Normalised Diffusion Cosine Similarity and Its Use for Image Segmentation

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Abstract: In many image-segmentation algorithms, measuring the distances is a key problem since the distance is often used to decide whether two image points belong to a single or, respectively, to two different image segments. The usual Euclidean distance need not be the best choice. Measuring the distances along the surface that is defined by the image function seems to be more relevant in more complicated images. Geodesic distance, i.e. the shortest path in the corresponding graph, or the \( k \) shortest paths can be regarded as the simplest methods. It might seem that the diffusion distance should provide the properties that are better since all the paths (not only their limited number) are taken into account. In this paper, we firstly show that the diffusion distance has the properties that make it difficult to use it for image segmentation, which extends the recent observations of some other authors. Afterwards, we propose a new measure called normalised diffusion cosine similarity that is more suitable. We present the corresponding theory as well as the experimental results.

1 INTRODUCTION

Measuring the distance is an important problem in clustering and image segmentation. The distance is used as a quantity that makes it possible to decide whether two image pixels belong to one or two different clusters (image segments). The Euclidean distance (i.e. the direct straight-line distance) need not be the best choice. In images, the image points form a certain surface in some space. Measuring the distance along this surface promises better results.

The geodesic distance (Papadimitriou, 1985; Surazhsky et al., 2005) measures the length of the shortest path lying entirely on the surface. The problem is that the geodesic distance can be influenced significantly by relatively small disturbances in image since only one (and "thin") path on the surface determines the distance. In (Eppstein, 1998), the possibility of computing \( k \) shortest paths is discussed. This can be viewed as an attempt to take into consideration the connection that is not thin, but has a certain width, which reduces the influence of disturbances and noise.

The resistance distance is a metric on graphs (Klein and Randić, 1993; Babić et al., 2002). The resistance distance between two vertices of graph is equal to the effective resistance between the corresponding nodes in an equivalent electrical network (regular grid in this case). The resistances of edges in the network increase with the increasing local image contrast. Intuitively, the resistance distance explores all the existing paths between two points whereas the geodesic distance explores only the shortest of them.

It was shown that the resistance distance is equivalent to so called commute-time distance (Fouss et al., 2007; Yen et al., 2007; Qiu and Hancock, 2007) which is the distance based on summing the diffusion distance in time. Diffusion is a process during which a certain substance, e.g. heat or electric charge diffuses from the places of its greater concentration to the places where the concentration is lower. The mathematical description can be built on the diffusion equation (i.e. can be physically based) or on the Markov matrices describing the random walker technique (Grady, 2006). The diffusion maps were systematically introduced in (Nadler et al., 2005; Coifman and Lafon, 2006). Although further papers appear, e.g. (Lipman et al., 2010), almost nothing is reported about successful use of diffusion distance for image segmentation. This can be regarded as surprising since, at a first glance, the method should have the properties that are useful. For measuring every distance, it examines many paths on the image surface.

In this paper, we show that the diffusion distance...
need not be beneficial for measuring distances in image segmentation. The reason is that the influence of different sizes of image segments may overshadow the influence of the edges between them (i.e. the differences in brightness or colour). This finding extends the observations of some other authors that appeared recently (von Luxburg et al., 2014). We introduce a new measure called normalised diffusion cosine similarity in which the mentioned problem is significantly reduced. The computational technique (as well as the time complexity) remains similar as is usually presented for the diffusion distance, i.e. it is based on the spectral decomposition of the Laplacian matrix.

The paper is organised as follows. In the following section, we recall the needed theoretical background. In Section 3, the problems of diffusion distance are explained. The new similarity is introduced in Section 4. Section 5 is devoted to the experimental results. The concluding remarks are given in Section 6.

2 DIFFUSION DISTANCE AND CLUSTERING

The diffusion-based methods are usually formulated by making use of the diffusion equation

\[
\frac{\partial f(t,x)}{\partial t} = \text{div}(g(f(t,x),x)\nabla f(t,x)),
\]

where \( f(t,x) \) is a potential function (e.g. concentration, temperature, charge) evolving in time; \( g(\cdot) \) is a diffusion coefficient (generally, it is a function). In some applications, the coefficient does not depend on \( f(t,x) \). If \( g(\cdot) \) reduces to a constant \( G \), the right-hand side of Eq. (1) reduces to \( G V^2 f(t,x) \). In our context, \( f(t,x) \) has the meaning of evolving image brightness or colour. The process of evolving starts at \( t = 0 \); \( f(0,x) \) is a given input image.

In the discrete case, the problem is formulated in a graph (Sharma et al., 2011). The diffusion properties are represented by edge weights that can be understood as proximity between the neighbouring nodes connected by the corresponding edge. The weights may again be considered evolving in time or constant. In this paper, we follow the latter option. The diffusion equation can now be written in the form of

\[
\frac{\partial \bar{f}(t)}{\partial t} = L \bar{f}(t),
\]

where \( L \) is the Laplacian matrix containing the weights of edges; \( \bar{f}(t) \) is a vector whose entries correspond to the potential in the particular graph nodes, i.e. \( \bar{f}(t) = (f_1(t), \ldots, f_n(t))^T \) (we suppose the graph with \( n \) nodes). The weight, denoted by \( w_{i,j} \), of the edge connecting the nodes \( i \) and \( j \) is often considered according to the formula

\[
w_{i,j} = e^{-|ci,j|^2/2\sigma^2},
\]

where \( ci,j \) denotes the grey-scale or colour contrast between the nodes.

The solution of Eq. (2) can be found in the form of (Sharma et al., 2011)

\[
\bar{f}(t) = H(t) \bar{f}(0),
\]

where \( H(t) \) is a diffusion matrix. The entry \( h_k(p,q) \) of \( H(t) \) expresses the amount of a substance that is transported from the \( q \)-th node into the \( p \)-th node (or vice versa since \( h_k(p,q) = h_k(q,p) \)) during the time interval \([0,t]\). It can be shown that the following formula for \( H(t) \) ensures that Eq. (2) is satisfied

\[
H(t) = \sum_{k=1}^{n} e^{-\lambda_k^2 t} u_{i,k} u_{j,k}^T,
\]

where \( \lambda_k \) and \( u_k \), respectively, stand for the \( k \)-th eigenvalue and the \( k \)-th eigenvector of \( L \). Let \( u_k \) be the \( i \)-th entry of the \( k \)-th eigenvector. For each graph vertex, the vector of new coordinates can be introduced

\[
\bar{x}(t) = (e^{-\lambda_1^2 t} u_{1,1}, \ldots, e^{-\lambda_k^2 t} u_{i,k}, \ldots, e^{-\lambda_n^2 t} u_{n,n}).
\]

If the coordinates are assigned in this way, we call it diffusion map (Coifman and Lafon, 2006; Lafon and Lee, 2006). This vector can be used for clustering the vertices, which will be discussed later. By making use of this vector, the entries of the diffusion matrix can be expressed as the following dot product

\[
\|\bar{x}(t) - \bar{x}(0)\|^2 = \sum_{i=1}^{n} [h_i(p,q) - h_i(i,q)]^2.
\]

The square of diffusion distance is defined as a sum of the squared differences of the concentrations caused by putting the unit concentration into the \( p \)-th node and into the \( q \)-th node, respectively, which corresponds to the formula

\[
d^2(p,q) = \sum_{i=1}^{n} [h_i(p,q) - h_i(i,q)]^2.
\]

After some effort, the following formula can be deduced from Eq. (8)

\[
d^2(p,q) = \|\bar{x}(p) - \bar{x}(q)\|^2,
\]

which shows that introducing the coordinates according to Eq. (6) may be seen as creating a diffusion map, which is a map created in a similar sense as in (Tenenbaum et al., 2000), where the idea was presented that measuring the distance along the data manifold in
some space can be done by transforming the problem into a new space in such a way that the Euclidean distance in the new space is equal to the distance measured on the data manifold in the original space.

Diffusion clustering is based on the idea to use the coordinates introduced in Eq. (6) for clustering the graph nodes, i.e. the image pixels (Nadler et al., 2005; Lafon and Lee, 2006; Huang et al., 2011). The time $t$ can be used to set the level of details that is desired. Often, the $k$-means clustering method is mentioned in this context (Lafon and Lee, 2006; Huang et al., 2011). It is believed that much less than $n$ coordinates are needed in practice.

3 THE PROBLEMS OF DIFFUSION DISTANCE

In this section, we show that the diffusion distance has the properties that make it difficult to use it for image segmentation. We show that the value of diffusion distance between two image points does not necessarily give a good clue whether or not they belong to one image segment. We note that a certain criticism in a similar sense has already been published for the commute-time distance. In (von Luxburg et al., 2014), the authors came to the conclusion that the commute-time distance in graph does not reflect its structure correctly if the graph is large. We continue in this direction and show some further problems that are relevant for image segmentation. We also show that the problems appear not only for the commute-time (resistance) distance, but also for the diffusion distance, i.e. they cannot be avoided by a certain suitable choice of time.

Consider two points, denoted by $p$, $q$, in image. We study two situations (Fig. 1): (i) Both the points are placed in an image containing one rectangular area with a constant brightness; the size of image is $w \times h$ pixels. (ii) The size of image is $w \times h$ pixels again, but the image area is now split by the vertical line into two halves (areas); the brightness is constant inside each area; the difference of brightness between the areas is equal to 1; each of the points is placed in one area. The Euclidean distance between $p$ and $q$ measured in the $xy$ plane is denoted by $a$ (Fig. 1). We traditionally call these situations as "without edge" and "with edge", respectively. Clearly, from the point of view of image segmentation, these two situations are substantially different. In the second case, we expect two image segments and a big distance between $p$ and $q$. In the first case, only one image segment and a small distance between $p$ and $q$ are expected.

A simple theoretical consideration might be used to set the level of details that is desired. With Edge $\sigma=0.4$ With Edge $\sigma=0.5$ With Edge $\sigma=0.6$ With Edge $\sigma=0.7$ Without Edge $\sigma=0.5$

Figure 1: Two points ($p,q$) placed into an image containing a single area (left image) or two areas (right image).

Figure 2: The dependence of diffusion distance on the length of the edge between the areas: The distance (vertical axis) is computed for the problem from Fig. 1 with/without the edge, for $a=15$, and for various values of $t$, $\sigma$, and for the increasing value of $h$ (the length of the edge between the areas); the width of the areas remains constant (the value of $w$). It can be seen that for one value of $t$ and $\sigma$, the value of distance depends on $h$. This is the distance between every two distinct points for obtaining the first intuitive overview. We compute the distance $d_\sigma(p,q)$ by making use of the formula from Eq. (8) for both mentioned cases. If we consider all possible sizes of image (from small to infinitely big) and all possible values of time ($0 \leq t < \infty$), we can easily see that the values of distance vary between 0 and $\sqrt{2}$ in both cases. (We note that the value of $\sqrt{2}$ is the distance between every two distinct points for $t = 0$.) It follows that it is threatening that from the value of diffusion distance itself, it will not be clear whether it was obtained for the case (i) or (ii).

For a more detailed insight, we present the computational simulation of the problem (Fig. 1). Various image sizes, values of time, and various values of $\sigma$ (Eq. (3)) are considered. The results show that the diffusion distance presented in Figs. 2, 3, and 4 between $p$ and $q$ depends on the length of the edge between the areas (Fig. 2), on the size of areas (Fig. 3), and on the distance of points in the $xy$ plane (Fig. 4). Special attention should be paid to the fact that, for some area sizes, it may happen that the diffusion distance between the points lying in one area (case (i)) is greater than in the case if the points lie in two areas (case (ii)). In Fig. 2, for example, we can see that for $t = 100$ and $\sigma = 0.5$, the distance for $(w = 30, h = 11)$ in the case (i) is greater than the distance for $(w = 30, h = 31)$ in the case (ii). As can be seen, the problem increases with the increasing value of $\sigma$. We note that the value of $\sigma$ must be big enough with respect to the noise intensity that is expected.

In image segmentation, the neighbouring segments may be of different sizes, which has not been
that the value of distance does not give the information that is needed for segmentation if we do not have any apriori knowledge about the size of segments or if the sizes may vary.

We also use this test set for evaluating the quality of measuring the distance and for comparing the classical diffusion distance with the new measure that is introduced in the next section. We introduce a discriminative capability of distance measuring method, which is defined by the following formula

\[
D(t) = \frac{\| \mu_e(t) - \mu_w(t) \|}{\sqrt{\sigma_e^2(t) + \sigma_w^2(t)}}, \quad (10)
\]

where \( \mu_e(t) \) and \( \sigma_e^2(t) \) stand for the mean value and variance, respectively, of the distance for the cases without edge. Similarly, \( \mu_w(t), \sigma_w^2(t) \) stand for the corresponding values for the cases with the edge. (We note that the mentioned values are all dependent on time.) The higher is the value of \( D(t) \), the better is the method. The formula in Eq. (10) simply reflects the fact that we would welcome if the distance measured for any case without edge were less than the distance measured for any case with edge. The computational simulation gave \( D(100) = 0.74 \) for the case without noise (Fig. 6). The discriminative capability shows the unsatisfactory behaviour of the classical diffusion distance again. As can be seen, the intervals corresponding to the cases with and without the edge overlap each other, which says again that the diffusion distance cannot distinguish between both cases.

For a certain visual illustration of the behaviour of diffusion distance, we finally present an example in Fig. 7. For a synthetic image with noise, the diffu-
The diffusion distance was computed for $t = 100$. The value of sigma from Eq. (3) was 0.0, 0.6, and 0.075 was added. Gaussian noise with $\sigma_n = 0.075$ was computed and depicted by brightness ($\mu_\sigma = 0.02398, \sigma_\sigma^2 = 0.22 \times 10^{-4}$).

In this section, we propose an improvement that reduces the problems with the diffusion distance that have been mentioned in the previous section. We firstly define our approach. Then we explain why it has been mentioned in the previous section. We compare it with Fig. 4. Further results will be presented in the next section.

For completeness, it should be pointed out that the value of normalised cosine similarity itself tells more clearly whether or not two points are close one to another (i.e. belong to one image segment). No other additional information is needed. The value of 1.0 expresses the maximum possible concordance, decreasing values mean increasing difference. We stress the following properties. The normalised cosine similarity is independent on the length of the edge along which two areas touch (see Fig. 8 and compare it with Fig. 2 for the diffusion distance). The normalised cosine similarity is much less dependent on the total size of area (see Fig. 9 and compare it with Fig. 3). The normalised cosine similarity is more less dependent on the distance between the points in the $xy$ plane (see Fig. 10 and compare it with Fig. 4). Further results will be presented in the next section.

For completeness, it should be pointed out that the idea of using the cosine similarity in a related area is not completely new. In (Brand, 2005), the author mentions the use of cosine similarity in the context of maximizing satisfaction and profit and in connection with the commute-time distance. The author, however, does not present similar analysis (focused on the use in the area of image segmentation) as we do in this paper. Neither he uses the normalisation.

We should now explain why the normalised diffusion cosine similarity is better than the diffusion distance. The reason is simple. The value of normalised cosine similarity itself tells more clearly whether or not two points are close one to another (i.e. belong to one image segment). No other additional information is needed. The value of 1.0 expresses the maximal possible concordance, decreasing values mean increasing difference. We stress the following properties. The normalised cosine similarity is independent on the length of the edge along which two areas touch (see Fig. 8 and compare it with Fig. 2 for the diffusion distance). The normalised cosine similarity is much less dependent on the total size of area (see Fig. 9 and compare it with Fig. 3). The normalised cosine similarity is much less dependent on the distance between the points in the $xy$ plane (see Fig. 10 and compare it with Fig. 4). Further results will be presented in the next section.

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4 NORMALISED DIFFUSION COSINE SIMILARITY

In this section, we propose an improvement that reduces the problems with the diffusion distance that have been mentioned in the previous section. We firstly define our approach. Then we explain why it should be better than the diffusion distance.

For a given image, we introduce the diffusion cosine similarity between $p, q$ at the time $t$ as follows

$$s_t(p,q) = \frac{\langle h_2(p,q) \rangle}{\sqrt{\langle h_2(p,p)\rangle \langle h_2(q,q) \rangle}}.$$  \hfill (11)

By substituting from Eq. (7), it can be easily seen that

$$s_t(p,q) = \frac{\langle \vec{x}_p(t), \vec{x}_q(t) \rangle}{\sqrt{\langle \vec{x}_p(t), \vec{x}_p(t) \rangle \langle \vec{x}_q(t), \vec{x}_q(t) \rangle}} = \frac{\langle \vec{x}_p(t), \vec{x}_q(t) \rangle}{\|\vec{x}_p(t)\| \|\vec{x}_q(t)\|}.$$  \hfill (12)

The value of $s_t(p,q)$ is equal to the value of the cosine of the angle between the vectors $\vec{x}_p(t)$ and $\vec{x}_q(t)$. Since the value of $h_t(p,q)$ is always non-negative, the value of $s_t(p,q)$ varies in the range of $[0, 1]$.

To obtain a normalised cosine similarity, we evaluate the diffusion cosine similarity two times. Firstly, for a given image. Secondly, for the corresponding reference image, which is the image of the same size as is the given input image, but with a constant brightness everywhere. The normalised cosine similarity is now the ratio between the similarity in the given image and the similarity in the reference image. We note that this ratio is only computed if the similarity in the reference image is not close to zero. Otherwise, the normalised cosine similarity is set to zero too, which means that it cannot be computed reliably. Since the diffusion cosine similarity in the given image is not greater than the similarity in the reference image, the maximal possible value of the normalised diffusion cosine similarity is 1.

5 EXPERIMENTAL RESULTS

We start with the tests using the synthetic images. Then the tests with the real-life images are also pre-
Figure 8: The dependency of normalised diffusion cosine similarity on the length of the edge between the areas: The similarity (vertical axis) is computed for the problem from Fig. 1 with/without the edge, for $a = 15$, and for various values of $t$, $\sigma$, and for the increasing length of the edge between the areas (the value of $h$); the width of areas remains constant. In contrast to the diffusion distance, the new similarity does not depend on the edge length in this test environment (compare with Fig. 2).

Figure 9: The dependency of normalised diffusion cosine similarity on the area size: The similarity (vertical axis) is computed for the problem from Fig. 1 with/without the edge, for $a = 15$, and for various values of $t$, $\sigma$, and for the increasing length of the edge between the areas and for the increasing width of the areas ($w$ and $h$ are changing). The dependence of similarity on the area size is much smaller than in the case of diffusion distance (Fig. 3).

As a first experiment, we evaluate the discriminative capability introduced in Eq. (10) based on computing the distance or similarity in various area configurations (Fig. 5). For the diffusion distance, the results have already been presented in Fig. 6. For the new method, the values are stated in Fig. 11. Notice that the intervals into which the values of normalised diffusion cosine similarity fall for the cases with and without the edge, respectively, do not overlap, which makes the discriminative capability very good.

Naturally, the behaviour of every method is also important in the presence of noise. We carried out the same test for the noisy images too. Gaussian noise was added to all test images (Fig 5). For each test image, 1000 samples were used in simulation (see Fig. 12 for further details). Even with a relatively big amount of noise, the results of the new method were better (Fig. 12) than the results obtained for the diffusion distance without noise.

As a further example, we also present the result for the image from Fig. 7. The normalised diffusion cosine similarity is depicted in Fig. 13. The similarity is measured between the image center point and all remaining pixels and is depicted as brightness. Since big similarity corresponds to a small distance, we also present an inverse image for more convenient comparison with the result for diffusion distance (Fig. 7). Although we do not present any quantitative evaluation in this case, we believe that the result of the new similarity may be regarded as visually better (Fig. 13).

In the rest of this section, we focus on the real-life images and their seeded (interactive) segmentation (Sinop and Grady, 2007). For this purpose, the similarity (proximity) between the pixel and area should be defined. Let $\sum_{i \in Q} l_i$ (collection) stand for the sum of the biggest $Q$ elements from a collection of real numbers. The normalised diffusion cosine proximity, denoted by $\tilde{s}_i(p, A)$, between a point $p$ and an area $A$...
can be introduced by the formula

\[
\hat{s}_t(p, A) = \frac{1}{Q} \sum_{q \in A} \{\hat{s}_t(p, q)\} \in A. \tag{13}
\]

The formula simply reflects the fact that \( p \) and \( A \) may be regarded as close if at least a certain number of points exist in \( A \) that are close to \( p \). The formula can also be easily adapted for the diffusion distance (instead of the \( Q \) points with the biggest similarities, \( Q \) points with the smallest distances are considered).

We note that the segmentation algorithm itself is not the direct focus of our work, i.e. we do not propose a new algorithm. Instead, by making use of a certain algorithm, we demonstrate the properties of the new similarity measure that might be useful in various known or future algorithms based on measuring the distance or similarity. The algorithm used for testing should make it possible to present the properties of the new measure clearly; understanding the results should not be made more difficult due to the properties of algorithm. For this reason, we use the simple one-step seeded segmentation.

The seeds of the objects and the background are defined manually. Once it is done, the distance to the seeds is computed for all remaining image pixels. If the distance of a pixel is lower to the object seed than to the background seed, the pixel is marked as an object pixel. Otherwise, it is marked as a background pixel. The algorithm can be easily adapted for the use of similarity instead of distance.

Several real-life images from the Berkeley Segmentation Dataset (Martin et al., 2001) were used (Fig. 14) and processed as follows. The conversion to greyscale was carried out, which was followed by the normalisation of intensity values into the interval \([0, 1]\). The normalised images were slightly filtered by making use of anisotropic diffusion filtering; the filtered images used for further processing are shown in Fig. 14 too. For all images, we used \( \sigma = 0.07 \) (Eq. 3), \( t = 150 \), \( Q = 10 \), and 750 eigenvectors. The size of images was \( 160 \times 240 \) pixels. The suitable values of \( t \) and \( Q \) were determined experimentally on the basis of visual evaluation of the results. For the diffusion distance as well as for the new similarity, the best results were obtained for \( 100 \leq t \leq 200 \), \( 4 \leq Q \leq 50 \). The results of the segmentation using the new normalised diffusion cosine similarity, the diffusion distance, and the cosine similarity mentioned in (Brand, 2005) are shown in Fig. 14. It can be seen that the new similarity gives visually better results than the remaining mentioned measures. Naturally, all the results could be improved by modifying the position of the seeds. However, we did not do so since we wanted to show the properties of the distance/similarity measures clearly.

Finally, we note that we did not aim at comparing the above segmentation algorithms with all other main state-of-the-art approaches. Instead, we used them to show that the theoretical findings and expectations presented before are correct and useful for the practice (see the conclusion for the discussion about our main goals and contributions).

\section{6 CONCLUSIONS}

Measuring the distances along the surface that is defined by the image function seems to be useful in more complicated situations. The use of geodesic distance is often mentioned in this context, but its disadvantages are known. One would intuitively say that the diffusion distance should have good properties for the mentioned purpose. We showed (including the computational simulations of the situations that are important for segmentation) that the diffusion distance need not be useful since the presence of edges may be overshadowed by the varying size of image segments (and the size is not often known in advance). We proposed a new measure called \textit{normalised diffusion cosine similarity} that suffers from these problems to a much lesser extent. We have also demonstrated that it can be used in image segmentation algorithms.

We believe that the geodesic distance and diffusion distance (resistance or commute-time distance) are two opposite approaches. While the geodesic distance only searches for the shortest path between the points, the diffusion distance takes into account all possible paths. The idea of simultaneously examining more paths seems to be generally useful. The question, however, remains how it should be exactly done. The diffusion distance does not seem to be the best solution. We believe that a certain gap exists in this area and that the corresponding efficient methods will probably be developed in the future. We intended this paper as a certain step in this direction rather than a paper proposing a new segmentation method for ev-
Figure 14: One-step seeded segmentation: The source images (the first row); the seeds for the objects and the background (the second row); the filtered images that were used for further processing (the third row); the normalised diffusion cosine similarity of pixels to the object seeds, the bright areas correspond to a high similarity (the fourth row); the objects extracted by making use of the new similarity (the fifth row); the diffusion distance from the object seeds, the dark areas correspond to a small distance (the sixth row); the objects extracted by making use of the cosine similarity mentioned in (Brand, 2005) (the last row).

As for everyday use. That is why we did not aim at comparing the algorithm mentioned in the previous section with various other state-of-the-art algorithms. The goal was to show that some alternatives exist in the area of the diffusion-like distances that may have a chance to be developed into useful and practical tools. We hope that introducing the new normalised diffusion cosine similarity can be regarded as a step in this direction.

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