A comparison study of ellipsoid fitting for pose normalization of hippocampal shapes

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Keywords
shapes, hippocampal, fitting, pose, comparison, ellipsoid, study, normalization

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A Comparison Study of Ellipsoid Fitting for Pose Normalization of Hippocampal Shapes

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Abstract—Pose normalization is an important step to establish shape correspondence for group comparison of anatomical structures. The most basic and widely used way is ellipsoid fitting, which provides three principal axes for shape alignment, and is often solved by least square fitting. In this paper, it is recognized that the deformation caused by neuro-degenerative diseases is usually locally irregular, behaving like the outliers to the majority of the anatomical surfaces. Therefore we hypothesize that the distance function in \( L^1 \)-norm may perform better than that in \( L^2 \)-norm for hippocampal surface fitting, and thus conduct a study to compare the influence of different distance functions. In particular, we show how to perform ellipsoid fitting via \( L^1 \)-norm based algebraic and geometric distances, and experimentally compare their performance together with the conventional \( L^2 \)-norm based distance functions. Our study demonstrates that \( L^1 \)-norm approach fits the majority of the surface, while \( L^2 \)-norm approach tends to fit the irregularity.

Keywords: hippocampal shapes; pose normalization; spherical harmonics; algebraic distance; geometric distance

I. INTRODUCTION

Analyzing anatomical shape variation from a population is one of the major issues in medical imaging, which aims to identify possible biomarkers for early diagnosis of diseases. For example, the shape change of hippocampus has been treated as a major biomarker for the prediction of Alzheimer’s disease (AD). It has been realized that the accuracy of the statistical shape analysis highly depends on the accuracy of the shape correspondence. Boundary or medial descriptions such as SPHARM [1], [2] or M-rep [3] are often used to establish the shape correspondence as well as representing the 3D shapes. However, these methods are usually not invariant to transformations. Therefore, a pose normalization step is often involved. Given two shapes, the translation can be removed by moving their centers of mass to the origin, and the rotation can be eliminated by aligning their principal axes. Ellipsoid fitting is a common way to compute the principal axes. For example, to remove rotations in SPHARM, a 3D anatomical shape is represented as an ellipsoid via the spherical harmonics of degree 1. The three axes of the ellipsoid are used to align their parameter spaces. Note that in literature ellipsoid fitting is usually solved as a least-square fitting [4], [5]. This is also true for SPHARM, where the first order SPHARM coefficients used to reconstruct the ellipsoid are calculated by least-square. In this paper, these approaches are referred to as the \( L^2 \)-norm based ellipsoid fitting.

As is known, an \( L^2 \)-norm based fitting may be more sensitive to outliers than an \( L^1 \)-norm based fitting. In this paper, it is pointed out that in brain structure analysis, the deformations, which are of great interest when investigating the effects of neuro-degenerative diseases, may be often locally irregular. The irregularities behave more or less like the outliers to the majority of the surface that is relatively smooth. Due to its natural properties, the \( L^2 \)-norm fitting might erase the discrimination by trying to fit the local irregularity. Therefore, in this paper, we hypothesize that an \( L^1 \)-norm ellipsoid fitting may outperform an \( L^2 \)-norm approach when the morphological changes caused by neuro-degenerative diseases are locally irregular. Our study is conducted on hippocampal shapes that are represented by landmark points sampled from their surfaces.

In this paper, two cost functions are investigated for the \( L^1 \)-norm ellipsoid fitting: the algebraic distance and the geometric distance. The study of the algebraic distance is intrigued by a successful work [6] in 2D least square ellipse fitting. In [6], using the algebraic distance in \( L^2 \)-norm, an analytical solution can be directly given to the least square fitting problem. Some efforts have been put to extend the work in [6] to 3D \( L^2 \)-norm ellipsoid fitting. However, the problem becomes much more complicated for ellipsoids than for ellipses. No analytical solution can be given. In this paper, along the line in [6], we provide our solution of the \( L^1 \)-norm based algebraic distance for ellipsoid fitting. Although the algebraic distance is not geometrically meaningful, it is worthy to study due to its simpler formulae compared with the geometric distance, and in general it is computationally cheap. Following that, a cost function corresponding to the geometric distance is also studied due to its robustness of approximation compared with the algebraic distance.

It is worth to clarifying the following issues about the contribution of this paper. Firstly, please note that the general effects of \( L^1/L^2 \)-norm to outliers are known to the community. One contribution of this paper is to identify the similarity between local anatomical abnormalities (which are still part of the anatomical shape) and the outliers, and conduct comparative studies to investigate the influence of cost functions on pose normalization. Examples of hippocampal surfaces belonging to both normal subjects and AD subjects are given in Fig 1. As shown, the similarity is not straight-forward. Secondly, there are broadly two groups of approaches to
establish dense surface correspondence: surface registration and surface parameterization. Both have a wide spectrum of applications. Compared with surface registration, surface parameterization represents the surface as well as establishing the correspondence, which is the focus of this paper. For surface parameterization approaches, a simple alignment method is preferred to remove rotation and translation if the parameterization approach is not invariant to these transforms, for example, SPHARM. The purpose of this paper is to discuss the influence of different cost functions on this alignment step instead of proposing an accurate shape registration method, although we do develop different approaches of ellipsoid fitting in this paper. Given the wide use of SPHARM in brain analysis only, we believe this study is necessary and significant. Finally, the contribution of this study is not only limited to ellipsoid fitting. It puts forwards an issue that should be considered but often ignored when designing algorithms for pose normalization of anatomical shapes.

This paper is organized as follows. At the beginning, a brief introduction of SPHARM representation is given as an example of the investigated problem. The necessity of pose normalization for SPHARM is shown and the reason why the conventional method is an $L_2$-norm based approach is explained. After that, two $L_1$-norm based approaches are developed using both algebraic and geometric distance functions. Their performance is compared and discussed in the experiment, together with the conventional $L_2$-norm based approach.

![AD and Normal hippocampal shapes](image)

Fig. 1. Examples of the left hippocampal shapes belonging to 4 AD subjects and 4 normal subjects.

II. METHODS

A. SPHARM Representation

SPHARM is a short term for spherical harmonics shape representation. It provides a multi-resolution representation for surfaces with spherical topology, and thus is often used to model brain cortex [7], hippocampus [1], caudate [8], ventricle [9] and other anatomical structures in brain imaging analysis. It seeks a one-to-one mapping from the surface to the unit sphere, and then decomposes the coordinates of surface vertices onto a set of orthonormal functions. In particular, a surface $f(\theta, \phi) = (x(\theta, \phi), y(\theta, \phi), z(\theta, \phi))^T$ is decomposed to

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_l^m Y_l^m(\theta, \phi),$$

where $Y_l^m(\theta, \phi)$ is the spherical harmonics of degree $l$ and order $m$, evaluated at the spherical parameters $(\theta, \phi)$ ($\theta \in [0, \pi], \phi \in [0, 2\pi]$). The coefficient $c_l^m$ is the three-dimensional coefficient vector $(c_{l1}^m, c_{l2}^m, c_{l3}^m)$, which is used to construct the shape descriptor. To estimate the coefficients, the following least square fitting problem is solved:

$$\hat{C} = \arg\min_C ||BC - F||^2; \quad (1)$$

where $B$ is a $n \times nc$ matrix with $B_{ij} = Y_j(\theta_i, \phi_i)$. The basis function $Y_j = Y_l^m$ uses a single index $j = l^2 + l + m$. Here $n$ is the number of the points sampled from the surface $f$ and $nc$ is the number of the SPHARM coefficients. The vector $F$ contains the coordinates of the $n$ sampled points.

SPHARM represents an object surface in multi-resolution by taking different degree spherical harmonics. With degree 1 expansion, an object shape degenerates to an ellipsoid. When the degree increases, higher frequency components are included and hence more details appear. Given a certain degree $l$, an object shape can be represented by a shape descriptor vector composing of $(l+1)^2 \times 3$ spherical harmonic coefficients

$$(c_0^0, c_0^1, c_0^2, c_1^0, c_1^2, c_1^1, c_2^0, c_2^1, c_2^2, c_2^1, c_2^0, c_3^0, c_3^1, \cdots),$$

or by a set of resampled surface points with established correspondence.

SPHARM is not rotation invariant. That means the shape descriptor constructed above depends on the orientation of the object. In some research works, a rotation invariant shape descriptor of SPHARM is proposed [10]. However, such method discards the phase information, which reduces its discrimination capacity. Moreover, the shape cannot be reconstructed by the shape descriptor alone. Therefore, in practice a pose normalization step is used in SPHARM. In this step, a shape is represented as an ellipsoid obtained by the spherical harmonics of degree 1, and then the parameter space is rotated to a standard position according to the three axes of the ellipsoid. The coefficients of spherical harmonics up to degree 1 are estimated in the least square way as shown in (1). Therefore, this approach is essentially an $L_2$-norm based ellipsoid approximation. Below, possible alternatives using $L_1$-norm based ellipsoid fitting are further explored.

B. Identifying quadratic surface

In this paper, the ellipsoid fitting is obtained via general quadratic surface function that can be expressed as:

$$f(x, y, z) = Ax^2 + By^2 + Cz^2 + Dxy + Eyz + Fxz + Gx + Hy + Jz + K = 0. \quad (2)$$

Let us denote
\[
Q_a = \begin{bmatrix}
A & D & F \\
D & B & E \\
F & E & C \\
\end{bmatrix} = \begin{bmatrix}
q_{11} & q_{12} & q_{13} \\
q_{21} & q_{22} & q_{23} \\
q_{31} & q_{32} & q_{33} \\
\end{bmatrix},
\]

(3)

where \(Q_a\) is the sub-discriminant of the quadratic surface, which is invariant under transformations and thus helpful to classify the quadratic surface. According to [11], the conditions for a quadratic surface to be an ellipsoid are:

\[
T_2 > 0
\]

\[\text{det}(Q_a) \times T_1 > 0.\]

\[
C. \text{ Algebraic Distance in } L_1\text{-norm}
\]

For a given point \(x\), its algebraic distance to the quadratic surface is \(f(x)\). Denote \(a = [A \ B \ C \ D \ E \ F \ H \ J \ K]^\top\) and \(D_i = \begin{bmatrix} x_i^2 & y_i^2 & z_i^2 & x_i y_i & y_i z_i & z_i x_i & y_i x_i & y_i y_i & z_i z_i \end{bmatrix}^\top\), \(i = 1, \ldots, n\). We only consider the ellipsoid constraint in (5) for two reasons: i) the constraint in (6) is too complicated for the optimization problem to be efficiently solved; ii) by solely considering the constraint in (5), our problem becomes comparable to the successful work of 2D \(L_2\)-norm ellipse fitting in [6]. To express the constraint in (5) in the form of matrix, a matrix \(C\) is constructed:

\[
C = \begin{bmatrix}
0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\
\end{bmatrix}
\]

Then the constraint in (5) can be rewritten as \(a^\top Ca > 0\). As suggested in [6], we can arbitrarily scale the parameters in \(a\) to make this inequality constraint become equality \(a^\top Ca = 1\). Therefore the optimization problem is:

\[
\min_{a} \|Da\|_1 = \min_{a} \sum_{i=1}^{n} \sum_{j=1}^{10} d_{ij} a_j
\]

\[\text{s.t. } a^\top Ca = 1.\]

(7)

To simplify the objective function, let \(\sum_{j=1}^{10} d_{ij} a_j \leq t_i\). The upper bound of the objective function is obtained:

\[
\sum_{i=1}^{n} \sum_{j=1}^{10} d_{ij} a_j \leq \sum_{i=1}^{n} t_i.
\]

Instead of minimizing the original optimization problem, we can minimize its upper bound. If only considering the constraint in Eq. 5, the optimization problem becomes:

\[
\min_{a, t} \ \ 1^\top_t t
\]

\[\text{s.t. } d_i a \leq t_i, \quad d_i a \geq -t_i, \quad t_i \geq 0 \quad a^\top Ca = 1\]

(8)

where \(1_n\) is an \(n \times 1\) vector with each element equal to 1, and \(t = (t_1, \ldots, t_n)^\top\).

Let \(v = [a^\top \ t]^\top\). The problem can be further written as:

\[
\min_{v} \ \ L v
\]

\[\text{s.t. } \begin{bmatrix} -D & I_n \\
0_{n \times 10} & I_n \end{bmatrix} v \geq 0_{3n \times 1} \quad v^\top \tilde{C} v = 1\]

(9)

where \(L = \begin{bmatrix} 0_{1 \times 10} & 1_{1 \times n} \end{bmatrix}\), \(\tilde{C} = \begin{bmatrix} C & 0_{10 \times n} \\
0_{n \times 10} & 0_{n \times n} \end{bmatrix}\). Let \(0_{m \times n}\) denote the \(m \times n\) matrix with all elements equal to 0, \(I_{m \times n}\) denote the \(m \times n\) matrix with all elements equal to 1, \(I_n\) denote the \(n \times n\) identity matrix. In this way, the original problem is converted to minimizing a linear objective function with 3n linear inequality constraints and one non-convex equality constraint. This is a non-convex polynomial optimization, which suggests that LMI (Linear Matrix Inequality) relaxation (with the toolkit GloptiPoly 3) might be used [12] to find the global optima. In LMI, by adding moderate number of lifting variables and constraints, the non-linear monomials are linearized, and hence a global optimality can be reached. It has succeeded in some computer vision problems [13] where the number of variables is no more than 10. However it is not applicable here, because the number of parameters to be estimated is relatively large (20 variables), a moderate order of LMI relaxation can lead to hundred thousands of inequalities. Hence the “fmincon” solver provided by Matlab is used instead, where both the objective function and the constraints can be nonlinear functions.

\[D. \text{ Geometric Distance in } L_1\text{-norm}\]

A cost function that corresponds to, but not strictly equals, the actual geometric distance is employed to measure the distance between the surface points and the model. This cost function is used to simplify the computation of the actual geometric distance in \(L_1\)-norm. The latter is very complicated so that the existence of too many local optima often prevents a good solution to be reached. Although the employed cost function is not strictly geometric distance, its advantage over the algebraic distance has been demonstrated visually and quantitatively in our experiment. For simplification, this distance is still called the “geometric distance”. Let us consider a standard ellipsoid whose center is at the origin, and three axes are aligned with the coordinate system. Without loss of generality, the longest axis is aligned with the \(x\)-axis, and
The angles \( \theta \) geometry:

It is solved by the Levenberg-Marquardt algorithm iteratively.

The term \( r(a) \) is the length of \( \mathbf{oP}_i \), which is a function of the ellipsoid parameter vector \( a \) as defined above. Since \( \mathbf{P}_i \) is a point on the ellipsoid surface, the term \( r(a) \) can be computed by

\[
\frac{r(a)^2 \sin^2 \phi}{l_a^2} + \frac{r(a)^2 \sin \phi \cos \phi}{l_b^2} + \frac{r(a)^2 \cos \phi}{l_c^2} = 1.
\]

The parameters \( l_a, l_b, \) and \( l_c \) in the standard form are calculated using the parameters in the general form in (2):

\[
\begin{align*}
    l_a &= \sqrt{M} / A', \\
    l_b &= \sqrt{M} / B', \\
    l_c &= \sqrt{M} / C', \\
    M &= \frac{G'^2}{4A'} + \frac{H'^2}{4B'} + \frac{J'^2}{4C'} - K, \\
    A' &= \lambda_1, \\
    B' &= \lambda_2, \\
    C' &= \lambda_3, \\
    G' &= G \mathbf{P}^T, \\
    H' &= H \mathbf{P}^T, \\
    J' &= J \mathbf{P}^T.
\end{align*}
\]

The process. We choose it as an ellipsoid constructed by the eigen-vectors obtained from the eigen-decomposition of the landmark covariance matrix. This ellipsoid has to be presented in the general form of a quadratic surface function. Suppose \( \mathbf{e}_1, \mathbf{e}_2, \) and \( \mathbf{e}_3 \) are the eigen-vectors sorted by their eigen-values \( \lambda_1, \lambda_2, \) and \( \lambda_3 \) in a decreasing order. Their lengths have been normalized to 1. Let \( \mathbf{e}_{ij} \) denotes the \( j \)-th element in \( \mathbf{e}_i, \) and \( \mu_x, \mu_y, \) and \( \mu_z \) the means of the \( x, y, \) and \( z \) coordinates of all the landmarks respectively. The coefficients of the general quadratic function are computed by

\[
\begin{align*}
    A &= p_1, \\
    B &= p_2, \\
    C &= p_3, \\
    D &= 2p_4, \\
    E &= 3p_5, \\
    F &= 2p_6, \\
    G &= -2(p_{1x} + p_{2y} + p_3z), \\
    H &= -2(p_{2y} + p_{3x} + p_4z), \\
    J &= -2(p_{3x} + p_{4x} + p_5y), \\
    K &= p_{1x}^2 + p_{2y}^2 + p_{3z}^2 + p_{4y}^2 + p_{5z}^2 + 1.0.
\end{align*}
\]

III. EXPERIMENT

The experiment studies two problems: i) which \( \ell_1 \)-norm based distance function is better for ellipsoid fitting; and ii) whether the \( \ell_1 \)-norm based ellipsoid fitting is better than the \( \ell_2 \)-norm based approach.

A. Comparison between \( \ell_1 \)-norm distance functions

The ellipsoid fitting is realized by optimizing both the \( \ell_1 \)-norm based algebraic distance and the \( \ell_1 \)-norm based geometric distance. The approximation accuracy is evaluated by the average Sampson distance (error) from the 1002 landmark points to the estimated surface model. The Sampson error is the distance from the points to the first order Taylor expansion of the surface function. The smaller the Sampson error, the better the fitting. Both methods are tested on 37 hippocampal shapes from subjects in 60-69 age cohort (from OASIS data set preprocessed by NICTA AASEDP project). The average Sampson errors (ASE) is 14.19 for the geometric distance, and 28.9 for the algebraic distance. Four examples are given in
Fig. 3. The ellipsoid fitting is compared between minimizing a $L_1$-norm based algebraic distance and minimizing a $L_1$-norm based geometric distance. The averaged Sampson errors (ASE) are computed to estimate the approximation. The geometric distance based approach consistently generates less ASE than the algebraic distance based approach.

Fig. 3. The estimated ellipsoids are displayed translucently and overlapped on the hippocampal surfaces to show the fitting. As the figure shows, the geometric distance consistently generates smaller ASE than the algebraic distance. This result suggests that the ellipsoid approximation by the geometric distance is better than that by the algebraic distance. Generally speaking, sometimes the algebraic distance may be satisfying when a good initialization is provided, and its optimization may be faster than that of the geometric distance. However, it is not the case in the the $L_1$-norm based ellipsoid fitting. The reason is two-fold. Firstly, the optimization of the algebraic distance in (9) introduces $n$ additional variables, where $n$ is the number of the surface points. The speed of the optimization significantly slows down when $n$ is large. Secondly, the surface model is general to all types of quadratic surfaces. The determination of an ellipsoid surface relies on the conditions in (5) and (6). However, to make the optimization simple, the complex constraint in (6) is just ignored. This is common in the literature of ellipsoid fitting [14]. Nevertheless, we find that the ignorance of (6) may cause a non-ellipsoid solution to the algebraic distance in (9). This problem is avoided in the geometric distance. Satisfying (11) guarantees an ellipsoid solution. An example is shown in Fig. 4. The initialization is the same ellipsoid for both the algebraic and the geometric distance. Eventually the geometric distance approach properly fits an ellipsoid, whereas the algebraic distance approach fits a cylinder.

B. Comparison between $L_1$-norm and $L_2$-norm distance functions

The ellipsoid fitting is compared between the $L_1$-norm and the $L_2$-norm geometric distance functions. The $L_2$-norm geometric distance only replaces the $L_1$-norm in (10) with the $L_2$-norm. The reason to investigate this approach is to test the influence of the $L_1$-norm and the $L_2$-norm on the same distance function.

In Fig. 5, six examples of the $L_1$-norm and $L_2$-norm ellipsoid fitting based on the geometric distance are displayed. As the figure shows, the $L_1$-norm distance function tries to fit the majority of the hippocampal surface, while the $L_2$-norm distance function tends to fit the irregularity as well. This phenomenon is salient in Subject II and Subject V. As Sampson error is essentially a least-square based distance, it biases the $L_2$-norm approach and fails to be a proper measurement for our comparison. Take subject II for example. Although visually the $L_1$-norm approach is more reasonable than the $L_2$-norm, the ASE is 10.52 for the $L_1$-norm, and 7.35 for the $L_2$-norm. The histogram of error values at each surface point is plotted in Fig. 6. It shows that the slope of the $L_1$-norm curve is sharper than that of the $L_2$-norm curve. This indicates that for this subject, the $L_1$-norm approach generates more points located in the small Sampson error area (around the origin) than the $L_2$-norm approach, which is a desired property. This phenomenon is more evident.
in AD subjects, where more shape irregularity is expected in hippocampus caused by the disease. In future work a more fair measurement than Sampson error should be sought for this comparison.

Fig. 5. The $L_1$-norm and $L_2$-norm ellipsoid fittings via optimizing the geometric distance are compared on two examples of hippocampal surfaces (the shapes in the wireframe). The fitted ellipsoids are translucent and overlapped on the hippocampus. The $L_1$-norm ellipsoid fitting tends to fit the majority of the hippocampal shape, while the $L_2$-norm ellipsoid fitting fits the irregularity as well.

Please note that, in Section III-A, both the geometric and the algebraic approaches in comparison are based on $L_1$-norm. The bias of the Sampson distance (towards $L_2$-norm) effects identically on these two approaches. Therefore the Sampson distance is still valid for comparing the degree of fitting in that case, which agrees well with the visual results in Fig. 3.

IV. CONCLUSION

In this paper, it has been studied if the distance function in $L_1$-norm can achieve better ellipsoid fitting than that in $L_2$-norm for the pose normalization of hippocampal shapes. Two $L_1$-norm based ellipsoid fitting are proposed via both the algebraic and geometric distances. They are compared with the conventional $L_2$-norm based approaches. Our experiment shows that: i) for the $L_1$-norm ellipsoid fitting, the geometric distance is better than the algebraic distance in three aspects: a more accurate approximation, less variables to optimize, and a guaranteed ellipsoid solution; ii) the $L_1$-norm approach fits the majority of the hippocampal shape, while the $L_2$-norm approach tends to fit the irregularity. These observations may help guide the design of pose normalization algorithms.

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