential form of the Euclidean metric in  $\Omega_2$ . Setting  $u_i = \varphi_i(x_i)$  so that  $du_i = \varphi'_i(x_i) dx_i$ , we get

$$\sum_{i=1}^n (du_i)^2 = \sum_{i=1}^n \varphi'_i(x_i)^2 (dx_i)^2 = \sum_{i=1}^n \frac{1}{2} F''_i(x_i) (dx_i)^2, \quad (10)$$

in which the last sum is the differential form of the metric defined by  $F$  and the second equality is required to get an isometry. This condition simplifies to

$$\varphi'_i(x_i) = \sqrt{\frac{1}{2}F''_i(x_i)}, \quad (11)$$

for  $1 \leq i \leq n$ . Since  $F$  is strictly convex, we have  $F''_i(x_i) > 0$  for every component function, so this equation has a solution.  $\square$

**From Fisher information to Euclidean distance.** We make use of Lemma 2 by constructing the isometry that relates the Fisher information metric in  $\mathbb{R}_+^n$  and in  $\Delta = \Delta^{n-1}$  with the Euclidean metric in  $\mathbb{R}_+^n$  and in  $\sqrt{2}\mathbb{S}_+^{n-1}$ , the latter being our notation for the positive orthant of the  $(n-1)$ -sphere with radius  $\sqrt{2}$  centered at the origin in  $\mathbb{R}^n$ . As mentioned before, this isometry is well known [2, 4], and we give the construction for completeness.

**Theorem 2** (Fisher Information to Euclidean Distance). *Let  $E: \mathbb{R}_+^n \rightarrow \mathbb{R}$  be the Shannon entropy, and  $x, y \in \mathbb{R}_+^n$ . Then*

$$d_E(x, y) = \sqrt{2 \sum_{i=1}^n (\sqrt{x_i} - \sqrt{y_i})^2}, \quad (12)$$

$$d_{E|\Delta}(x, y) = \sqrt{2} \arccos \sum_{i=1}^n \sqrt{x_i y_i}, \quad (13)$$

where we assume  $x, y \in \Delta \subseteq \mathbb{R}_+^n$  in (13). Furthermore, the balls under  $d_E$  and  $d_{E|\Delta}$  are convex.

PROOF. We prove both equations with the diffeomorphism  $\varphi: \mathbb{R}_+^n \rightarrow \mathbb{R}_+^n$  that distorts the Fisher information metric to the Euclidean metric. Since  $E$  decomposes into identical components, so does  $\varphi$ . By Equation (11) in the proof of Lemma 2, the derivative of this component satisfies  $p'(t) = 1/\sqrt{2t}$ . We get  $p(t) = \sqrt{2t}$  by integration. As illustrated in Figure 2, the diffeomorphism maps a point  $x$  with coordinates  $x_i > 0$  to the point  $\varphi(x)$  with coordinates  $p(x_i) = \sqrt{2x_i} > 0$ . The squared Euclidean distance between  $\varphi(x)$  and  $\varphi(y)$  is  $\sum_{i=1}^n (\sqrt{2x_i} - \sqrt{2y_i})^2$ , which implies (12).

The image of the standard simplex,  $\varphi(\Delta)$ , consists of all points with coordinates  $u_i = p(x_i) > 0$  that satisfy  $u_1^2 + u_2^2 + \dots + u_n^2 = 2$ . This is the equation of the sphere with radius  $\sqrt{2}$  centered at the origin in  $\mathbb{R}^n$ . Denoting the positive portion of this sphere by  $\sqrt{2}\mathbb{S}_+^{n-1}$ , we get an isometry  $\varphi|_\Delta: \Delta \rightarrow \sqrt{2}\mathbb{S}_+^{n-1}$ . Given points  $u, v \in \sqrt{2}\mathbb{S}_+^{n-1}$ , the shortest spherical path connecting them is a portion of the great-circle that passes through  $u$  and  $v$ . Its length is  $\sqrt{2}$  times the angle between the vectors  $u, v \in \mathbb{R}_+^n$ . This implies (13).

To prove convexity, let  $x \in \mathbb{R}_+^n$ , consider the function  $d_x: \mathbb{R}_+^n \rightarrow \mathbb{R}$  defined by  $d_x(y) = d_E^2(x, y)$ , and note that  $d_x^{-1}[0, r^2]$  is the ball with center  $x$  and radius  $r \geq 0$  under the Fisher information metric. It is the preimage of the function  $f_u: \mathbb{R}_+^n \rightarrow \mathbb{R}$  defined by  $f_u(v) = \sum_{i=1}^n (v_i - u_i)^2$ , with  $u_i = \sqrt{2x_i}$  and  $v_i = \sqrt{2y_i}$ , for  $1 \leq i \leq n$ . Hence,  $d_x$  is decomposable with  $d_x(y) = 2 \sum_{i=1}^n (\sqrt{y_i} - \sqrt{x_i})^2$ . The components are convex because  $-\sqrt{t}$  is convex. By Lemma 1,  $d_x$  is convex, and because  $x$  can be any point in  $\mathbb{R}_+^n$ , all balls under  $d_E$  are convex. To finally see that every ball under  $d_{E|\Delta}$  is convex, we note that it is the

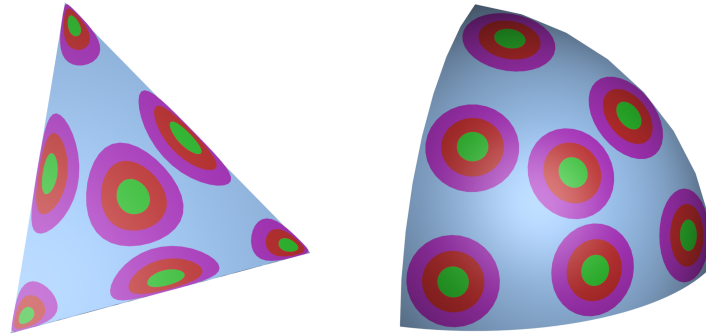


Figure 2: *Left*: three Fisher information disks each for seven points inside the standard triangle. *Right*: the images of the disks in the positive portion of the sphere. For aesthetic reasons, we scale the sphere by a factor  $1/\sqrt{2}$  relative to the triangle.

preimage of the intersection between  $\sqrt{2}\mathbb{S}_+^{n-1}$  and a Euclidean ball. This preimage is the intersection between  $\Delta$  and a ball under  $d_E$ , which is again convex.  $\square$

REMARK 5: Using the isometry specified in Theorem 2, we can map data from Fisher information space to Euclidean space. This allows us to glean information about data living in the Fisher information space, using standard mathematical and computational tools specialized to the Euclidean case. Furthermore, the presented derivation works for any Bregman divergence, provided it is decomposable, which ensures the Hessian is diagonal.

#### 4 Information and Loss

In this section, we reverse the direction and measure divergences *to* a point. We use these readings to define the Jensen–Shannon divergence, whose square root we compare to the Fisher information metric. Furthermore, in Appendix C, we consider the Burbea–Rao divergence that is based on the Burg entropy.

**Jensen–Shannon divergence.** The *Jensen–Shannon divergence* of a pair  $x, y \in \mathbb{R}_+^n$  is the average relative entropy from  $x$  and  $y$  to the average of the two points:

$$\text{JS}(x, y) = \frac{1}{2}[D_E(x|\mu) + D_E(y|\mu)] = \frac{1}{2}[E(x) + E(y)] - E(\mu) \quad (14)$$

$$= \frac{1}{2} \sum_{i=1}^n [x_i \ln \frac{2x_i}{x_i+y_i} + y_i \ln \frac{2y_i}{x_i+y_i}], \quad (15)$$

in which  $\mu = \frac{x+y}{2}$  and we get (15) by noting that  $x + y - 2\mu = 0$ . As pointed out in [19], it measures the loss of efficiency when we encode signals from two probability distributions using their average.

If we substitute any other point  $z \in \mathbb{R}_+^n$  for  $\mu$ , the average relative entropy increases. To prove this, we define  $f(z) = \frac{1}{2}[D_E(x|z) + D_E(y|z)]$ , noting that  $f(\mu) = \text{JS}(x, y)$ . The following lemma can also be found in [5].



**Lemma 3** (Local Minimum). *Let  $\mu$  be the average of the points  $x, y \in \mathbb{R}_+^n$ . Then  $f(\mu) \leq f(z)$  for every  $z \in \mathbb{R}_+^n$ , with equality if and only if  $z = \mu$ .*

PROOF. Computing  $f(z) - f(\mu)$  from the definition, most terms cancel and only  $E(\mu) - E(z) - \langle \nabla E(z), \mu - z \rangle$  remains, which implies  $f(z) - f(\mu) = D_E(\mu \| z)$ . It is non-negative by definition and 0 if and only if  $z = \mu$ .  $\square$

As proved in [19],  $\mathbb{R}_+^n$  together with the square root of the Jensen–Shannon divergence is a metric space. It is however not a *length metric space* because it does not agree with the corresponding *intrinsic metric*, in which the length of a path is measured by taking infinitesimal steps; see also Section 3. It is not difficult to see that the intrinsic metric defined by the Jensen–Shannon divergence is half the intrinsic metric defined by the relative entropy, which is of course the Fisher information metric. Being a metric, the square root of the Jensen–Shannon divergence satisfies the triangle inequality, which implies that it is bounded from above by the corresponding intrinsic metric.

**Jensen–Shannon divergence versus Fisher information metric.** Since the Fisher information metric is twice the intrinsic metric defined by the Jensen–Shannon divergence, we get  $4\text{JS}(x, y) \leq d_E^2(x, y)$ . We will confirm this inequality with an independent argument shortly and prove  $\frac{4}{\ln 2} = 5.770\dots$  as a tight upper bound on the expansion.

**Theorem 3** (Jensen–Shannon Divergence vs. Fisher Information). *The Jensen–Shannon divergence and the squared Fisher information metric satisfy*

$$4\text{JS}(x, y) \leq d_E^2(x, y) \leq \frac{4}{\ln 2} \text{JS}(x, y), \quad (16)$$

$$4\text{JS}(x, y) \leq d_{E|\Delta}^2(x, y) \leq \frac{\sqrt{2}\pi}{\ln 2} \text{JS}(x, y), \quad (17)$$

in which (16) applies to  $\mathbb{R}_+^n$  and (17) to the standard  $(n - 1)$ -simplex.

PROOF. Restricting  $\mathbb{R}_+^n$  to  $\Delta$ , the Jensen–Shannon divergence is unaffected, but the Fisher information metric expands because the shortest paths correspond to great-circle arcs rather than line segments in Euclidean space. The expansion is larger for longer paths, and the supremum expansion rate is  $\pi/\sqrt{8}$ , which is the length of a quarter great-circle over the length of the straight edge connecting its endpoints. Since  $\frac{4}{\ln 2} \frac{\pi}{\sqrt{8}} = \frac{\sqrt{2}\pi}{\ln 2}$ , (16) implies (17).

Returning to  $\mathbb{R}_+^n$ , we note that both the Jensen–Shannon divergence and the squared Fisher information metric are decomposable. It suffices to prove (16) in  $n = 1$  dimension, where we write  $a$  for  $x$  and  $b$  for  $y$ . From (12) and (15), we get  $d_E^2(a, b) = 2(\sqrt{a} - \sqrt{b})^2$  and  $\text{JS}(a, b) = \frac{1}{2}[a \ln \frac{2a}{a+b} + b \ln \frac{2b}{a+b}]$ . Observe that  $d_E^2(Ca, Cb) = C d_E^2(a, b)$  and  $\text{JS}(Ca, Cb) = C \text{JS}(a, b)$  for every  $C > 0$ . We use these properties to eliminate one degree of freedom by setting  $b = t^2 a$  to get

$$\frac{1}{a} d_E^2(a, b) = d_E^2(1, t^2) = 2(1 - t)^2, \quad (18)$$

$$\frac{1}{a} \text{JS}(a, b) = \text{JS}(1, t^2) = \frac{1}{2} \left[ \ln \frac{2}{1+t^2} + t^2 \ln \frac{2t^2}{1+t^2} \right]. \quad (19)$$

We will see shortly that the ratio of these two functions behaves monotonically within  $1 < t < \infty$ , attaining its extreme values in the two limits. These extreme values are the constants

in (16), with monotonicity proving the inequalities. Setting  $f(t) = \text{JS}(1, t^2)/d_E^2(1, t^2)$ , the inequalities in (16) are equivalent to

$$\frac{\ln 2}{4} \leq f(t) \leq \frac{1}{4}. \quad (20)$$

Plugging the right-hand sides of (18) and (19) into the definition of the ratio, we get

$$f(t) = \frac{1}{4(t-1)^2} \left[ \ln \frac{2}{t^2+1} + t^2 \ln \frac{2t^2}{t^2+1} \right]. \quad (21)$$

When  $t$  goes to infinity, the first term in (21) goes to 0, while the second term goes to  $\frac{\ln 2}{4}$ , the lower bound in (20). To take the other limit, when  $t$  goes to 1, we use the l'Hopital rule and differentiate the numerator and the denominator twice. For the numerator, we get

$$g(t) = t^2 \ln t^2 - (t^2 + 1) \ln \frac{t^2+1}{2}, \quad (22)$$

$$g'(t) = 2t \ln t^2 - 2t \ln \frac{t^2+1}{2}, \quad (23)$$

$$g''(t) = 2 \ln t^2 - 2 \ln \frac{t^2+1}{2} + \frac{4}{t^2+1}. \quad (24)$$

Setting  $t = 1$ , we get  $g(1) = g'(1) = 0$  and  $g''(1) = 2$ . Similarly, the denominator and its first derivate vanish at  $t = 1$ , its second derivative is 8, and  $f(t)$  goes to  $\frac{1}{4}$ , the upper bound in (20). It remains to show that the ratio is monotonically decreasing, from  $\frac{1}{4} = 0.25$  at  $t = 1$  to  $\frac{\ln 2}{4} = 0.173\dots$  at  $t = \infty$ . We accomplish this by computing the derivative of  $f$  as written in (22):

$$f'(t) = \frac{(t \ln t^2 + t)(t-1)^2}{2(t-1)^4} - \frac{t^2(t-1) \ln t^2}{2(t-1)^4} - \frac{(t \ln \frac{t^2+1}{2} + t)(t-1)^2}{2(t-1)^4} + \frac{(t^2+1) \ln \frac{t^2+1}{2}(t-1)}{2(t-1)^4} \quad (25)$$

$$= \frac{t(t-1) \ln \frac{2t^2}{t^2+1}}{2(t-1)^3} - \frac{t^2 \ln \frac{2t^2}{t^2+1}}{2(t-1)^3} + \frac{\ln \frac{t^2+1}{2}}{2(t-1)^3} = \frac{1}{2(t-1)^3} \left[ \ln \frac{t^2+1}{2} - t \ln \frac{2t^2}{t^2+1} \right]. \quad (26)$$

To prove that  $f'(t)$  is negative for all  $t > 1$ , we rewrite the numerator and compute its first two derivatives:  $u(t) = (t+1) \ln \frac{t^2+1}{2} - t \ln t^2$ ,  $u'(t) = \ln \frac{t^2+1}{2} + \frac{2t(t+1)}{t^2+1} - \ln t^2 - 2$ ,  $u''(t) = \frac{1}{t(t^2+1)^2} [-2t^3 + 2t^2 + 2t - 2]$ . The numerator of the second derivative factors into  $(t-1)(-2t^2 + 2)$ , which is clearly negative for all  $t > 1$ . Note that  $u(1) = u'(1) = 0$ . Because  $u''$  is negative, we have  $u'(t) < 0$  and  $u(t) < 0$  for all  $t > 1$ . The latter inequality is equivalent to  $f'(t) < 0$  for all  $t > 1$ , which implies that  $f$  is monotonically decreasing. This implies (20) and completes the proof.  $\square$

## 5 TDA in Information Space

While the preceding sections shed light on distances with information-theoretic foundations, we will now connect them to topological data analysis. We begin with the introduction of standard results from topological data analysis, which we will then use to shed light on relations between different notions of distance. In particular, we focus on the half-diameter functions and the radius functions, which correspond to two popular constructions: the Vietoris–Rips complex and the Čech complex.

**Half-diameter functions.** It will be convenient to consolidate notation by writing  $\mathbb{X}$  for a topological space and  $\theta: \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R}$  for a distance. Here we consider  $\mathbb{X}$  to either be  $\mathbb{R}_+^n$  or  $\Delta^{n-1}$ , and  $\theta$  to either be the square root of the Jensen–Shannon divergence,  $\sqrt{\text{JS}}$ , or the Fisher information metric,  $d_E$ . When we consider the set of all subsets, we will always exclude the empty set and write  $\mathcal{P}_0(\mathbb{X}) = \{Q \subseteq \mathbb{X} \mid Q \neq \emptyset\}$ . Given  $\mathbb{X}$  and  $\theta$ , the *half-diameter function*  $\mathcal{D}_\theta: \mathcal{P}_0(\mathbb{X}) \rightarrow \mathbb{R}$  is defined by mapping every non-empty subset  $Q \subseteq \mathbb{X}$  to

$$\mathcal{D}_\theta(Q) = \frac{1}{2} \sup_{x,y \in Q} \theta(x,y), \quad (27)$$

which we call the *half-diameter* of  $Q$ . Since  $\theta$  is a metric, we can define the *Hausdorff distance* between two subsets of  $\mathbb{X}$  as the larger of the two directed such distances:  $\mathcal{H}_\theta(P, Q) = \max\{\mathcal{H}_\theta(P\|Q), \mathcal{H}_\theta(Q\|P)\}$ , in which  $\mathcal{H}_\theta(P\|Q) = \max_{x \in P} \min_{y \in Q} \theta(x, y)$ . This is a metric on the compact sets in  $\mathcal{P}_0(\mathbb{X})$ , and under it, the half-diameter function is 1-Lipschitz and therefore continuous. Finally, we note that the half-diameter function is *monotonic*, that is:  $\mathcal{D}_\theta(P) \leq \mathcal{D}_\theta(Q)$  whenever  $\emptyset \neq P \subseteq Q \subseteq \mathbb{X}$ .

Data analysis starts with a finite set of points,  $X \subseteq \mathbb{X}$ . Let  $K = \mathcal{P}_0(X)$ , noting that this is a full simplex, and write  $f: K \rightarrow \mathbb{R}$  for the restriction of the half-diameter function. For each  $r \geq 0$ , we write  $K_r = f^{-1}[0, r]$  for the corresponding sublevel set, which consists of all simplices in  $K$  with half-diameter  $r$  or less. By the monotonicity of  $f$ , each sublevel set is a subcomplex of  $K$ . We refer to  $K_r$  as the *Vietoris–Rips complex* of  $X$  and  $\theta$  for radius  $r$ . By construction,  $K_r$  is a *clique complex*: a simplex belongs to  $K_r$  if and only if all edges of the simplex belong to  $K_r$ . It follows that the edges in  $K_r$  determine the entire complex. This has computational advantages because triangles and higher-dimensional simplices can be treated implicitly, computing their properties from the edges only when needed; see e.g. the Ripser software of Bauer [6]. It has modeling disadvantages because triangles and higher-dimensional simplices carry no new structural information. We will return to this point when we consider Čech complexes as an alternative construction.

**Persistent homology.** Persistent homology groups have been introduced in [16] to measure holes in proteins. The concept has since found many applications inside and outside mathematics. The idea is however older, and the earliest reference we know is a paper by Morse [28], which develops the concept as a tool in the study of minimal surfaces.

The concept starts with the classic notion of homology groups, which formalize our notion of how a complex or really any topological space is connected; see e.g. [21]. It does so by counting the holes as ranks of abelian groups. Choosing the coefficients in the construction of these groups as elements of a field, the groups are vector spaces and their ranks are the familiar dimensions from linear algebra. Returning to  $f: \mathcal{P}_0(X) \rightarrow \mathbb{R}$ , we index the finitely many sublevel sets consecutively from 1 to  $m$ . Mapping each complex  $K_\ell$  to its  $p$ -th homology group, for some fixed integer  $p$ , we get a sequence of vector spaces,  $H_\ell = H_p(K_\ell)$ :

$$\begin{array}{ccccccc} \dots & \subseteq & K_{i-1} & \subseteq & K_i & \subseteq & \dots & \subseteq & K_{j-1} & \subseteq & K_j & \subseteq & \dots \\ & & \downarrow & & \downarrow & & & & \downarrow & & \downarrow & & \\ \dots & \rightarrow & H_{i-1} & \rightarrow & H_i & \rightarrow & \dots & \rightarrow & H_{j-1} & \rightarrow & H_j & \rightarrow & \dots \end{array}$$

The inclusions  $K_i \subseteq K_j$  induce linear maps  $h_{i,j}: H_i \rightarrow H_j$ , and by the functoriality of

homology, the inclusions commute with these maps. We call the row of complexes a *filtration* and the row of vector spaces together with the maps connecting them a *persistence module*. This is the essential concept that permits us to measure how long holes persist in the filtration. To be specific, let  $1 \leq i \leq j \leq m$  and call the image of the map from  $H_i$  to  $H_j$  a *persistent homology group*,  $\text{im } h_{i,j} \subseteq H_j$ . Its rank is the number of holes in  $K_i$  that are still holes in  $K_j$ . A homology class  $\alpha$  in  $H_i$  is *born* at  $K_i$  if  $\alpha$  does not belong to the image of  $H_{i-1}$ , and it *dies entering*  $K_j$  if  $\alpha$  enters the preimage of  $H_{i-1}$  when we go from  $K_{j-1}$  to  $K_j$ . Writing  $r_i$  for the smallest value such that  $K_i = f^{-1}[0, r_i]$ , we define the *persistence* of  $\alpha$  as  $|r_j - r_i|$ .

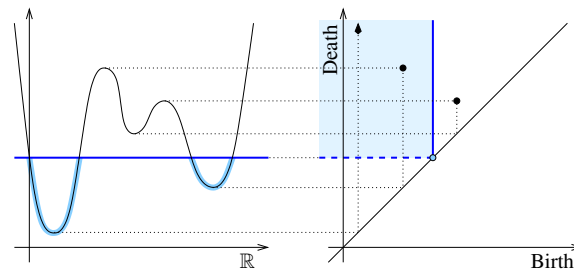


Figure 3: *Left*: the graph of a function on  $\mathbb{R}$ . *Right*: the persistence diagram of the function, with two finite points and one point at infinity. The components of the highlighted sublevel set are counted by the two points in the corresponding upper-left quadrant.

To summarize the information in the persistence module, we represent a coset of homology classes born at  $K_i$  and dying entering  $K_j$  by the point  $(r_i, r_j)$ ; see Figure 3, setting  $r_j = \infty$  if the classes never die. The result is a multiset of points in the extended plane, which we refer to as the *persistence diagram* of  $f$ , denoted  $\text{Dgm}(f)$ . The ranks of the persistent homology groups can be read as the numbers of points in the upper-left quadrants defined by corners on or above the diagonal; see again Figure 3.

**Stability.** An important property of persistence diagrams is their stability with respect to perturbations. To explain this, we define the *bottleneck distance* between two persistence diagrams as the length of the longest edge in a minimizing matching. To finesse the difficulty caused by different cardinalities, we add infinitely many copies of every point along the diagonal to each diagram and define  $W_\infty(\text{Dgm}(f), \text{Dgm}(g)) = \inf_\beta \sup_A \|A - \beta(A)\|_\infty$ , in which  $\beta: \text{Dgm}(f) \rightarrow \text{Dgm}(g)$  is a bijection and  $A$  is a point in  $\text{Dgm}(f)$ . The original proof of stability in [13] bounds the bottleneck distance by the  $L_\infty$ -distance between the functions. In later developments, [7, 12] compare the diagrams directly with the persistence modules they summarize. Letting  $\mathcal{F}$  and  $\mathcal{G}$  be the persistence modules defined by the sublevel sets of  $f$  and  $g$ , indexed by real numbers for convenience, we say they are  $\varepsilon$ -interleaved if there are maps  $\phi_r: \mathbf{F}_r \rightarrow \mathbf{G}_{r+\varepsilon}$  and  $\psi_r: \mathbf{G}_r \rightarrow \mathbf{F}_{r+\varepsilon}$  that commute with the maps within the modules. The *interleaving distance*, denoted  $I(\mathcal{F}, \mathcal{G})$ , is the infimum  $\varepsilon \geq 0$  for which  $\mathcal{F}$  and  $\mathcal{G}$  are interleaved. With this notation, we have

$$W_\infty(\text{Dgm}(f), \text{Dgm}(g)) = I(\mathcal{F}, \mathcal{G}) \leq \|f - g\|_\infty. \quad (28)$$

Suppose  $\theta$  is a metric, and  $X, Y \subseteq \mathbb{X}$  are finite sets with Hausdorff distance  $\varepsilon$ . Letting  $f$  and  $g$  be the restrictions of the half-diameter function to  $\mathcal{P}_0(X)$  and to  $\mathcal{P}_0(Y)$ , it is not difficult

to see that the interleaving distance between the corresponding persistence modules is at most  $\varepsilon$ . We state this straightforward consequence of stability for later reference.

**Theorem 4** (Stability for Metrics). *Let  $\theta: \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R}$  be a metric,  $X, Y \subseteq \mathbb{X}$  finite, and  $f: \mathcal{P}_0(X) \rightarrow \mathbb{R}$ ,  $g: \mathcal{P}_0(Y) \rightarrow \mathbb{R}$  induced by the half-diameter function of  $\mathbb{X}$  and  $\theta$ . Then the bottleneck distance between  $\text{Dgm}(f)$  and  $\text{Dgm}(g)$  is bounded from above by the Hausdorff distance between  $X$  and  $Y$ .*

**Approximation.** Since  $\sqrt{\text{JS}}$  and  $d_E$  are both metrics, Theorem 4 applies. Specifically, the mapping from the subsets of  $\mathbb{X}$  to the space of persistence diagrams defined by  $\sqrt{\text{JS}}$  is 1-Lipschitz, and so is the mapping defined by  $d_E$ . Writing  $f_j, f_i: X \rightarrow \mathbb{R}$  for the maps in which  $j = \sqrt{\text{JS}}$  and  $i = \frac{1}{2}d_E$ , the persistence diagrams of  $f_j$  and  $f_i$  are generally different, and we can use this difference to compare the two distances. By Theorem 3, we have

$$\frac{1}{C} j(x, y) \leq i(x, y) \leq C j(x, y) \tag{29}$$

for  $C^2 = 1/\ln 2 = 1.442\dots$ , in which the two distances between  $x$  and  $y$  are measured in  $\mathbb{R}_+^n$ . Rewriting (29) in terms of sublevel sets, we get  $f_j^{-1}[0, \frac{1}{C}r] \subseteq f_i^{-1}[0, r] \subseteq f_j^{-1}[0, Cr]$ . To get constant interleaving distance, we re-index the vector spaces in the persistence modules  $\mathcal{F}_j$  of  $f_j$  and  $\mathcal{F}_i$  of  $f_i$  by substituting  $\ln r$  for  $r$ . Hence,  $I(\mathcal{F}_j, \mathcal{F}_i) \leq \ln C = 0.183\dots$ . By (28), this implies that the persistence diagrams of  $\mathcal{F}_j$  and  $\mathcal{F}_i$  are very similar, with bottleneck distance at most  $0.183\dots$ . We get slightly different results if we measure the distances in  $\Delta$ . Specifically, we get  $C^2 = \sqrt{2}\pi/(4 \ln 2) = 1.602\dots$  in (29) and interleaving distance at most  $\ln C = 0.235\dots$

**Theorem 5** (Approximation). *Let  $j = \sqrt{\text{JS}}$  and  $i = \frac{1}{2}d_E$ ,  $X \subseteq \mathbb{X}$  finite, and  $\mathcal{F}_j, \mathcal{F}_i$  the persistence modules defined by the restrictions of  $\ln \mathcal{D}_j, \ln \mathcal{D}_i$  to  $\mathcal{P}_0(X)$ . Then  $\mathcal{F}_j$  and  $\mathcal{F}_i$  are interleaved, with the interleaving distance labeling the first edge in Figure 4.*

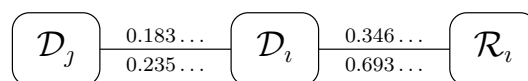


Figure 4: Recall that  $j = \sqrt{\text{JS}}$ ,  $i = \frac{1}{2}d_E$ , and  $\mathcal{D}_j, \mathcal{D}_i, \mathcal{R}_i$  are the corresponding half-diameter and radius functions. Each edge is labeled by two interleaving distances: above the edge for  $\mathbb{X} = \mathbb{R}_+^n$  and below the edge for  $\mathbb{X} = \Delta$ .

REMARK 6: The two constants labeling the first edge in Figure 4 can be improved by taking advantage of the asymmetry of the inequalities in (16) and (17). Indeed, while being symmetric, (29) is strictly weaker than (16).

**Radius function by comparison.** We contrast the half-diameter functions with a different construction, which we introduce for the Fisher information metric. Given  $\mathbb{X}$ , the radius function  $\mathcal{R}_i: \mathcal{P}_0(\mathbb{X}) \rightarrow \mathbb{R}$  is defined by mapping every non-empty subset to

$$\mathcal{R}_i(Q) = \inf_{z \in \mathbb{X}} \sup_{x \in Q} d_E(z, x), \tag{30}$$

which we call the *radius* of  $Q$ . Again, the radius function is monotonic, but in contrast to the half-diameter functions, the simplices of dimension 2 and higher encode structural information that is not already contained in the edges. To explain, we write  $B_r(x)$  for the set of points  $d_E(x, z) \leq r$ . The radius function signals at which radius the balls defined by  $Q$  have a non-empty common intersection:  $r \geq \mathcal{R}_i(Q)$  if and only if  $\bigcap_{x \in Q} B_r(x) \neq \emptyset$ .

To see why this property is useful, consider a finite set  $X \subseteq \mathbb{X}$ , write  $g: \mathcal{P}_0(X) \rightarrow \mathbb{R}$  for the restriction of the radius function, and note that  $G_r = g^{-1}[0, r]$  is a subcomplex of  $G = \mathcal{P}_0(X)$ . We refer to  $G_r$  as the *Čech complex* of  $X$  and  $i$  for radius  $r$ . Furthermore, write  $X_r = \bigcup_{x \in X} B_r(x)$  for the union of the balls with radius  $r$ . We thus have two filtrations: the complexes  $G_r$  and the subspaces  $X_r$  of  $\mathbb{X}$ . The Nerve Theorem implies that  $G_r$  and  $X_r$  have isomorphic homology groups [9, 26], and this property extends:

**Theorem 6** (Isomorphism of Modules). *The persistence modules defined by the complexes  $G_r = g^{-1}[0, r]$  and the subspaces  $X_r = \bigcup_{x \in X} B_r(x)$  are isomorphic and the corresponding persistence diagrams are equal.*

Theorem 6 suggests we consider the common persistence diagram of the subspaces  $X_r$  and the Čech complexes  $G_r$  the "correct" diagram of the data set,  $X$ . Not surprisingly, the persistence diagram of the corresponding Vietoris–Rips complexes is generally different. We therefore have the opportunity to quantify the error we tolerate when we compute persistence for the Vietoris–Rips instead of the Čech complexes. Clearly,  $\mathcal{D}_i(Q) \leq \mathcal{R}_i(Q)$ , but how different can the two values be? Considering first the case  $\mathbb{X} = \mathbb{R}_+^n$ , we recall Theorem 2 (12). As proved in [15, page 62], the radius of a simplex in Euclidean space is at most  $\sqrt{2}$  times the half-length of its longest edge. The isometry between the Fisher information distance and the Euclidean distance implies  $\mathcal{R}_i(Q) \leq \sqrt{2}\mathcal{D}_i(Q)$  in  $\mathbb{R}_+^n$  equipped with the Fisher information metric. Hence,  $\frac{1}{C}\mathcal{D}_i(Q) \leq \mathcal{R}_i(Q) \leq C\mathcal{D}_i(Q)$  with  $C^2 = 2$ . The corresponding interleaving distance is  $\ln C = 0.346\dots$ , as recorded in Figure 4. The calculation of the interleaving distance for points in  $\Delta$  is similar, except that we do not have a Euclidean result ready to use. We will prove shortly that for simplices  $Q \subseteq \mathbb{S}_+^{n-1}$ , we have  $\frac{1}{C}\mathcal{D}_i(Q) \leq \mathcal{R}_i(Q) \leq C\mathcal{D}_i(Q)$  with  $C^2 = 4$ . The corresponding interleaving distance is  $\ln C = 0.693\dots$ . We thus observe that there is a higher penalty for using Vietoris–Rips complexes in  $\Delta$  than there is in  $\mathbb{R}_+^n$ . We finally prove the required Euclidean result. We recall that the radius and half-diameter of a set  $Q$  are defined in (27) and (30).

**Lemma 4** (Interleaving on the Sphere). *Let  $Q$  be a finite set of points in  $\mathbb{S}_+^{n-1}$ . Measuring distances in the  $(n-1)$ -sphere, the radius of  $Q$  is at most twice the half-diameter of  $Q$ , and this bound is tight as  $n$  goes to infinity.*

PROOF. Suppose first that  $Q$  is a regular  $(n-1)$ -simplex. It cannot be larger than the  $(n-1)$ -simplex  $Q_0$  that covers the entire positive orthant of the sphere. Its vertices are the  $n$  unit coordinate vectors, and its center lies on the diagonal, with all coordinates equal to  $1/\sqrt{n}$ . The scalar product of the vectors connecting the origin to the center and a vertex of  $Q_0$  is  $1/\sqrt{n}$ , which goes to 0 as  $n$  goes to infinity. It follows that the spherical distance between the two points approaches  $\frac{\pi}{2}$ . Since the half-diameter of  $Q_0$  is  $\frac{\pi}{4}$  and the radius of  $Q_0$  approaches  $\frac{\pi}{2}$  as  $n$  goes to infinity, the claimed inequality holds for regular  $(n-1)$ -simplices and cannot be improved unless we assume a fixed finite dimension.

To see that the claimed inequality holds for general sets  $Q$ , we recall that the spherical distance is a metric. Let  $B_r(x)$  be the ball with Fisher information radius  $r$  centered at  $x \in Q$ . Setting  $r$  equal to the diameter of  $Q$ , every such ball contains all points of  $Q$ , which implies that the common intersection is non-empty. Hence, the radius is at most the diameter.  $\square$

## 6 Discussion

The main contribution of this paper is a connection between information theory and topological data analysis, thus complementing the established field of information geometry [3] with topological methods. Concretely, we study notions of distance with information theoretic foundations, focusing on properties relevant in their application in topological data analysis. As an immediate practical gain, we can now use computational topology tools that work for Euclidean distance to analyze data measured with Fisher information metric. It is thus easy to experiment with data in information space without developing new and specialized software. Another option is to construct Vietoris–Rips complexes with the Ripser software [6], which at the time of writing this paper is significantly more efficient than constructing nerves of entropy balls.

The first concrete application of the theory set up in this paper is described in [17], where Euclidean and Fisher information point processes are studied and compared through the lens of integral geometry. Many challenges remain before topology can be fully utilized in high-dimensional data analysis tasks. In particular, a proof of stability of topological descriptors based on Bregman divergences remains elusive, and we hope that the results presented here are a step in this direction.

We now turn to applications in data science. The cosine dissimilarity is an effective measure for text documents in the vector space model [22]. It represents each document as a discrete probability distribution, and — just like the Antonelli isometry — maps this distribution to a point in the positive orthant of a sphere. This resembles the Fisher information distance in  $\Delta$ , except that the latter uses the angle rather than its cosine. This suggests an information-theoretic interpretation for the cosine measure. Using the generalized Antonelli isometry, we can devise similarly simple measures for other decomposable Bregman divergences. Will they prove equally effective in practice?

In general, choosing a suitable dissimilarity measure for a given task can have a big impact on performance, and certain dissimilarity measures are known to work well for certain tasks [22]. Metric learning [24] algorithms can be used to tailor a dissimilarity measure to a task at hand. In the context of topological data analysis, some interesting open problems arise: How does the choice of a dissimilarity measure affect the persistence diagrams? Can we guide the choice by examining the diagrams? What is the effect of substituting a decomposable Bregman divergence with the corresponding (generalized) Fisher information metric?

## A Burg Entropy by Comparison

To offer a perspective, we contrast Theorem 1 with the analysis of balls defined for a Legendre type function different from the Shannon entropy. The *Burg entropy* is the function  $G: \mathbb{R}_+^n \rightarrow \mathbb{R}$  defined by  $G(x) = \sum_{i=1}^n [1 - \ln x_i]$ . The corresponding divergence,

$$D_G(x||y) = G(x) - [G(y) + \langle \nabla G(y), x - y \rangle] = \sum_{i=1}^n [\ln \frac{y_i}{x_i} + \frac{x_i}{y_i} - 1], \quad (31)$$

is known as the *Itakura–Saito divergence* [23]. We note that the Burg entropy is strongly decomposable, which implies that every one of its divergence functions is strongly decomposable. By Lemma 1, these functions are convex if and only if their components are convex. Furthermore, the divergence functions of different points can be obtained by stretching the domain along coordinate directions. To explain this, let  $\mathbf{1} = (1, 1, \dots, 1) \in \mathbb{R}_+^n$  and write  $y/x = (y_1/x_1, y_2/x_2, \dots, y_n/x_n)$ .

**Lemma 5** (Stretch Deformation). *Let  $G: \mathbb{R}_+^n \rightarrow \mathbb{R}$  be the Burg entropy, and  $x \in \mathbb{R}_+^n$ . Then the divergence function of  $x$  satisfies  $D_x(y) = D_{\mathbf{1}}(y/x)$ .*

PROOF. Note that  $x/x = \mathbf{1}$ . Hence,  $D_{\mathbf{1}}(y/x)$  is equal to  $D_G(x/x||y/x) = \sum_{i=1}^n [\ln \frac{y_i}{x_i} + \frac{x_i}{y_i} - 1]$ , which is  $D_x(y) = D_G(x||y)$ .  $\square$

Scaling the components does not affect the convexity or nonconvexity of the sublevel sets. Hence,  $B_r(x)$  is convex if and only if  $B_r(\mathbf{1})$  is convex. We use this insight to show that under the Burg entropy, all balls beyond a certain size are nonconvex.

**Theorem 7** (Nonconvex Divergence Balls). *Let  $G: \mathbb{R}_+^n \rightarrow \mathbb{R}$  be the Burg entropy in  $n \geq 2$  dimensions. Then a ball  $B_r(x)$  of the Itakura–Saito divergence is convex if  $r^2 \leq \ln 2 - \frac{1}{2}$  and nonconvex if  $r^2 > 2 \ln 2 - 1$ .*

PROOF. Writing  $g(t) = 1 - \ln t$  for the component function of the Burg entropy, the component function of the divergence function of  $\mathbf{1} \in \mathbb{R}_+^n$  is  $d(t) = g(1) - [g(t) + g'(t)(1-t)] = \ln t + \frac{1}{t} - 1$ . Its first and second derivatives are  $d'(t) = \frac{1}{t} - \frac{1}{t^2} = \frac{t-1}{t^2}$  and  $d''(t) = -\frac{1}{t^2} + \frac{2}{t^3} = \frac{-t+2}{t^3}$ . Hence,  $d$  is convex for  $t \leq 2$  and concave for  $t \geq 2$ . This implies that  $d^{-1}[0, r^2]$  is convex as long as  $r^2 \leq d(2) = \ln 2 - \frac{1}{2}$ . By Lemma 1,  $B_r(\mathbf{1})$  is convex for  $r^2 \leq \ln 2 - \frac{1}{2} = 0.193\dots$  To prove the upper bound, we note that Remark 3 applies here. Setting  $x = (a, b, 1, \dots, 1)$  and  $y = (b, a, 1, \dots, 1)$ , with  $a = 2 + \varepsilon$ ,  $b = 2 + 2\varepsilon$ , and  $\varepsilon > 0$ , we get a nonconvex ball of squared radius  $r^2 = D_{\mathbf{1}}(x) = D_{\mathbf{1}}(y) = d(a) + d(b)$ . Hence,  $r^2 = 2 \ln 2 - 1 + f(\varepsilon)$ , in which  $f(\varepsilon)$  approaches 0 as  $\varepsilon$  goes to 0. Since  $\varepsilon$  can be chosen arbitrarily small, this implies that  $B_r(\mathbf{1})$  is nonconvex for all  $r^2 > 2 \ln 2 - 1 = 0.386\dots$  By Lemma 5, the same is true for all balls  $B_r(x)$ ,  $x \in \mathbb{R}_+^n$ .  $\square$

## B Burg Information Metric by Comparison

We wish to compare the metrics defined by the Shannon entropy and the Burg entropy. Recall that the latter is the Legendre type function  $G: \mathbb{R}_+^n \rightarrow \mathbb{R}$  defined by mapping  $x$



to  $G(x) = \sum_{i=1}^n [1 - \ln x_i]$ , which is twice differentiable. Using its Hessian, we define the corresponding *Burg information metric*,  $d_G: \mathbb{R}_+^n \times \mathbb{R}_+^n \rightarrow \mathbb{R}$ .

**Theorem 8** (Burg Information to Euclidean Distance). *Let  $G: \mathbb{R}_+^n \rightarrow \mathbb{R}$  be the Burg entropy, and  $x, y \in \mathbb{R}_+^n$ . Then*

$$d_G(x, y) = \sqrt{\frac{1}{2} \sum_{i=1}^n (\ln x_i - \ln y_i)^2}. \quad (32)$$

PROOF. Let  $\psi: \mathbb{R}_+^n \rightarrow \mathbb{R}$  be the diffeomorphism that distorts the Burg information metric to the Euclidean metric. It decomposes into  $n$  copies of  $q: \mathbb{R}_+ \rightarrow \mathbb{R}$ . By Equation (11), the derivative of the component function is  $q'(t) = 1/\sqrt{2t^2}$ . We get  $q(t) = \ln t/\sqrt{2}$  by integration. The diffeomorphism maps a point  $x$  with coordinates  $x_i > 0$  to the point  $\psi(x)$  with coordinates  $q(x_i) = \ln x_i/\sqrt{2}$ , which may be positive, zero, or negative. The squared Euclidean distance between  $\psi(x)$  and  $\psi(y)$  is  $\frac{1}{2} \sum_{i=1}^n (\ln x_i - \ln y_i)^2$ , which implies (32).  $\square$

While the Burg information metric in  $\mathbb{R}_+^n$  has a satisfactory description given in Theorem 8, the situation is more complicated when we restrict the domain to  $\Delta \subseteq \mathbb{R}_+^n$ . The image of the standard simplex,  $\psi(\Delta)$ , consists of all points with coordinates  $u_i = q(x_i)$  that satisfy  $e^{\sqrt{2}u_1} + e^{\sqrt{2}u_2} + \dots + e^{\sqrt{2}u_n} = 1$ . The thus specified  $(n-1)$ -dimensional surface is the graph of a smooth and strictly concave function whose graph is close to the boundary of the negative orthant. Denoting this surface by  $\mathbb{H}^{n-1}$ , we get an isometry  $\psi|_{\Delta}: \Delta \rightarrow \mathbb{H}^{n-1}$ .

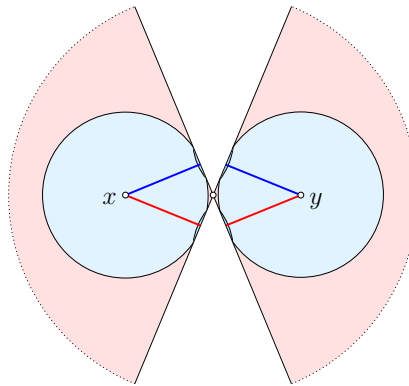


Figure 5: An unfolding of the cone that is the boundary of the negative orthant in  $\mathbb{R}^3$ . The two disks contain both shortest connecting paths and form a hole that contains the apex.

It is not difficult to show that the shortest path between two points in  $\Delta$  is not unique. We illustrate this by approximating  $\mathbb{H}^2$  with the cone that has an angle  $\frac{3\pi}{2}$  at the apex; see Figure 5. Indeed, this cone is isometric to the boundary of the negative orthant. To draw the cone in the plane, we cut it symmetrically along two half-lines. Let  $x$  and  $y$  be opposite from each other at unit distance from the apex. There are two shortest paths connecting them, by-passing the apex on different sides. The disks of radius  $\cos \frac{\pi}{16}$  centered at  $x$  and at  $y$  cover both paths but not the apex. Indeed, the union of the two disks is an annulus with a hole containing the apex. To create this hole, the two disks intersect in two disconnected pieces. The configuration depicted in Figure 5 can be approximated

arbitrarily closely for  $\mathbb{H}^2$ , namely if we increase the radii of the two disks as needed. In other words, the balls in the Burg information metric violate the essential assumption of the Nerve Theorem [9, 26], namely the contractibility of non-empty common intersections, and can therefore not be convex in  $\Delta$ .

### C Burbea–Rao Divergence by Comparison

The Jensen–Shannon divergence and the Fisher information metric both generalize to the case of the Burg entropy, but not all results do. In particular, the left inequality in (16) extends, while there is no counterpart to the right inequality. We call the generalization of the Jensen–Shannon divergence to Legendre type functions the *Burbea–Rao divergence*. For the Burg entropy and points  $x, y \in \mathbb{R}_+^n$ , it is

$$\text{BR}_G(x, y) = \frac{1}{2}[D_G(x||\mu) + D_G(y||\mu)] = \frac{1}{2}[G(x) + G(y)] - G(\mu) = \frac{1}{2} \sum_{i=1}^n \left[ \ln \frac{(x_i + y_i)^2}{4x_i y_i} \right], \quad (33)$$

in which  $\mu = \frac{x+y}{2}$ . The squared distance between  $x$  and  $y$  according to the Burg information metric is given in (32) as

$$d_G^2(x, y) = \frac{1}{2} \sum_{i=1}^n [\ln x_i - \ln y_i]^2. \quad (34)$$

**Theorem 9** (Burbea–Rao Divergence vs. Burg Information). *The Burbea–Rao divergence and the squared Burg information metric satisfy  $4 \text{BR}_G(x, y) \leq d_G^2(x, y)$  for all  $x, y \in \mathbb{R}_+^n$ . Furthermore, for any  $C > 0$ , there are points  $x, y \in \mathbb{R}_+^n$  for which  $d_G^2(x, y) > C \text{BR}_G(x, y)$ .*

PROOF. Both the Burbea–Rao divergence and the squared Burg information metric are decomposable, so it suffices to consider the 1-dimensional case in which we write  $a$  for  $x$  and  $b$  for  $y$ . From (33) we get  $\text{BR}_G(Ca, Cb) = \text{BR}_G(a, b)$ , and from (34) we get  $d_G^2(Ca, Cb) = d_G^2(a, b)$ , for any  $C > 0$ . Setting  $b = ta$  and  $C = \frac{1}{a}$ , we thus get  $\text{BR}_G(a, b) = \text{BR}_G(1, t)$  and  $d_G^2(a, b) = d_G^2(1, t)$ . We will show that the ratio of the two functions decreases monotonically within  $1 < t < \infty$ , attaining its extreme values in the two limits. Setting  $g(t) = \text{BR}_G(1, t) / d_G^2(1, t)$ , we have  $g(t) = \frac{2 \ln(t+1) - \ln(4t)}{(\ln t)^2}$ . As  $t$  goes to infinity, the denominator grows faster than the numerator, which implies  $\lim_{t \rightarrow \infty} g(t) = 0$ . In other words, for every  $C > 0$ , there is a sufficiently large  $t$  such that  $d_G^2(1, t) > C \text{BR}_G(1, t)$ , as claimed. At  $t = 1$ , we get  $g(1) = \frac{0}{0}$ . To resolve this ambiguity, we write  $g(t) = \frac{u(t)}{v(t)}$  and use the l'Hopital rule by differentiating twice:

$$u'(t) = \frac{t-1}{t(t+1)}, \quad u''(t) = \frac{-t^2+2t+1}{t^2(t+1)^2}, \quad (35)$$

$$v'(t) = \frac{2 \ln t}{t}, \quad v''(t) = \frac{2 - \ln t}{t^2}. \quad (36)$$

The second derivatives at  $t = 1$  are  $u''(1) = \frac{1}{2}$  and  $v''(1) = 2$ , which gives  $\lim_{t \rightarrow 1} g(t) = \frac{1}{4}$ , as required. To prove that  $g$  decreases monotonically, from  $\frac{1}{4}$  at  $t = 1$  to 0 at  $t = \infty$ , we compute the first derivative:

$$g'(t) = \frac{(t-1) \ln t - 4(t+1) \ln(t+1) + 2(t+1) \ln(4t)}{t(t+1)(\ln t)^3}. \quad (37)$$

The denominator is positive so it suffices to show that the numerator is negative, for all  $t > 1$ . Writing  $w(t)$  for the numerator of  $g'(t)$ , we have  $w(1) = -8 \ln 2 + 4 \ln 4 = 0$ . The first two derivatives are

$$w'(t) = 3 \ln t - 4 \ln(t + 1) + 4 \ln 2 - 1 + \frac{1}{t}, \quad (38)$$

$$w''(t) = -\frac{(t-1)^2}{t^2(t+1)}. \quad (39)$$

We have  $w'(1) = 0$  and  $w''(t) < 0$  for all  $t > 1$ , which implies  $w'(t) < 0$  for all  $t > 1$ . Hence,  $g'(t) < 0$  for all  $t > 1$ , so  $g$  is indeed monotonically decreasing, as required.  $\square$

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