Improved Laplacian Eigenmaps

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ABSTRACT

This paper presents an improvement to the Laplacian Eigenmaps technique for manifold learning. The Laplace-Beltrami operator on a Riemannian manifold is re-investigated and a discretization scheme based on the theory of Riemannian integration is proposed. The result is a more accurate analogue of the continuous operator for graphs, which by comparison, outperforms the previously reported operators in extracting the structure of the data. The proposed method, similar to Laplacian Eigenmaps, preserves both the local and global structures of the data.

Keywords

Dimensionality reduction, Laplace-Beltrami operator, manifold learning.

1. INTRODUCTION

In many practical machine perception problems, the sensory data belong to a high dimensional space. For instance in machine vision, a 40× 40 gray-scale image can be thought of as a point in a 1600-dimensional Euclidean space, whose components along the axes are the gray-scale values of different pixels. The question is: *May all points in this space be considered as valid sensory data?* A randomly selected point in our example, is nothing but salt-and-pepper noise. As a matter of fact the set of all images that belong to our context are rare events when considered as outcomes of a random selection in the high dimensional space. Mathematically speaking the set of data points which are outcomes of the sensing, have a singular distribution. This means that they do not fill the whole input space, but lie on a lower dimensional manifold, embedded in the high dimensional Euclidean space.

Given a set of data instances which belong to a low dimensional manifold, embedded in a high dimensional Euclidean space, manifold learning seeks to find a possibly global coordinate system on the manifold and represent the data instances in this coordinate system. For example if the data instances are a set of images taken from an apple, in which the distance from the camera to the apple is constant, and the camera is aimed at the apple, the images differ by the two angles the camera can take while moving on a sphere. It is natural to expect that the images belong to an embedded sphere. Manifold learning seeks to find a low dimensional representation of this sphere. From this point of view, manifold learning is a *concept abstraction* tool.

A growing interest in research on manifold learning has been witnessed during the past few years. Tenenbaum et al. [6] proposed a method based on approximating the geodesic distances between data points by the length of the shortest path connecting the points on the proximity graph. This method acts well for isometrically embedded manifolds where the geodesic distances can be identified as the Euclidean distances of the points in their low dimensional representation. The method is named after this fact, ISOMAP. Later the authors extended their method to conformally embedded manifolds under some assumptions [7]. Although ISOMAP preserves the global properties of the manifold, it is restricted to manifolds very similar to Euclidian spaces. It cannot handle a surface with a hole for instance.

Another method proposed by Roweis and Saul [5] is Locally Linear Embedding (LLE). The key idea in this method is that every smooth manifold is locally similar (mathematically speaking diffeomorphic) to a Eucledian space. By dividing the manifold into patches and realigning these patches one would expect to get a flat manifold, or a lower dimensional Euclidean space. LLE accomplishes this by preserving the local relative geometry of the data points, while representing them in a lower dimensional space. This method is local and fails to code the global properties of the manifold.

Belkin and Niyogi [1, 2] have recently proposed a third method based on advanced topics from differential geometry. Laplacian Eigenmaps, as it is called, uses the eigenfunctions of the Laplacian-Beltrami operator on the manifold, as its natural global coordinates. A discretized version is used to deal with the fact that the data are sampled from the manifold. The important feature of these eigenfunctions is that they code the topological properties of the manifold, such as its De Rham cohomology, and as a result are able to handle manifolds with holes globally.

In this paper we propose a more accurate method for discretization of the Laplace-Beltrami operator and derivation of the graph Laplacian based on the theory of Riemannian integration. The operator is applied to a number of artificial and real data sets. Superior results to previously proposed methods have been obtained, where both the local and global properties of the manifold are preserved in the low dimensional representation.

The rest of this paper is organized as follows. In Section 2 we will introduce the Laplace-Beltrami operator on compact Riemannian manifolds. In Section 3 Laplacian eigenmaps is reviewed. The proposed method for defining the graph Laplacian is presented in Section 4. Section 5 is devoted to the algorithm outline and some examples. We conclude the paper in Section 6.

2. THE LAPLACE-BELTRAMI OPERATOR ON RIEMANNIAN MANIFOLDS

Let $\mathcal{M}$ be a compact m-dimensional Riemannian manifold embedded in R^n .Assume that the Riemannian metric on $\mathcal{M}$ is the one induced by the standard Riemannian metric on R^n . The Laplace-Beltrami operator on $\mathcal{M}$ is a second order differential operator defined on $C^\infty(\mathcal{M})$, i.e. the set of continuously differentiable real-valued functions defined on $\mathcal{M}$:

$$L : C^{\infty}(M) \to C^{\infty}(M), \tag{1}$$

$$L : f(.) \to -\mathrm{div}\nabla f(.). \tag{2}$$

A continuous real-valued function on $\mathcal{M}$ can be thought of as a function assigning a global coordinate to each point of the manifold. We look for a coordinate function, for which the points which are close on the manifold, have close coordinate values. Such a function presents an optimal 1-dimensional embedding of $\mathcal{M}$, as it preserves the local properties.

Assume that x is a point on $\mathcal{M}$ and $x+\delta x$ is a point in its vicinity. Assume that $f : M \to R$ is a coordinate function for the points on $\mathcal{M}$. The difference in coordinate values of x and $x+\delta x$ can be approximated by

$$\left|f(x+\delta x) - f(x)\right| \approx \left\|\nabla f\right\| \left\|\delta x\right\|, \tag{3}$$

where ∇f is the gradient of *f*. Hence if $\left\|\nabla f\right\|$ is small, neighboring points will have close coordinate values. An optimal coordinate function can thus be sought by solving

$$\arg\min_{f \quad \|f\|_{L^2(M)}=1} \int_M \left\|\nabla f\right\|^2. \tag{4}$$

The restriction has been imposed on the integral of $\left|f\right|^2$ to normalize the function.

To solve the optimization problem, we note that by Stoke's theorem, −div and ∇ are adjoint operators, i.e. for a real-valued function f and a vector field A defined on $\mathcal{M}$

$$\int_M \left\langle A, \nabla f \right\rangle = \int_M -div(A) f. \tag{5}$$

We can apply this identity to (4) and obtain the following optimization problem,

$$\arg\min_{f \quad \|f\|_{L^2(M)}=1} \int_M L(f) f. \tag{6}$$

It can be shown that the Laplace-Beltrami operator is a self-adjoint positive semidefinite operator [4]. Therefore the solution to the above optimization problem exists, and the function which minimizes $\int_M \left\|\nabla f\right\|^2$ is an eigenfunction of L corresponding to its minimum eigenvalue.

Another important property of the Lapalce-Beltrami operator on *compact* manifolds is that it has a discrete spectrum [4]. This, together with the fact that all eigenvalues are nonnegative enables us to sort them in ascending order. The operator always has an eigenvalue of zero which corresponds to the constant function on the manifold. For connected manifolds, it can be shown that this is the only eigenfunction with a zero eigenvalue [2]. The next eigenfunction provides the global coordinate map we were seeking.

An embedding of a higher dimension can similarly be sought. The details for the discrete case are presented by Belkin and Niyogi [1]. In this case the eigenfunctions corresponding to the smallest nonzero eigenvalues are selected as the coordinates of the points in the embedding.

3. LAPLACIAN EIGENMAPS

In this section we review Laplacian Eigenmaps as proposed by Belkin and Niyogi [1, 2]. An expression for computing the Laplacian of a function at a point can be derived by studying the equation of heat diffusion. If $f : M \to R$ is the initial temperature distribution on $\mathcal{M}$ and $u(x,t)$ is the temperature distribution at time *t*, the PDE that governs the heat diffusion in $\mathcal{M}$ can be written as

$$\frac{\partial u}{\partial t} = Lu. \tag{7}$$

The solution to this equation is given by $u(x,t) = \int_M H_t(x,y) f(y)$ where H_t is the heat kernel (the Green's function for this PDE). The heat kernel can be approximated locally by

$$H_t(x,y) \approx (4\pi t)^{-m/2} \exp\left(-\frac{\left\|x-y\right\|^2}{4t}\right), \tag{8}$$

where it is assumed that $\left\|x-y\right\|$ and *t* are sufficiently small and m is the dimension of $\mathcal{M}$. Therefore $Lf(x)$ can be written as

$$\begin{aligned} Lf(x) &= \left.\frac{\partial u}{\partial t}\right|_{t=0} \\ &= \frac{\partial}{\partial t}\int_M (4\pi t)^{-m/2} \exp\left(-\frac{\left\|x-y\right\|^2}{4t}\right) f(y) dy \end{aligned}, \tag{9}$$

and can be approximated by

$$Lf(x) = -\frac{1}{t}\left(f(x) - (4\pi t)^{-m/2}\int_M \exp\left(-\frac{\left\|x-y\right\|^2}{4t}\right) f(y) dy\right). \tag{10}$$

In manifold learning applications rather than a complete description of the manifold on which the data lie, one is faced with a set of sample points belonging to this manifold. Let these points be denoted by $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ where $\mathbf{x}_i \in R^n$. The points are assumed to lie on a manifold $\mathcal{M}$ of dimension *m*. Belkin and Niyogi [1, 2] have proposed the following scheme for discretization of the Laplace-Beltrami operator, to give the graph Laplacian:

$$\begin{aligned} Lf(\mathbf{x}_i) \approx -\frac{1}{t}\Bigg[& f(\mathbf{x}_i) \\ & -\frac{1}{k}(4\pi t)^{-m/2} \sum_{\substack{\mathbf{x}_j \\ 0<\left\|\mathbf{x}_j-\mathbf{x}_i\right\|<\varepsilon}} \exp\left(-\frac{\left\|\mathbf{x}_i-\mathbf{x}_j\right\|^2}{4t}\right) f(\mathbf{x}_j) \Bigg] \end{aligned}. \tag{11}$$

A number of points about the last equation are in order. First note the linearity in $f(\mathbf{x}_j)$, which makes it possible to represent the graph Laplacian by a matrix. Next note that the coefficient $1/t$ is global, and acts as a scaling factor. It does not affect the eigenfunctions of the operator and can be neglected if one is only interested in the eigenfunctions. Also note that for

each $\mathbf{x}_i$ the summation is taken over $\mathbf{x}_j$'s which are in an ϵ-neighborhood of the point. This is due to the fact that when $t \to 0$ the exponential function decays very fast and the far-away points can be neglected to yield a sparse matrix which facilitates numerical calculations. And finally it seems that the dimension of $\mathcal{M}$ must be known to calculate the coefficient $(4\pi t)^{-m/2}$. But this coefficient scales $f(\mathbf{x}_i)$ i.e. the value of the function at the point where the Laplacian is being calculated, with respect to $f(\mathbf{x}_j)$, i.e. the value of the function at neighboring points. As mentioned before, the constant function is always an eigenfunction of the Laplace-Beltrami operator with an eigenvalue of zero. By artificially requiring the constant function to be an eigenfunction of the graph Laplacian with an eigenvalue of zero, one can dispose of this coefficient.

Summing up, the graph Laplacian can be defined as the matrix $L = D - W$ where

$$W_{ij} = \begin{cases} \exp\left(-\dfrac{\left\|\mathbf{x}_i - \mathbf{x}_j\right\|^2}{4t}\right) & \text{if } \left\|\mathbf{x}_i - \mathbf{x}_j\right\| < \varepsilon \\ 0 & \text{otherwise,} \end{cases} \tag{12}$$

and D is a diagonal matrix defined as

$$D_{ii} = \sum_j W_{ji} \,. \tag{13}$$

The Laplacian of a real-valued function defined at $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ is then given by

$$\begin{bmatrix} Lf(\mathbf{x}_1) \\ \vdots \\ Lf(\mathbf{x}_k) \end{bmatrix} = L \begin{bmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_k) \end{bmatrix}. \tag{14}$$

4. PROPOSED METHOD: IMPROVED LAPLACIAN EIGENMAPS

In this section, we propose a more accurate discretization scheme for (10). First we review integration by Riemann sums from Edwards [3]. A closed interval in R^n is a set $I = I_1 \times I_2 \times \cdots \times I_n$, where $I_j = [a_j, b_j] \subset R$, $j = 1, \ldots, n$. The volume of I is, by definition, $v(I) = (b_1 - a_1)(b_2 - a_2)\cdots(b_n - a_n)$. Assume that Q is an interval in R^n. A *partition* of the interval Q is a collection $P = \{Q_1, Q_2, \ldots, Q_k\}$ of closed intervals, with disjoint interiors, such that $Q = \bigcup_{i=1}^{k} Q_i$. By the *mesh* of P we are referring to the maximum of the diameters of the Q_i. A *selection* for P is a set $S = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$ of points such that $\mathbf{x}_i \in Q_i$ for each i. If $f : R^n \to R$ is a function such that $f = 0$ outside of Q, then the Riemann sum for f corresponding to the partition P and selection S is

$$R(f, P, S) = \sum_{i=1}^{k} f(\mathbf{x}_i) v(Q_i) \,. \tag{15}$$

Theorem 3.4 from Edwards [3] then reads:

Theorem.(*Edwards*) *Suppose* $f : R^n \to R$ *is bounded and vanishes outside the interval Q. Then f is integrable with* $\int f = A$ *iff, given ε > 0, there exists δ >0 such that*

$$\left|A - R(f, P, S)\right| < \varepsilon \tag{16}$$

whenever P is a partition of Q with mesh < δ and S is a selection for P.

The theorem actually says that if f is integrable, we can approximate its integral by its Riemann sum and the accuracy of the approximation increases as the intervals become smaller.

In the case of manifold learning, we are dealing with general Riemannian manifolds, and not the Euclidian R^n. Nevertheless, we do not see the need to go into the mathematical technicalities of dealing with a general metric. As noted before we assume that the Riemannian metric on $\mathcal{M}$ is the one induced by the standard Riemannian metric on R^n.

We now turn our attention to the problem of discretization of the Laplace-Beltrami operator as given by (10) and the derivation of the graph Laplacian. (For convenience we have repeated the equation here.)

$$Lf(x) = -\frac{1}{t}\left(f(x) - (4\pi t)^{-m/2} \int_M \exp\left(-\frac{\|x - y\|^2}{4t}\right) f(y) dy \right). \tag{17}$$

As stated before in manifold learning applications rather than a complete description of the manifold on which the data lie, one is faced with a set of sample points belonging to this manifold. Let these points be denoted by $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ where $\mathbf{x}_i \in R^n$. The points are assumed to lie on the manifold $\mathcal{M}$ which has dimension m. These points are in essence a selection S based on which we would like to approximate the integral in (17). As can be seen from (15) the value of the integrand at these points is not enough for the formation of the Riemann sum. Rather the volume (or measure) of the interval (or patch) from which the selection was made is also necessary. Therefore the measure of these patches must be approximated.

We note that there exists a fundamental difference between numerical integration of a function f on a manifold $\mathcal{M}$ and approximating this integral from samples of f. In the former case, one is able to freely partition the manifold, make a selection and then calculate the numerical sum (15) to get an approximation of the integral. In the latter case, the only available information is the selection, i.e. a set of points $\mathbf{x}_i$ and the value of f at these points. In this case one has to build the partition for numerical integration a posteriori (Fig. 1).

Here we propose a method for approximating the measure of Q_i in (15). By κ_i, $i = 1, \ldots, k$ we denote the number of points $\mathbf{x}_j$ in an ϵ-neighborhood of $\mathbf{x}_i$. Therefore in a ball of volume

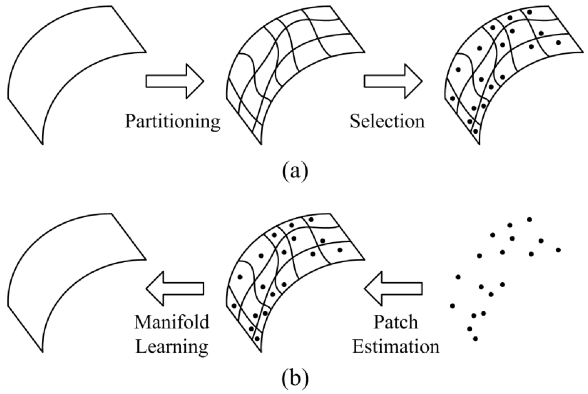

Figure 1. A comparison of (a) numerical integration and (b) integration from samples

$\alpha_n \varepsilon^n$ centered at $\mathbf{x}_i$ there exist κ_i points.[1] We would like to choose a ball around $\mathbf{x}_i$ such that it contains only one point, namely $\mathbf{x}_i$. So it is natural to choose the volume of such a ball as

$$v_i = \frac{\alpha_n \varepsilon^n}{\kappa_i}. \tag{18}$$

Due to the fact that the metric we have chosen on $\mathcal{M}$ is the one induced by the standard Riemannian metric on R^n, the measure of Q_i can be approximated by the area of the intersection of this ball with $\mathcal{M}$, i.e.

$$v(Q_i) = \frac{\alpha_m \varepsilon^m}{\kappa_i}. \tag{19}$$

One should easily identify this measure as the inverse of the empirical approximation to the a posteriori pdf of points on the manifold.

A more precise approximation of (17) can thus be made by the use of (19). Formation of the Riemann sum of (17) by the use (19) yields

$$Lf(\mathbf{x}_i) \approx -\frac{1}{t}\left[f(\mathbf{x}_i) - \frac{(4\pi t)^{-m/2}}{\alpha_m \varepsilon^m} \sum_{\substack{\mathbf{x}_j \\ 0<\|\mathbf{x}_j-\mathbf{x}_i\|<\varepsilon}} \exp\left(-\frac{\|\mathbf{x}_i-\mathbf{x}_j\|^2}{4t}\right)\frac{f(\mathbf{x}_j)}{\kappa_j}\right]. \tag{20}$$

The graph Laplacian can now be modified to take into account the effect of κ_j. The W matrix is defined as

$$W_{ij} = \begin{cases} \frac{1}{\kappa_j}\exp\left(-\frac{\|\mathbf{x}_i-\mathbf{x}_j\|^2}{4t}\right) & \text{if } \|\mathbf{x}_i-\mathbf{x}_j\|<\varepsilon \\ 0 & \text{otherwise,} \end{cases} \tag{21}$$

and D and L are as before

$$D_{ii} = \sum_j W_{ij} \quad \text{and} \quad L = W - D. \tag{22}$$

A comparison of (21) and (12) reveals that in improved Laplacian eigenmaps, the columns of W are weighted by $1/\kappa_j$, where κ_j is proportional to the local density of points around the j^{th} data point. This factor compensates for the nonuniform distribution of data on the manifold. Hence the proposed method extracts the structure of the manifold regardless of this distribution.

5. CASE STUDIES

5.1 Implementation

The algorithm for implementation of improved Laplacian eigenmaps is the same as that for Laplacian eigenmaps and is outlined here for convenience [1]. Given k points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ in R^n the following steps are taken:

1. (constructing the Proximity Graph) The neighboring points $\mathbf{x}_j$ of each data point $\mathbf{x}_i$ are determined. These are the points which satisfy
$$0 < \|\mathbf{x}_j - \mathbf{x}_i\| < \varepsilon. \tag{23}$$
The number of these points is denoted by κ_i.

2. (Determining the Laplacian) The weight matrix of the proximity graph is determined from (21) and the graph Laplacian from (22).

3. (Finding the Eigenmaps) The eigenvalues and eigenvectors of L are found
$$L\mathbf{y} = \lambda\mathbf{y}. \tag{24}$$
The eigenvalues are sorted in ascending order
$$0 = \lambda_0 \le \lambda_1 \le \cdots \le \lambda_{k-1}. \tag{25}$$

4. (Embedding) The optimal representation of $\mathbf{x}_i$ when embedded in R^m is then given by
$$[\mathbf{y}_1(i), \ldots, \mathbf{y}_m(i)]^T, \tag{26}$$
where $\mathbf{y}_j$ is the eigenvector corresponding to eigenvalue λ_j, and $\mathbf{y}_j(i)$ is its i^{th} component.

In the following subsections we present the results of application of this algorithm to a number of artificial as well as a real-world data set.

5.2 Case Study: Artificially Generated Data Sets

Improved Laplacian eigenmaps has been applied to a number of artificially generated data sets and a comparison is made between this method and the weighted Laplacian eigenmaps as presented in [1] and the Laplacian eigenmaps as presented in [2]. Figure 2

[1] The coefficient α_n is actually equal to $\pi^{n/2}/\Gamma(1+n/2)$.

summarizes the results. In column (a) the original data is depicted. The points in the rows from top to bottom are sampled respectively from a circle, an eight shape, a disc, a ring, a square, a sphere, and a cylinder. Depicted in columns (b), (c) and (d) are the results of the retrieval of each manifold from its sample points using weighted Laplacian eigenmaps [1], Laplacian eigenmaps [2], and improved Laplacian eigenmaps respectively. Although the first two methods are able to preserve the structure of the manifold, deformations are present in the retrieved manifolds. Improved Laplacian eigenmaps on the other hand avoids these deformations.

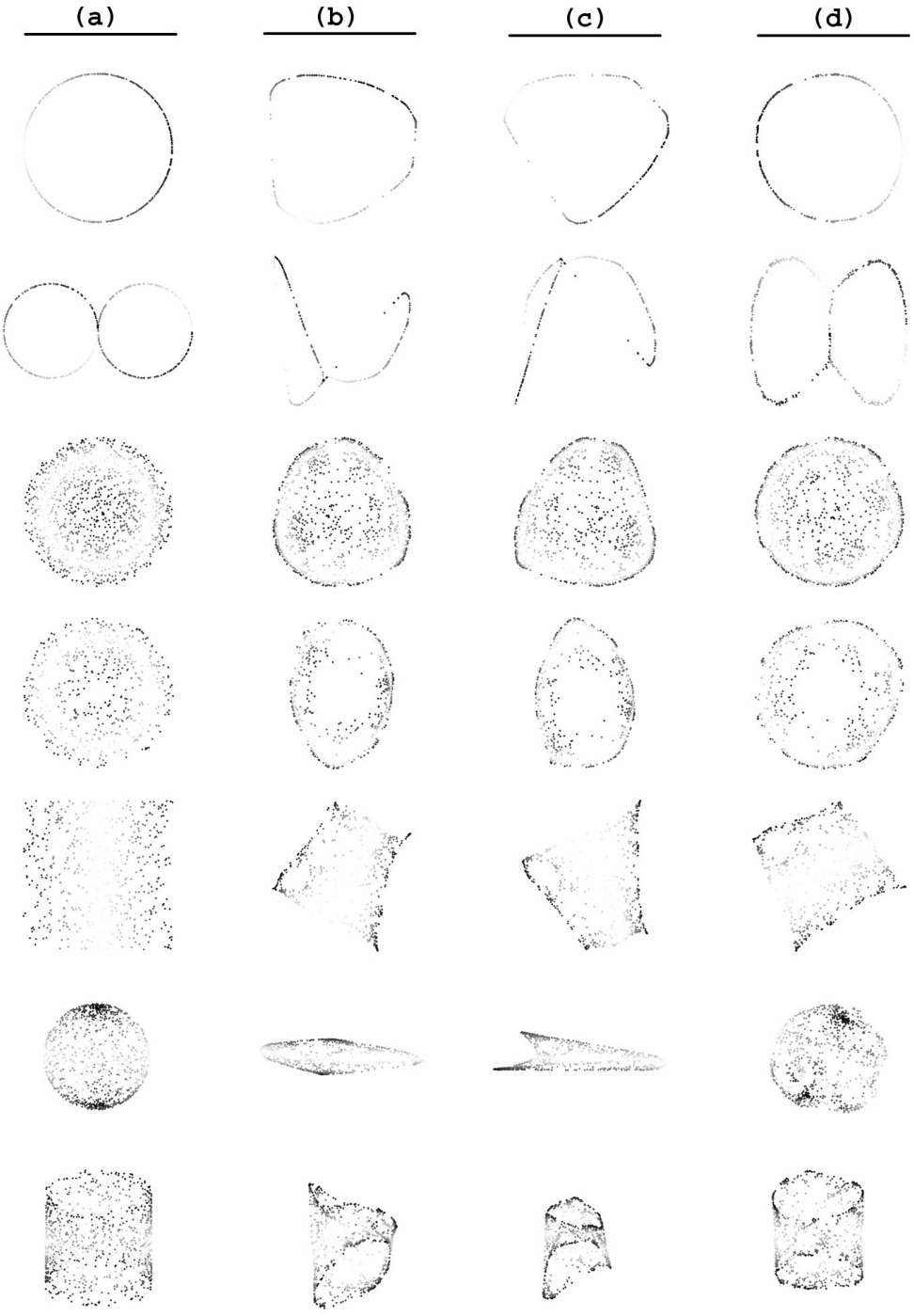

Figure 2. A comparison of (b) Laplacian eigenmaps, (c) weighted Laplacian eigenmaps, and (d) improved Laplacian eigenmaps. Column (a) represents the original data, while the other columns are the embeddings found by the three methods

5.3 Case Study: Real-World Data Set

The proposed method has been applied to a data set of 2000, 40× 40 gray-scale images as used in Verbeek et al. [8]. The images contain two degrees of variation in the pose of the face; The head turns from left to right, and from up to down. The data was first mapped to a 100-dimensional space using PCA, and improved Laplacian eigenmaps was applied. We shall note on the use of PCA in the last section. The results are depicted in Figure 3. Part (a) shows the two dimensional embedding found. Different regions of (a) have been magnified and shown in (b)–(f). In (b)–(e) every other 10^{th} point has been labelled by its corresponding image. In (f) the labelling is done for every other 50^{th} point. Part (g) shows different regions of the retrieved manifold for reference. Part (h) is the three dimensional embedding found.

As can be seen the retrieved manifold is essentially two dimensional, which is consistent with our expectation; When we move from region (1) to (2) the head turns from right to left, and from region (3) to (4) then to (5) the head turns down and up again. Nevertheless, the folding in region 5 makes it impossible to embed the manifold in two dimensions, and a three dimensional ambient space as in (h) is required. The effect is seen in (f) where the right and left poses of the face interchange their places.

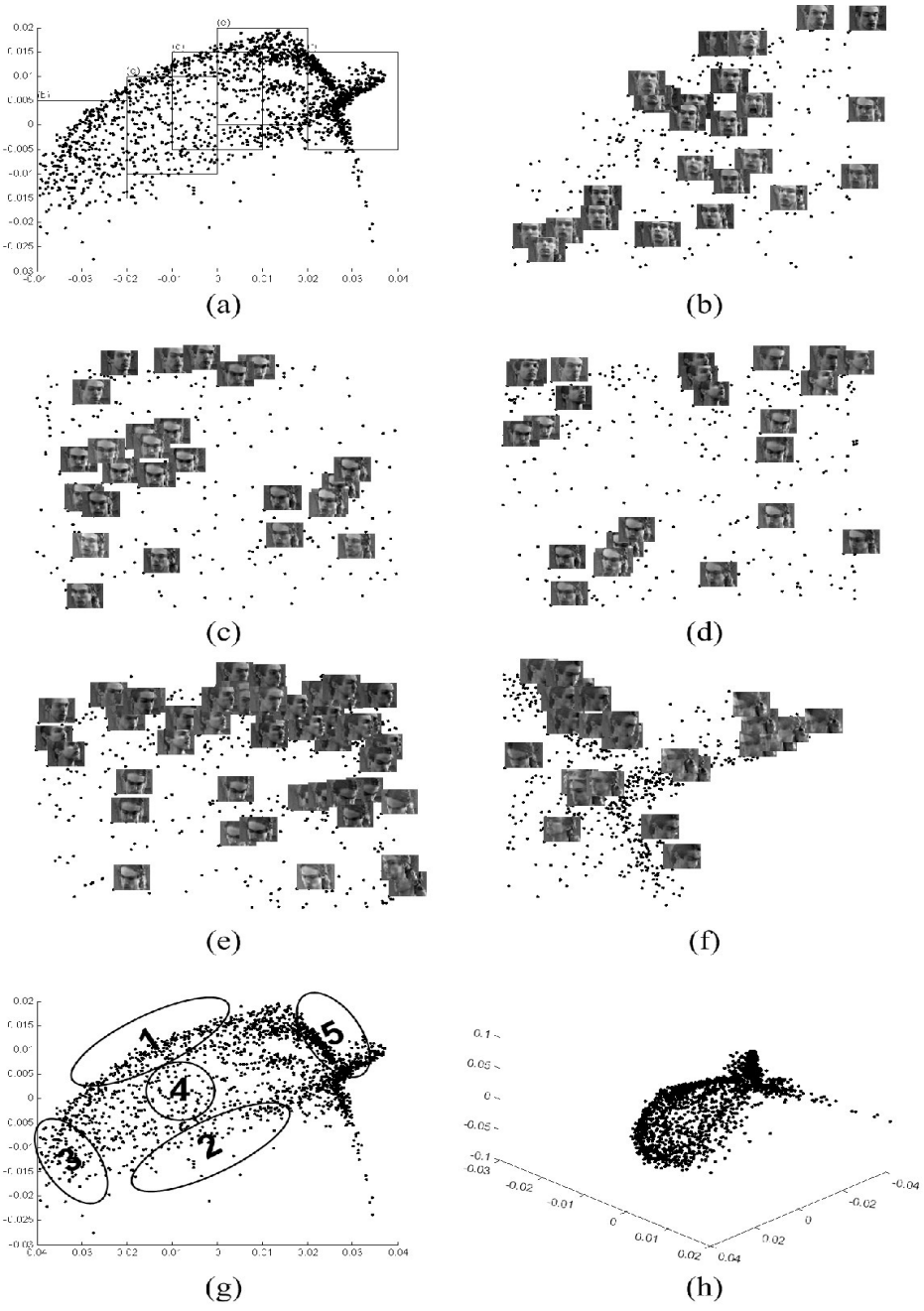

Figure 3. Face image data set (a) two dimensional embedding (b)-(f) different regions of *(a)* zoomed in and labeled by images (g) regions of the manifold numbered for reference (h) three dimensional embedding

6. CONCLUSION AND FUTURE WORK

We have proposed a more accurate method for discretization of the Laplace-Beltrami operator on Riemannian manifolds. This was accomplished by weighting the integrand by the inverse of the empirical distribution of points on the manifold. When the points are selected from a nonuniform pdf on the manifold, this method compensates for the nonuniformity and retrieves the structure of the manifold, independent of the distribution of points. When the points are selected from a uniform pdf, still the posterior distribution of points on the manifold is nonuniform, and the method should be applied to compensate this nonuniformity.

The method was applied to a number of artificially generated data sets and its superiority was demonstrated by a comparison with previously proposed methods. A real-world set of images was also studied and the data were mapped to a two dimensional manifold embedded in a three dimensional space. In this case the data were first projected to a 100-dimensional space using PCA. As a matter of fact applying the method directly to the images does not yield a satisfactory result. This is due to a fundamental problem which arises when applying any manifold learning approach to image data sets. *How should one choose the measure of similarity between images, such that it is proportional to the perceptual difference of them?* The Euclidian distance

$$d(A,B) = \sqrt{\sum_{i,j} \left(A_{ij} - B_{ij}\right)^2} \tag{27}$$

is by no means an appropriate measure, since it does not take into account the proximity information of the pixels in the image and all pixels are equally apart in this model. This is an issue to be addressed before any manifold learning approach can satisfactorily abstract the concepts present in image data sets.

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