# Comprehensive Survey on Distance/Similarity Measures between Probability Density Functions 

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#### Abstract

Distance or similarity measures are essential to solve many pattern recognition problems such as classification, clustering, and retrieval problems. Various distance/similarity measures that are applicable to compare two probability density functions, pdf in short, are reviewed and categorized in both syntactic and semantic relationships. A correlation coefficient and a hierarchical clustering technique are adopted to reveal similarities among numerous distance/similarity measures.


Keywords-Distance, Histogram, Probability Density Function, Similarity.

## A <br> I. Introduction

BEIT the concept of Euclidean distance has prevailed in different cultures and regions for millennia, it is not a panacea for all types of data or pattern to be compared. The $20^{\text {th }}$ century witnessed tremendous efforts to exploit new distance/similarity measures for a variety of applications. There are a substantial number of distance/similarity measures encountered in many different fields such as anthropology, biology, chemistry, computer science, ecology, information theory, geology, mathematics, physics, psychology, statistics, etc.

There have been considerable efforts in finding the appropriate measures among such a plethora of choices because it is of fundamental importance to pattern classification, clustering, and information retrieval problems [1]. Such endeavors have been conducted throughout different fields [2-5]. Despite such comparative studies on diverse distance/similarity measures, further comprehensive study is necessary because even names for certain distance/similarity measures are fluid and promulgated differently.

From the scientific and mathematical point of view, distance is defined as a quantitative degree of how far apart two objects are. Synonyms for distance include dissimilarity. Those distance measures satisfying the metric properties are

[^0]simply called metric while other non-metric distance measures are occasionally called divergence. Synonyms for similarity include proximity and similarity measures are often called similarity coefficients. A distance measure and a similarity measure are denoted as $d_{x}$ and $s_{x}$, respectively throughout the rest of the paper.

The choice of distance/similarity measures depends on the measurement type or representation of objects. Here the probability density function or pdf in short which is one of the most popular pattern representations, is considered. Let $X$ be a set of $n$ elements whose possible values are discrete and finite. A histogram $H(X)$ of a set $X$ represents the frequency of each value as shown in Figure 1. The frequency value of the $i$ th bin is denoted as $H_{i}(X)$, e.g., $H_{2}(X)=4$ and $H_{3}(Y)=2$ in Figure 1.


Fig. 1 Histogram Representation.

Let $d$ be the number of bins in the histogram. There are different types of histograms [6]. Here only the nominal type histogram where each level or bin is independent from other levels or bins is considered and other types of histogram are abstained. When each bin is divided by $n$, the probability density function which represents a probability distribution is produced. A pdf for a corresponding histogram is produced by dividing each level by $n: P=H(X) / n$. For example, let $P$ and $Q$ be pdfs for $H(X)$ and $H(Y)$ and then $P_{2}=0.4$ and $Q_{3}=0.2$ in Figure 1.

In this paper, various distance/similarity measures that are applicable to compare two probability density functions are perambulated and categorized. All measures appearing in this
paper have the shuffling invariant property [6] and thus naturally imply the level independency.

There are two approaches in pdf distance/similarity measures: vector and probabilistic. Since each level is assumed to be independent from other levels, a histogram or pdf can be considered as a vector, i.e., a point in the Euclidean space or a Cartesian coordinate system. Hence, numerous geometrical distances can be applied to compare two pdf's. There is much literature regarding discrete versions of various divergences in probability and information theory fields $[7,8]$. Computing the distance between two pdf's can be regarded as the same as computing the Bayes (or minimum misclassification) probability [1]. This is equivalent to measuring the overlap between two pdfs as the distance. The probabilistic approach is based on the fact that a histogram of a measurement provides the basis for an empirical estimate of the pdf.

The rest of the paper is organized as follows. In section 2, various distance/similarity measures are enumerated according to their syntactic similarities. In order to provide a better perspective on distance/similarity measures, section 3 presents the hierarchical cluster tree using the correlations between different measures. Finally, section 4 concludes this work.

## II.DEFINITIONS

Table 1. $L_{p}$ Minkowski family

| 1. Euclidean $L_{2}$ | $d_{E u c}=\sqrt{\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|^{2}}$ |  |
| :--- | :--- | :--- |
| 2. City block $L_{1}$ | $d_{C B}=\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|$ | (1) |
| 3. Minkowski $L_{\mathrm{p}}$ | $d_{M k}=\sqrt{r} \sqrt{\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|^{p}}$ | (2) |
| 4. Chebyshev $L_{\infty}$ | $d_{\text {Chee }}=\max _{i}\left\|P_{i}-Q_{i}\right\|$ |  |

A couple of thousand years ago, Euclid stated that the shortest distance between two points is a line and thus the eqn (1) is predominantly known as Euclidean distance. It was often called Pythagorean metric since it is derived from the Pythagorean Theorem. In the late $19^{\text {th }}$ century, Hermann Minkowski considered the city block distance [9]. Other names for the eqn (2) include rectilinear distance, taxicab norm, and Manhattan distance. Hermann also generalized the formulae (1) and (2) to the eqn (3) which is coined after Minkowski. When $p$ goes to infinite, the eqn (4) can be derived and it is called the chessboard distance in 2D, the minimax approximation, or the Chebyshev distance named after Pafnuty Lvovich Chebyshev [10].

Table 2. $L_{1}$ family
5. Sørensen

$$
\begin{equation*}
d_{s o r}=\frac{\sum_{i=1}^{d}\left|P_{i}-Q_{i}\right|}{\sum_{i=1}^{d}\left(P_{i}+Q_{i}\right)} \tag{5}
\end{equation*}
$$

| 6. Gower | $d_{\text {gow }}=\frac{1}{d} \sum_{i=1}^{d} \frac{\left\|P_{i}-Q_{i}\right\|}{R_{i}}$ |
| :--- | :--- | :--- |
| $=\frac{1}{d} \sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|$ | $d_{s g}=\frac{\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|}{\sum_{i=1}^{d} \max \left(P_{i}, Q_{i}\right)}$ |
| 7. Soergel | $d_{k u l}=\frac{\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|}{\sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)}$ |
| 8. Kulczynski $d$ | $d_{\text {Can }}=\sum_{i=1}^{d} \frac{\left\|P_{i}-Q_{i}\right\|}{P_{i}+Q_{i}}$ |
| 9. Canberra | $d_{\text {Lor }}=\sum_{i=1}^{d} \ln \left(1+\left\|P_{i}-Q_{i}\right\|\right)$ |
| 10. Lorentzian |  |
| * $L_{1}$ family <br> Czekanowski (16), Ruzicka (21), Tanimoto (23), etc \}. |  |

Several distance measures listed in Table 2 facilitate the $L_{1}$, more precisely the absolute difference. The eqn (5), which is widely used in ecology [11], is known as Sorensen distance [12] or Bray-Curtis [2,4,13]. When it is used for comparing two pdfs, it is nothing but the $L_{1}$ divided by 2 . Gower distance [14] in the eqn (6) scales the vector space into the normalized space and then uses the $L_{1}$. Since the pdf is already normalized space, Gower distance is the $L_{1}$ divided by $d$. Other $L_{1}$ family distances that are non-proportional to the $L_{1}$ include Soergel and Kulczynski distances given in the eqns (8) [4] and (9) [2] respectively. At first glance, Canberra metric given in the eqn $(10)[2,15]$ resembles Sorensen but normalizes the absolute difference of the individual level. It is known to be very sensitive to small changes near zero [15]. The eqn (11) [2], attributed to Lorentzian, also contains the absolute difference and the natural logarithm is applied. 1 is added to guarantee the non-negativity property and to eschew the $\log$ of zero.

## Table 3. Intersection family

| 11. Intersection | $s_{l S}=\sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)$ |
| :---: | :---: |
| $d_{\text {non }-I S}=1-s_{I S}=\frac{1}{2} \sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|$ |  |
| 12. Wave Hedges | $\begin{aligned} & d_{W H}=\sum_{i=1}^{d}\left(1-\frac{\min \left(P_{i}, Q_{i}\right)}{\max \left(P_{i}, Q_{i}\right)}\right) \\ & =\sum_{i=1}^{d} \frac{\left\|P_{i}-Q_{i}\right\|}{\max \left(P_{i}, Q_{i}\right)} \end{aligned}$ |
| 13. Czekanowski | $s_{C z e}=\frac{2 \sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)}{\sum_{i=1}^{d}\left(P_{i}+Q_{i}\right)}$ |
|  | $d_{C z e}=1-s_{C z e}=\frac{\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|}{\sum_{i=1}^{d}\left(P_{i}+Q_{i}\right)}$ |


| 14. Motyka $s_{\text {Mot }}=\frac{\sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)}{\sum_{i=1}^{d}\left(P_{i}+Q_{i}\right)}$ | (18) |
| :---: | :---: |
| $d_{\text {Mot }}=1-s_{\text {Mot }}=\frac{\sum_{i=1}^{d} \max \left(P_{i}, Q_{i}\right)}{\sum_{i=1}^{d}\left(P_{i}+Q_{i}\right)}$ | (19) |
| 15. Kulczynski $s$ $s_{K u l}=\frac{1}{d_{K u l}}=\frac{\sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)}{\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|}$ | (20) |
| 16. Ruzicka $s_{R u z}=\frac{\sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)}{\sum_{i=1}^{d} \max \left(P_{i}, Q_{i}\right)}$ | (21) |
| 17. Tanimoto $\begin{aligned} & d_{\text {Tani }}=\frac{\sum_{i=1}^{d} P_{i}+\sum_{i=1}^{d} Q_{i}-2 \sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)}{\sum_{i=1}^{d} P_{i}+\sum_{i=1}^{d} Q_{i}-\sum_{i=1}^{d} \min \left(P_{i}, Q_{i}\right)} \\ & =\frac{\sum_{i=1}^{d}\left(\max \left(P_{i}, Q_{i}\right)-\min \left(P_{i}, Q_{i}\right)\right)}{\sum_{i=1}^{d} \max \left(P_{i}, Q_{i}\right)} \end{aligned}$ | (22) <br> (23) |

The intersection between two pdfs in the eqn (12) is a widely used form of similarity [1] where the non-overlaps between two pdfs defined in the eqn (13) is nothing but the $L_{1}$ divided by 2 [6]. Hence, most similarity measures pertinent to the intersection enumerated in Table 3 can be transformed into the $L_{1}$ based distance measures using the technique, i.e., $d_{\mathrm{x}}(P, Q)=1-s_{\mathrm{x}}(P, Q)$ with a few of exceptions. The eqn (14) is called Wave Hedges [16] and its $L_{1}$ based distance form is given in the eqn (15). Czekanowski Coefficient in the eqn (16) [15] has its distance form identical to Sørensen (5). Half of the Czekanowski Coefficient is called Motyka similarity in the eqn (18) [2]. The eqn (20) is known as Kulczynski similarity [2]. Unlike the other similarity and distance relationship, Kulczynski has skul $s_{\mathrm{kul}}(P, Q)=1 / d_{\mathrm{kul}}(P, Q)$. The eqn (22) is referred to as Tanimoto distance [1] a.k.a., Jaccard distance. Soergel distance in the eqn (8) is identical to Tanimoto. 1 $d_{\text {Tani }}$ is Ruzicka similarity given in the eqn (21) [2]. The eqn (23) is given to help understand their equivalencies.

Table 4. Inner Product family

| 18. Inner Product | $s_{I P}=P \bullet Q=\sum_{j=1}^{d} P_{i} Q_{i}$ |
| :--- | :--- |
| 19. Harmonic <br> mean | $s_{H M}=2 \sum_{i=1}^{d} \frac{P_{i} Q_{i}}{P_{i}+Q_{i}}$ |
| 20. Cosine | $s_{C o s}=\frac{\sum_{i=1}^{d} P_{i} Q_{i}}{\sqrt{\sum_{i=1}^{d} P_{i}^{2}} \sqrt{\sum_{i=1}^{d} Q_{i}^{2}}}$ |


| 21. Kumar- <br> Hassebrook (PCE) | $s_{J a c}=\frac{\sum_{i=1}^{d} P_{i} Q_{i}}{\sum_{i=1}^{d} P_{i}^{2}+\sum_{i=1}^{d} Q_{i}^{2}-\sum_{i=1}^{d} P_{i} Q_{i}}$ | (27) |
| :---: | :---: | :---: |
| 22. Jaccard | $s_{J a c}=\frac{\sum_{i=1}^{d} P_{i} Q_{i}}{\sum_{i=1}^{d} P_{i}^{2}+\sum_{i=1}^{d} Q_{i}^{2}-\sum_{i=1}^{d} P_{i} Q_{i}}$ | (28) |
|  | $d_{J a c}=1-s_{J a c}=\frac{\sum_{i=1}^{d}\left(P_{i}-Q_{i}\right)^{2}}{\sum_{i=1}^{d} P_{i}^{2}+\sum_{i=1}^{d} Q_{i}{ }^{2}-\sum_{i=1}^{d} P_{i} Q_{i}}$ | (39) |
| 23. Dice | $s_{\text {Dice }}=\frac{2 \sum_{i=1}^{d} P_{i} Q_{i}}{\sum_{i=1}^{d} P_{i}^{2}+\sum_{i=1}^{d} Q_{i}^{2}}$ | (40) |
|  | $d_{\text {Dice }}=1-s_{\text {Dice }}=\frac{\sum_{i=1}^{d}\left(P_{i}-Q_{i}\right)^{2}}{\sum_{i=1}^{d} P_{i}^{2}+\sum_{i=1}^{d} Q_{i}^{2}}$ | (31) |

Table 4 deals exclusively with similarity measures which incorporate the inner product , $P \bullet Q$ explicitly in their definitions. The inner product of two vectors in the eqn (24) yields a scalar and is sometimes called the scalar product or dot product [1]. The inner product is also called the number of matches or the overlap if it is used for binary vectors. The eqn (25) is the harmonic mean [2]. The eqn (26) is the normalized inner product and called the cosine coefficient because it measures the angle between two vectors and thus often called the angular metric [2]. Other names for the cosine coefficient include Ochiai [2,4] and Carbo [4]. Kumar and Hassebrook utilized $P \bullet Q$ to measure the Peak-to-correlation energy, $P C E$ in short [17] in the eqn (27). Jaccard coefficient [18], a.k.a. Tanimoto [19], defined in the eqn (28) is another variation of the normalized inner product. Dice coefficient in the eqn (30) [20] is occasionally called Sorensen, Czekannowski, HodgkinRichards [4] or Morisita [21]. The eqns $(24,26,28,30)$ are frequently encountered similarity measures in the fields of information retrieval and biological taxonomy for the binary feature vector comparison (see $[2,22]$ for the exhaustive list of distance and similarity measures for the binary feature vectors).

Table 5. Fidelity family or Squared-chord family

| 24. Fidelity | $s_{F i d}=\sum_{i=1}^{d} \sqrt{P_{i} Q_{i}}$ |
| :--- | :--- |
| 25. Bhattacharyya | $d_{B}=-\ln \sum_{i=1}^{d} \sqrt{P_{i} Q_{i}}$ |
| 26. Hellinger | $d_{H}=\sqrt{2 \sum_{i=1}^{d}\left(\sqrt{P_{i}}-\sqrt{Q_{i}}\right)^{2}}$ |
|  | $=2 \sqrt{1-\sum_{i=1}^{d} \sqrt{P_{i} Q_{i}}}$ |


| 27. Matusita | $d_{M}=\sqrt{\sum_{i=1}^{d}\left(\sqrt{P_{i}}-\sqrt{Q_{i}}\right)^{2}}$ |
| :--- | :--- |
| $=\sqrt{2-2 \sum_{i=1}^{d} \sqrt{P_{i} Q_{i}}}$ |  |
| 28. Squared-chord | $d_{s q c}=\sum_{i=1}^{d}\left(\sqrt{P_{i}}-\sqrt{Q_{i}}\right)^{2}$ |
| $s_{s q c}=1-d_{s q c}$ | $s_{s q c}=2 \sum_{i=1}^{d} \sqrt{P_{i} Q_{i}}-1$ |

The sum of geometric means in the eqn (32) is referred to as Fidelity similarity, a.k.a. Bhattacharyya coefficient or Hellinger affinity [2]. Bhattacharyya distance given in the eqn (33), which is a value between 0 and 1 , provides bounds on the Bayes misclassification probability [23]. Other approaches closely related to Bhattacharyya include Hellinger [2] and Matusita [24] in eqns (34) and (36) respectively. The basic form in the eqn (38), i.e., Matusita without the square root is called Squared-chord distance [5] and thus all Fidelity based measures have their alternative representation using the squared-chord distance.

Table 6. Squared $L_{2}$ family or $\chi^{2}$ family

| 29. Squared <br> Euclidean | $d_{\text {sqe }}=\sum_{i=1}^{d}\left(P_{i}-Q_{i}\right)^{2}$ |
| :--- | :--- |
| 30. Pearson $\chi^{2}$ | $d_{P}(P, Q)=\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{Q_{i}}$ |
| 31. Neyman $\chi^{2}$ | $d_{N}(P, Q)=\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{P_{i}}$ |
| 32. Squared $\chi^{2}$ | $d_{S q C h i}=\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{P_{i}+Q_{i}}$ |
| 33. Probabilistic <br> Symmetric $\chi^{2}$ | $d_{P C h i i}=2 \sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{P_{i}+Q_{i}}$ |
| 34. Divergence | $d_{D i v}=2 \sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{\left(P_{i}+Q_{i}\right)^{2}}$ |
| 35. Clark | $\left.d_{C I k}^{d}=\sqrt{\sum_{i=1}^{d}} \frac{\left\|P_{i}-Q_{i}\right\|}{P_{i}+Q_{i}}\right)^{2}$ |
| 36. Additive <br> Symmetric $\chi^{2}$ | $d_{\text {AdChi }}=\sum_{i=1}^{b} \frac{\left(P_{i}-Q_{i}\right)^{2}\left(P_{i}+Q_{i}\right)}{P_{i} Q_{i}}$ |

$\begin{aligned} & \text { 33. Probabilistic } \\ & \text { Symmetric } \chi^{2}\end{aligned} \quad d_{P C h i i}=2 \sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{P_{i}+Q_{i}}$
35. Clark $d_{C l k}=\sqrt{\sum_{i=1}^{d}\left(\frac{\left|P_{i}-Q_{i}\right|}{P_{i}+Q_{i}}\right)^{2}}$
$\begin{aligned} & \text { 36. Additive } \\ & \text { Symmetric } \chi^{2}\end{aligned} \quad d_{\text {AdChi }}=\sum_{i=1}^{b} \frac{\left(P_{i}-Q_{i}\right)^{2}\left(P_{i}+Q_{i}\right)}{P_{i} Q_{i}}$

* Squared $L_{2}$ family $\supset\{$ Jaccard (29), Dice (31) $\}$

Several distance measures containing the Squared Euclidean distance in the eqn (40) as the dividend are corralled in Table 6. Jaccard and Dice distance forms in the eqns (29) and (31) also belong to this family. The cornerstone to the $\chi^{2}$ family (eqns (41) $\sim(47)$ ) is Pearson $\chi^{2}$ divergence in the eqn (41) [25] which embodies the Squared Euclidean distance. Of particular concern to mathematicians is that Pearson $\chi^{2}$ divergence is asymmetric. Neyman $\chi^{2}$ in the eqn (42) [26] is $d_{\mathrm{P}}(P, Q)=d_{\mathrm{P}}(Q, P)$. Various symmetric versions of the $\chi^{2}$ have been exploited. The eqn (43) is called the squared $\chi^{2}$ distance [5] or triangular discrimination [27,28]. Twice of
the eqn (44) is called the probabilistic symmetric $\chi^{2}$ [2] which is equivalent to Sangvi $\chi^{2}$ distance between populations [2]. The term 'divergence' is pronominal to refer non-metric distance. Notwithstanding the eqn (45) has been commonly called divergence [29]. The squared root of half of the divergence is called Clark in the eqn (46) [2].

One of techniques to transform asymmetric distances into symmetric form utilizes the addition method; $d_{\mathrm{sym}}(P, Q)=$ $d_{\text {asym }}(P, Q)+d_{\text {asym }}(Q, P)$, e.g., The eqn (47) is $d_{\text {AdChi }}(P, Q)=$ $d_{\mathrm{P}}(P, Q)+d_{\mathrm{P}}(Q, P)[2,3]$. Albeit the eqn (47) is occasionally called 'symmetric $\chi^{2}$ divergence', let's call it the additive symmetric $\chi^{2}$ here in order to distinguish other symmetric versions of $\chi^{2}$. Other techniques that are not listed in the above table would include max, min, and avg methods; $d_{\text {max }}$ $\operatorname{sym}(P, Q)=\max \left(d_{\text {asym }}(P, Q), \quad d_{\text {asym }}(Q, P)\right), \quad d_{\text {min-sym }}(P, Q)=$ $\min \left(d_{\text {asym }}(P, Q), \quad d_{\text {asym }}(Q, P)\right), \quad$ and $\quad d_{\text {avg-sym }}(P, Q)=$ $\operatorname{avg}\left(d_{\text {asym }}(P, Q), d_{\text {asym }}(Q, P)\right)$.

Table 7. Shannon's entropy family

| 37. Kullback- <br> Leibler | $d_{K L}=\sum_{i=1}^{d} P_{i} \ln \frac{P_{i}}{Q_{i}}$ |
| :--- | :--- |
| 38. Jeffreys | $d_{J}=\sum_{i=1}^{d}\left(P_{i}-Q_{i}\right) \ln \frac{P_{i}}{Q_{i}}$ |
| 39. K divergence | $d_{\text {Kdiv }}=\sum_{i=1}^{d} P_{i} \ln \frac{2 P_{i}}{P_{i}+Q_{i}}$ |

40. Topsøe

$$
\begin{equation*}
d_{\text {Top }}=\sum_{i=1}^{d}\left(P_{i} \ln \left(\frac{2 P_{i}}{P_{i}+Q_{i}}\right)+Q_{i} \ln \left(\frac{2 Q_{i}}{P_{i}+Q_{i}}\right)\right) \tag{51}
\end{equation*}
$$

41. Jensen-Shannon

$$
\begin{equation*}
d_{J S}=\frac{1}{2}\left[\sum_{i=1}^{d} P_{i} \ln \left(\frac{2 P_{i}}{P_{i}+Q_{i}}\right)+\sum_{i=1}^{d} Q_{i} \ln \left(\frac{2 Q_{i}}{P_{i}+Q_{i}}\right)\right] \tag{52}
\end{equation*}
$$

$$
\begin{align*}
& \text { 42. Jensen difference } \\
& d_{J D}=\sum_{i=1}^{b}\left[\frac{P_{i} \ln P_{i}+Q_{i} \ln Q_{i}}{2}-\left(\frac{P_{i}+Q_{i}}{2}\right) \ln \left(\frac{P_{i}+Q_{i}}{2}\right)\right] \tag{53}
\end{align*}
$$

Eqns (48~53) in Table 7 are primary due to Shannon's concept of probabilistic uncertainty or "entropy" $\mathrm{H}(\mathrm{P})=\sum_{i=1}^{\mathrm{d}}$ $P_{\mathrm{i}} \ln P_{\mathrm{i}}$ [30]. Kullback and Leibler [31] introduced the eqn (48) called KL divergence, relative entropy, or information deviation [2]. The symmetric form of the KL divergence using the addition method is in the eqn (49) [31-33] and it is called Jeffreys or J divergence. The eqn (50) is called the K divergence and its symmetric form using the addition method is given in the eqn (51) and called Topsøe distance [2] or information statistics [5]. The half of the Topsøe distance is called Jensen-Shannon divergence $[2,34]$ which uses the avg method to make the K divergence symmetric. Sibson [35] studied the idea of information radius for a measure arising due to concavity property of Shannon's entropy and introduced the Jensen difference in the eqn (53) [33]. All eqns (48~53) can be expressed in terms of entropy.

Table 8. Combinations

| 44. Kumar- <br> Johnson | $d_{K J}=$ |
| :--- | :--- |
| 45. $\operatorname{Avg}\left(L_{1}, L_{\infty}\right)$ | $\left(\frac{\left(P_{i}{ }^{2}-Q_{i}{ }^{2}\right)^{2}}{2\left(P_{i} Q_{i}\right)^{3 / 2}}\right)$ |
|  | $d_{A C C}=\frac{\sum_{i=1}^{d}\left\|P_{i}-Q_{i}\right\|+\max _{i}\left\|P_{i}-Q_{i}\right\|}{2}$ |

Table 8 exhibits distance measures utilizing multiple ideas or measures. Taneja utilized both arithmetic and geometric means came up with the arithmetic and geometric mean divergence in the eqn (54) [36]. Symmetric $\chi^{2}$, arithmetic and geometric mean divergence is given in the eqn (55) [37]. The average of city block and Chebyshev distances in the eqn (56) appears in [9].

| Table 9. Grouping of distance/similarity measures by <br> caveats to implementation |  |  |  |  |
| :--- | :--- | :---: | :---: | :---: |
| Vector <br> Ops | Eqns (1~9), (11~13), (16~19), (21~23), <br> $(26 \sim 40)$, and (56~57) |  |  |  |
| $0 / 0$ | Canberra (10), Wave Hedges (14), Harmonic <br> mean (25), Squared $\chi^{2} \quad(43), \quad$ Probabilistic <br> Symmetric $\chi^{2}(44)$, Divergence (45), Clark (46), <br> and Additive Symmetric $\chi^{2}(47)$ |  |  |  |
| division <br> by zero | Kulczynski (9) (20), Pearson $\chi^{2}(41)$, Neyman <br> $\chi^{2}(42)$, KL (48), Jeffreys (49), Taneja (54), and <br> Kumar-Johnson (55) |  |  |  |
| 0 log0 | KL (48), K divergence (50), Topsøe (51), <br> Jensen-Shannon (52), Jensen difference (53), <br> and Taneja (54) |  |  |  |
| Log of 0 | Jeffreys (49) |  |  |  |

Those readers who wish to implement some distance/similarity measures presented in this section will face some technical problems. Table 9 identifies measures with their caveats to implementation. While most measures can be efficiently computed using simple vector operators, some measures prone to the division by zero and the log of zero cases deserve careful attention. Measures like Canberra belong to the zero divided by zero caveat group. When the divisor becomes zero, the dividend is always zero as well. It should be noted that $0 / 0$ are treated as 0 . Similarly, $0 \log 0$ is treated as 0 as well. For the division by zero and log of zero group cases, the zero is replaced by a very small value.

## III. Hierarchical Clustering on Distance/Similarity Measures

Hitherward, the focus is moved from the syntactic similarity to the semantic similarity between distance/similarity measures. So as to assess how similar distance/similarity measures are, the following experiments were conducted using the cluster analysis. $n$ samples whose values are between 1 and $d$ are randomly selected to build a histogram. Next, each bin is divided by $n$ to produce the pdf. Let $R$ be the set of $r$ number of reference pdfs and $q$ be a query pdf. Then $r$
number of distance values are produced using a certain distance measure $d_{x}\left(r_{i}, q\right)$ for $\forall i . r_{i}$ and $q$ are randomly generated pdfs.

Figure 2 presents the upper triangle matrix of correlation between $d_{x}\left(r_{\mathrm{i}}, q\right)$ and $d_{y}\left(r_{\mathrm{i}}, q\right)$ plots for selected distance or similarity measures where $n=20, b=8$, and $r=30$. Each plot in Figure 2 represents the relation between two distance measures. In order to quantify the correlation between distance/similarity measures, a correlation coefficient measure in the eqn (57) is used.

$$
\begin{gather*}
\operatorname{Corr}\left(d_{x}, d_{y}\right)=\frac{\sum_{i=1}^{r}\left(d_{x}\left(r_{i}, q\right)-\overline{d_{x}}\right)\left(d_{y}\left(r_{i}, q\right)-\overline{d_{y}}\right)}{\sqrt{\sum_{i=1}^{r}\left(d_{x}\left(r_{i}, q\right)-\overline{d_{x}}\right)^{2} \sum_{i=1}^{r}\left(d_{y}\left(r_{i}, q\right)-\overline{d_{y}}\right)^{2}}}  \tag{57}\\
\text { where } \overline{d_{x}}=\frac{\sum_{i=1}^{r} d_{x}\left(r_{i}, q\right)}{r}
\end{gather*}
$$

It indicates the strength and direction of a linear relationship between two distance measures. If the value gets close to 1 , it represents a good fit, i.e., two distance measures are semantically similar. As the fit gets worse, the correlation coefficient approaches zero. When either two distance or two similarity measures are compared, the correlation coefficient is a positive value. When a distance measure and a similarity measure are compared, the correlation coefficient is a negative value e.g., the squared $\chi^{2}$ and probabilistic symmetric $\chi^{2}$ divergences have $d_{S s q C h i}=.5 d_{P r C h i}$ and Corr $\left(d_{S s q C h i}, d_{P r C h i}\right)=1$ whereas Motyka similarity (20) and Sørensen (5) have $s_{M o t}=1$ $-d_{S o r}$ and Corr $\left(s_{M o t}, d_{S o r}\right)=-1$.
To adequately understand the similarities among distance/similarity measures, cluster analysis is adopted. The correlation coefficient is converted into the distance in the eqn (58) to find clusters of distance or similarity measures shown in Figure 3.

$$
\begin{equation*}
d_{D M}\left(d_{x}, d_{y}\right)=1-\left|\operatorname{Corr}\left(d_{x}, d_{y}\right)\right| \tag{58}
\end{equation*}
$$

The dendrogram representing the hierarchical clusters of distance/similarity measures is produced by averaging 30 independent trials of the above experiment. It is built using the agglomerative single linkage with the average clustering method [1]. The vertical scale on the left represents various distance/similarity measures and the horizontal scale represents the closeness between two clusters of distance/similarity measures. The dendrogram provides intuitive groupings of distance/similarity measures. Some distance measures in syntactic groups are interspersed in the semantic groups. Here are a few simple observations.
Observation 1: if two measures are proportional to each other, i.e., $d_{x}=c d_{y}, d_{D M}\left(d_{x}, d_{y}\right)=0$.
Observation 2: if two measures are in distance/similarity relation such that $d_{x}=1-s_{y}$,
$d_{D M}\left(d_{x}, d_{y}\right)=0$.
Observation 3: if two measures are in distance/similarity relation such that $s_{y}=1 / d_{x}, d_{D M}\left(d_{x}, d_{y}\right) \geq 0$. e.g, Kulczynski has $s_{k u l}=1 / d_{k u l}$ and $d_{D M}\left(s_{k u l}, d_{k u l}\right)>0$.

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Fig. 2 Upper triangle matrix of correlation plots between two distance measures.


Fig 3 Dendrogram for pdf distance/similarity measures

Observation 4: Angular based similarity coefficients such as cosine, Jaccard, and Dice are closely related to the Euclidean distance.


It is because histograms are of the same size. As depicted in Figure 4 (a), pdf or histogram space of the same size is only subpart of the entire vector space. The pdf space in the $d$ dimensional vector space is a segmented $d-1$ space which has three corners in Figure 4 (c) case. Figure 4 (b) illustrates the intuitive close relation between the angle and the Euclidean distances.

## IV. CONCLUSION

This article built the edifice of distance/similarity measures by enumerating and categorizing a large variety of distance/similarity measures for comparing nominal type histograms. Grouping aforementioned measures has concentrated upon three general aspects: syntactic similarity, implementation caveats, and semantics. The importance of finding suitable distance/similarity measures cannot be overemphasized. There is a continual demand for better ones.

Table 10. Vicissitude

| Vicis-Wave Hedges | $d_{\text {emanonl }}=\sum_{i=1}^{d} \frac{\left\|P_{i}-Q_{i}\right\|}{\min \left(P_{i}, Q_{i}\right)}$ | (60) |
| :---: | :---: | :---: |
| VicisSymmetric $\chi^{2}$ | $d_{\text {emanon } 2}=\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{\min \left(P_{i}, Q_{i}\right)^{2}}$ | (61) |
| VicisSymmetric $\chi^{2}$ | $d_{\text {emanon } 3}=\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{\min \left(P_{i}, Q_{i}\right)}$ | (62) |
| VicisSymmetric $\chi^{2}$ | $d_{\text {emanon } 4}=\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{\max \left(P_{i}, Q_{i}\right)}$ | (63) |
| max- <br> Symmetric <br> $\chi^{2}$ | $\left(\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{P_{i}}, \sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{Q_{i}}\right)$ | (64) |


| min- |
| :--- |
| symmetric |
| $\chi^{2}$ |$\quad d_{e 6}=\min \left(\sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{P_{i}}, \sum_{i=1}^{d} \frac{\left(P_{i}-Q_{i}\right)^{2}}{Q_{i}}\right)$

Table 10 exhibits a few distance measures that are not in literature. Similar syntactic relationship between Sørensen and Canberra can be applied to Kulczynski which yields the eqn (60). When squared, a new kind of symmetric $\chi^{2}$ divergence can be derived in the eqn (61). Evolving from this point, two symmetric $\chi^{2}$ divergences can be generated given in eqns (62) and (63). They are not the same as using the max and min method to make the $\chi^{2}$ divergence symmetric given in eqns (64) and (65). A large number of new distance/similarity can be relayed by studying the syntactic relations and may be useful in some applications.

## References

[1] Duda, R.O., Hart, P.E., and Stork, D.G., Pattern Classification, $2^{\text {nd }}$ ed. Wiley, 2001
[2] Deza E. and Deza M.M., Dictionary of Distances, Elsevier, 2006
[3] Zezula P., Amato G., Dohnal V., and Batko M., Similarity Search The Metric Space Approach, Springer, 2006
[4] Monev V., Introduction to Similarity Searching in Chemistry, MATCH Commun. Math. Comput. Chem. 51 pp. 7-38, 2004
[5] Gavin D.G., Oswald W.W., Wahl, E.R., and Williams J.W., A statistical approach to evaluating distance metrics and analog assignments for pollen records, Quaternary Research 60, pp 356-367, 2003
[6] S. Cha and S. N. Srihari, On Measuring the Distance between Histograms, in Pattern Recognition, Vol 35/6, pp 1355-1370, June 2002
[7] T. Kailath, The divergence and bhattacharyya distance measures in signal selection, IEEE Trans. Commun. Technol. COM-15 (1) (1967) 52-60.
[8] G.T. Toussaint, Bibliography on estimation of misclassification, IEEE Trans. Inform. Theory 20 (4) (1974) 472-479. pp. 21-24.
[9] Krause E.F., Taxicab Geometry An Adventure in Non-Euclidean Geometry
[10] David M. J. Tax, Robert Duin, and Dick De Ridder (2004). Classification, Parameter Estimation and State Estimation: An Engineering Approach Using MATLAB. John Wiley and Sons.
[11] Looman, J. and Campbell, J.B. (1960) Adaptation of Sorensen's K (1948) for estimating unit affinities in prairie vegetation. Ecology 41 (3): 409416
[12] Sørensen, T. (1948) A method of establishing groups of equal amplitude in plant sociology based on similarity of species and its application to analyses of the vegetation on Danish commons. Biologiske Skrifter / Kongelige Danske Videnskabernes Selskab, 5 (4): 1-34.
[13] Bray J. R., Curtis J. T., 1957. An ordination of the upland forest of the southern Winsconsin. Ecological Monographies, 27, 325-349.
[14] Gower, J.C. General Coefficient of Similarity and Some of Its Properties, Biometrics 27, pp857-874 1971
[15] Gordon, A.D., Classification. $2^{\text {nd }}$ edition London-New York 1999
[16] Hedges, T.S., 1976, "An empirical modication to linear wave theory". Proc. Inst. Civ. Eng. , 61, 575-579.
[17] B. V. K. Vijaya Kumar and L. G. Hassebrook, "Performance measures for correlation filters," Appl. Opt. 29, 2997-3006 (1990).
[18] Jaccard P., Étude comparative de la distribution florale dans une portion des Alpes et des Jura. Bulletin del la Société Vaudoise des Sciences Naturelles 37, 1901, 547-579.
[19] Tanimoto, T.T. (1957) IBM Internal Report 17th Nov. 1957.
[20] Dice, L. R., Measures of the amount of ecologic association between species, Ecology, 26:297-302, 1945
[21] Morisita M. Measuring of interspecific association and similarity between communities. Mem. Fac. Sci. Kyushu Univ. Ser. E (Biol.) 3:65-80, 1959.
[22] Cha, S.-H. and Tappert, C.C., Enhancing Binary Feature Vector Similarity Measures, in Journal of Pattern Recognition Research (JPRR), Vol 1 No 1, 2006, pp 63-77
[23] A. Bhattacharyya, "On a measure of divergence between two statistical populations defined by probability distributions", Bull. Calcutta Math. Soc., vol. 35, pp. 99-109, 1943.
[24] K. Matusita, Decision rules, based on the distance, for problems of fit, two samples, and estimation, Ann. Math. Statist. 26 (1955) 631-640
[25] Pearson, K. On the Criterion that a given system of deviations from the probable in the case of correlated system of variables is such that it can be reasonable supposed to have arisen from random sampling, Phil. Mag.,1900, 50, 157-172.
[26] J. Neyman. Contributions to the theory of the $\$ \backslash c h i^{\wedge} 2 \$$ test. In Proceedings of the First Berkley Symposium on Mathematical Statistics and Probability, 1949.
[27] S. S. DRAGOMIR, J. SUNDE and C. BUSE, New Inequalities for Jeffreys Divergence Measure, Tamsui Oxford Journal of Mathematical Sciences, 16(2)(2000), 295-309.
[28] F. TOPSØE, Some Inequalities for Information Divergence and Related Measures of Discrimination, IEEE Trans. on Inform. Theory, IT46(2000), 1602-1609.
[29] Cox, T.F. and Cox, M.A.A., Multidimensional Scaling, Chapman \& Hall/CRC $2^{\text {nd }} e d .2001$
[30] C.E. Shannon, A mathematical theory of communication, Bell System Tech. J. 27 (1948) 379-423, 623-656.
[31] S. Kullback, R.A. Leibler, On information and sufficiency, Ann. Math. Statist. 22 (1951) 79-86.
[32] JEFFREYS, H. (1946), "An Invariant Form for the Prior Probability in Estimation Problems", Proc. Roy. Soc. Lon., Ser. A, 186, 453-461.
[33] TANEJA. I.J. (2001), Generalized Information Measures and Their Applications, on-line book: www.mtm.ufsc.br/~taneja/book/book.html
[34] Jianhua Lin. 1991. Divergence measures based on the Shannon entropy. IEEE Transactions on Information Theory, 37(1):145-151.
[35] SIBSON, R. (1969), "Information Radius", Z. Wahrs. und verw Geb., 14, 149-160.
[36] TANEJA, I.J. (1995), "New Developments in Generalized Information Measures", Chapter in: Advances in Imaging and Electron Physics, Ed. P.W. Hawkes, 91, 37-135.
[37] Kumar P. and Johnson A., 2005, On a symmetric divergence measure and information inequalities, Journal of Inequalities in pure and applied Mathematics, Vol 6, Issue 3, article 65.

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