Exploration of Shape Variation Using Localized Components Analysis

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Abstract—Localized Components Analysis (LoCA) is a new method for describing surface shape variation in an ensemble of objects using a linear subspace of spatially localized shape components. In contrast to earlier methods, LoCA optimizes explicitly for localized components and allows a flexible trade-off between localized and concise representations, and the formulation of locality is flexible enough to incorporate properties such as symmetry. This paper demonstrates that LoCA can provide intuitive presentations of shape differences associated with sex, disease state, and species in a broad range of biomedical specimens, including human brain regions and monkey crania.

Index Terms—Feature representation, size and shape, life and medical sciences.

1 INTRODUCTION

The parameterization of an ensemble of shapes is a key step in a broad array of applications that require quantification or manipulation of the shape properties of objects. In this paper, shape parameterization refers to the problem of converting a representation of the delineating boundary of an object in 2D or 3D into a concise vector of numbers that captures its salient shape characteristics. Converting the shape of an object such as an organ or bone into a small set of shape parameters facilitates a variety of statistical analyses, including the characterization of shape variability across an ensemble, comparison of object shape between groups, and the tracking of shape change over time.

Often, converting shapes into concise parameter vectors is intended to make the compression, transmission, classification, and modification of shape data more computationally efficient. In contrast, we focus on finding an intuitive shape parameterization. In biology and medicine, presenting the results of shape analyses in an intuitive way can encourage the connection of shape properties to domain-specific physical or biological processes; for instance, the interpretability of brain shape parameterization could be enhanced if each parameter represents an easily grasped aspect of the brain, such as the size of an identifiable, anatomically localized brain region. The use of an intuitive parameterization could, in turn, promote interpretations of brain shape differences between healthy and sick individuals in terms of disease causes or effects. In graphics and vision, using each parameter to represent a single, intuitive aspect of shape could enhance the usability of user interfaces for shape model manipulation and simplify automated methods for object recognition based on the shape of object parts.

Here, we define an intuitive parameterization to be one that is both concise (capturing salient shape characteristics in a small number of parameters) and spatially localized (accounting for the shape of a spatially restricted subregion in each parameter). Our hypothesis is that spatially localized shape parameterizations are more intuitive since they allow users to conceptualize object shape in terms of a small number of object parts, which might be affected differentially by physical phenomena or may simply be of interest. In the above brain shape example, for instance, shape change due to disease processes is known to occur in spatially localized brain subregions in a variety of disorders (e.g., [1]). Concise parameterizations are attractive both for comprehensibility and because the statistical power of tests on those parameters is reduced as little as possible by corrections for multiple comparisons [2].

We follow the linear subspace paradigm of expressing each shape as a linear combination of prototypical, or basis shapes. That is, if each shape is represented as a vector \( v \) of the 2m or 3m coordinates of \( m \) points sampled from its boundary (i.e., \( v = [v_1, v_2, \ldots, v_m] \), \( v_{j,k} = [x_j, y_k] \) for 2D shapes), \( v \) is approximated as a linear combination of \( k \) basis vectors \( \{e_1, e_2, \ldots, e_k\} \):

\[
v_j = \sum_{i=1}^{k} \alpha_{j,i} \cdot e_i + \mu,
\]

where \( \mu \) represents the mean of the data vectors \( v_j \). The shape parameters are the coefficients \( \alpha_{j,i} \). Linear subspace methods are attractive because their linearity in \( e_i \) allows them to be manipulated using standard tools from linear algebra.

Fig. 1a depicts a typical \( e_i \) generated by the classical linear subspace method, Principal Components Analysis (PCA), applied to tracings of human corpora callosa (CC). The basis shape summarizes a complex pattern of shape characteristics across the entirety of the CC. Therefore, if the corresponding \( \alpha_i \) differs between groups, the explanation of the group difference in physical terms is complex. Localized Components Analysis (LoCA), in contrast, optimizes the \( e_i \) for spatial locality and conciseness simultaneously. It improves on previous linear subspace methods by explicitly optimizing for localized shape parameters and allowing the user to modulate the trade-off between locality and conciseness with greater flexibility than previous methods. Fig. 1b shows the \( e_i \) vectors from three increasingly localized LoCA bases; differences in the corresponding \( \alpha_i \) between groups give rise to a simple physical explanation in terms of the \( i \)th CC subregion whose shape is captured by the \( e_i \) at the far right.

We emphasize that we impose spatial locality onto our callosal shape components because doing so encourages simple anatomical
interpretations of the corpus callosum; it is not necessarily always the case that spatially localized shape components will be optimal for every shape analysis task. For example, if the shape analysis goal is to examine correlations between the shape characteristics of distal parts of an extended shape, spatially localized shape components will be unlikely to capture these correlations because they will be discouraged from placing highly correlated distal parts into the same component.

LoCA was introduced in a related conference paper [3]. This paper used three biomedical shape data sets to suggest that LoCA can provide shape parameterizations that are more effective than PCA and related linear subspace methods at modulating the trade-off between shape basis locality and conciseness. This paper uses additional experiments to demonstrate that these shape parameterizations provide advantages over PCA for scientifically relevant shape analysis tasks and are not extremely difficult to compute numerically. In this paper, we begin by summarizing related work in Section 2 and then we present LoCA in Section 3 (for more details and examples, see [3]). Then, in Section 4, we use LoCA to illustrate the shape differences between groups in three data sets. We examine how well-established sex differences in 2D sections of human CCs are expressed by LoCA, and we use LoCA to isolate specific shape differences in the crania of closely related cobaline monkeys.

2 RELATED WORK

PCA has been used to find concise bases for shape spaces in medical image analysis [4], morphometrics [5], computer graphics [6], and many other contexts. In PCA, \(e_i\) is the \(i\)th eigenvector of the covariance matrix of the example \(v_j\) vectors; therefore, \(e_i\) is orthogonal and \(\sum_i e_i^2\) is the best \(i\)th-order approximation of \(v_j\) under the \(L_2\) norm. Related algorithms such as Sparse PCA (S-PCA) [7], [8], [9], independent components analysis (ICA), or principal factor analysis (PFA) do not directly optimize a locality-related objective function, but they appear to generate spatially localized components anyway [9], [10], [11], [12]. Alternatively, predefined spatially located regions of interest can be integrated into PCA [13]. Our approach is inspired by S-PCA and follows a similar strategy of adjusting \(e_i\) provided by PCA, but we explicitly optimize for locality and allow the user to explicitly modulate the trade-off between conciseness and locality.

Other recent techniques have been proposed to capture localized shape differences. Networks of localized medial primitives [14] seem computationally more difficult than LoCA, while direct comparison of corresponding \(v_{j,k}\) [1] suffers from a reduction in statistical sensitivity as compared to methods employing dimension reduction.

3 METHODS

PCA produces the most concise basis possible under the \(L_2\) norm; that is, for each \(k\), \(\sum_j (v_j - v_k^*)^2\) is minimized when \(e_1 \cdots e_k\) are the first \(k\) eigenvectors of the covariance matrix of \(v_j\). We use a formulation of PCA as the minimization of an energy function \(E_{var}\) as in [7] and modify it by minimizing \(E_{var} + \lambda E_{loc}\), where \(E_{loc}\) is a new energy term that summarizes the spatial locality of \(e_i\). The parameter \(\lambda\) balances the trade-off between the competing interests of conciseness and locality (Fig. 1).

3.1 Energy Function

Each successive PCA component accounts for as much shape variation as possible, that is, the distribution of shape variation over the PCA basis vectors is as concentrated as possible on the leading \(e_i\). More formally, one can define the relative variance \(\beta_i\) of each basis vector \(e_i\) as

\[
\beta_i = \frac{\sum_j (v_j - \mu)^2}{\sum_j (v_j - \mu)^2}.
\]

The entropy of the distribution of relative variances, \(\sum_i \beta_i \log(\beta_i)\), is minimized over all orthogonal bases by the PCA basis, so we define this to be \(E_{var}\) as in [7]. Each \(e_i\) consists of a list of 2D or 3D vectors \(e_{i,j}\) each of which corresponds to the displacement of one of the surface points (i.e., \(e_i = [e_{i,1}, e_{i,2}, \ldots e_{i,n}], e_{i,j} = [e_{i,j,1}, e_{i,j,2}]\) for 2D shapes). We encourage each \(e_i\) to have simultaneous nonzero entries corresponding to points \(p_1\) and \(p_2\) (i.e., simultaneous nonzero entries in \(e_{i,1}\) and \(e_{i,2}\) if and only if \(p_1\) and \(p_2\) are close to each other. To do so, we introduce a pairwise compatibility matrix \(B\) whose entries \(B[i,j]\) tend toward 1 when \(p_i\) and \(p_j\) are near each other and tend toward 0 when they are distant. The exact B matrices we use for our experiments vary as appropriate for the data set. For instance, in a variant of our method called Symmetric LoCA, \(B[i,j]\) tends toward 1 when \(p_i\) and \(p_j\) are either close or symmetric near each other after one of the points is reflected across a symmetry plane defined on the object. We use the B matrix to define a cost function \(C(e_i, p_c)\) which evaluates each surface point \(p_c\) as a potential center point for \(e_i\). The surface point \(p_c\) is a good center point for \(e_i\) if the deformation described by \(e_i\) is localized around \(p_c\). Specifically,

\[
C(e_i, p_c) = \sum_{j=1}^m |B[c,j] - ||e_{i,j}\|^2|\epsilon.
\]
The variables $e_i$ have unit length, so both $B[c, j]$ and $\|e_i\|$ vary between 0 and 1. Center points $p_c$ for which $e_i$ move significantly and for which the entries in $e_i$ respect the compatibilities between $p_c$ and other surface points incur a low cost. We found experimentally that setting $\alpha$ to a value less than 2 (1.5 in all experiments below) helped us ameliorate outlier effects in our experiments.

A vector $e_i$ is well localized if we can find one (or more) good center points $p_c$, but we need to consider one additional complication: some $p_c$ may be favored as center points by the object geometry, as expressed by the compatibilities in matrix $B$, irrespective of the deformations in the input data $v_j$; specifically, those near the center of the object. Therefore, for a given $p_c$, we normalize $C(e_i, p_c)$ by the maximum value that $C(e_i, p_c)$ could take over all possible $e$. Our final locality term for each vector is the normalized $C(e_i, p_c)$ for the minimal choice of $p_c$:

$$E_{loc} = \sum_{p_c} \min_{e_i} \frac{C(e_i, p_c)}{\max_e C(e_i, p_c)}.$$  

The denominator for a given $p_c$ is simply $\sum_j \max_e (|B[c, j] - 1|, |B[c, j] - 0|)^\lambda$. It needs to be computed only once for each $p_c$.

### 3.2 Optimization

We assume that we are given an ensemble of $n$ objects, each represented by $m$ points on its boundary and the compatibility matrix $B$. Overall differences in object scale, rotation, and translation over the ensemble are removed through generalized Procrustes alignment [5]. The resulting scaled and aligned data sets are used as input to the numerical optimization.

Our optimization procedure is similar to that used in [7]. PCA provides an initial orthonormal basis $e$, and every possible pair $e_i, e_j$ is rotated together in the 2D plane that they span so that the basis remains orthonormal. Each pair is rotated by the angle $\theta$ that minimizes $E_{var} + \lambda E_{loc}$. The optimal $\theta$ is found numerically using Brent’s method [15]. As illustrated in Fig. 2, the global minimum is almost always found at each iteration, even though changes of center point produce slope discontinuities.

The pairs are rotated in decreasing order of shape variation accounted for. The set of all $e_i, e_j$ pairs are adjusted repeatedly, and optimization ceases when adjusting them changes the objective function less than a fixed threshold. Between 50 and 150 iterations were required for each experiment discussed below.

### 4 Results

Below, we compare LoCA to PCA on three data sets, two from brain imaging and one from primate morphology: CCs, lateral ventricles, and colobine monkey crania.

LoCA behavior depends strongly on $\lambda$, the parameter that modulates the trade-off between conciseness and locality (Fig. 1). For $\lambda = 0$, LoCA reduces to PCA. For small $\lambda$, LoCA basis vectors accounting for the highest amount of shape variation resemble PCA basis vectors, while the rest of the basis is clearly localized. For larger $\lambda$, all LoCA basis vectors are local, and the bases require more basis vectors to account for shape variation in the data. In Figs. 3 and 5, LoCA basis vectors are depicted for the smallest value of $\lambda$ for which the bases lacked global basis vectors. Reconstruction error for all three data sets is graphed in Table 1, in which we can see that strongly local bases (i.e., higher $\lambda$) require more vectors for accurate reconstruction.

### 4.1 Corpora Callosa

The CC data set represents 31 AIDS patients and 19 HIV-seronegative controls (mean age 42.64 ± 11.28 S.D.), who underwent high-resolution magnetic resonance brain scans as part of a previously described study [16]. As part of that study, each scan was rigidly aligned to the ICBM-53 template based on intensity cues, and all scans were then further aligned to each other in a groupwise fashion, based on manual sulcal landmarks. The CC was manually traced on the midsagittal slice of each scan using the Witelson criteria [17], and automatically marked with 103 surface correspondences [18].

We compared the ability of LoCA and PCA to detect what is likely the most firmly established difference in CC morphology between men and women, based on postmortem [17] and imaging-based [19], [20] findings: that women have larger isthmuses (i.e., posterior midbodies). We selected the LoCA and PCA coefficients for the shape components that captured 90 percent of the CC shape variation: the top 7 for PCA and the top 26 for LoCA (see Fig. 3). For each shape component, gender differences in its coefficients were tested in linear statistical models that controlled for other factors known to affect CC morphology: presence of AIDS, handedness, and age. The significance of the gender differences were assessed by F-tests in an ANOVA design.

Among the top 26 LoCA shape components, only components 5 and 9 had coefficients that differed significantly by gender at the $p < 0.05$ level, indicating thicker superior and inferior aspects of the isthmus in women (component 5: $F = 5.44, p = 0.024$; component 9: $F = 4.24, p = 0.045$, $p$-values uncorrected). This gender difference has been reported extensively (e.g., [17], [19], [20]). Only the first PCA component differed significantly between men and women ($F = 5.41, p = 0.024$); it represents a complex pattern of elongation, rotation, bending, and twisting of the entire structure. The complexity makes the shape component relatively difficult to interpret in simple anatomical terms. Also, some of the represented modes of CC deformation have not been reported to differ between genders in the literature, so their validity is uncertain.

### 4.2 Lateral Ventricles

Lateral ventricles were also traced manually in 3D on 54 of the 55 group-aligned scans of healthy and HIV/AIDS patients from a prior study [16]. The boundaries of the frontal, temporal, and occipital horns were traced on each slice based on a reliable, repeatable protocol described previously [21]. Dense one-to-one correspondences between subjects at homologous surface points were established by threading medial curves down the center of each of the frontal, temporal, and occipital horns, and resampling each horn to contain a fixed number of axis-aligned parallel traces [16]. Within each trace, rays were cast outward from the medial curve point toward the ventricular surface every $\theta$ radians. Across subjects, 330 correspondences were established between points in analogous traces and analogous $\theta$ radians. Geodesic distances were computed between pairs of resampled surface points, and the distances were used to compute compatibilities. The resampled surface points were the input to the shape parameterization methods.

We used PCA and Symmetric LoCA to assess differences in shape component coefficients between AIDS and control groups, and compared the results to differences between these groups that were previously presented using an established radial ventricular mapping approach [16]. The radial mapping approach has been strongly validated and used to characterize ventricular shape variation across a large number of medical covariates [21], [1], [22]. At each surface point, local thickness values were computed by calculating the distance from the surface point to the medial curve; mean thickness values were computed for AIDS and control groups. The ratios of mean local thicknesses between AIDS and control groups were computed and mapped to color values in a 3D rendering of the ventricular surface (Fig. 4). Red regions represent portions of the ventricular surface that were extremely dilated in AIDS patients compared to controls. Coefficients for the top PCA and Symmetric LoCA shape components accounting for...
90 percent of ventricular shape variation were analyzed in statistical models (17 PCA components and 36 LoCA components; the initial vectors in each basis appear in Fig. 5). The LoCA shape components that differed significantly at the $p < 0.05$ level between groups, in two-tailed $t$-tests with Bonferroni correction for multiple comparisons, are shown in Fig. 4. The ventricular regions covered by these shape components roughly correspond to the (red) regions that are grossly dilated in AIDS patients on the spatial maps, including the lateral walls, superior ridge, and anterior tip of the frontal horns; the superior and lateral aspects of the occipital horns; and the tips of the temporal horns. The only statistically significant PCA component was the second (Fig. 5, $p = 8.59e - 05, t = 26.25$), which represents nearly uniform inflation of the entire ventricular surface with no indication that some portions of the surface are more or less dilated in the AIDS group.

### 4.3 Colobine Monkey Crania

A shape space was built from a set of 238 colobine monkey crania (Subfamily Colobinae, Family Cercopithecidae) representing 17 species (2 of them outgroups). Various primate morphologists collected 45 landmark points on each cranium using a Microscribe 3D digitizer as part of data collection for a long-term project on Old World monkey cranial evolution. Twenty-nine of the landmarks were collected from the dorsal aspect of the cranium and 16 were collected from the ventral aspect (see [23] for details). The landmark sets were rescaled to remove the influence of size differences and aligned using GPA. Since we did not have surface models for each of the specimens, but only the landmarks, we estimated geodesic distance between landmarks by connecting them with a graph representing adjacency on the skull surface, and using distance in the weighted graph to form the compatibility matrix $B$.

We used a value of $\lambda$ that produced a completely localized Symmetric LoCA basis, which required 61 components to account
for 90 percent of the shape variance (Sym LoCA (61) in Table 1). We then compared branching groups in the evolutionary tree, testing the statistical significance of the PCA and LoCA vectors for discriminating between the two groups. We employed Welch’s two sample $t$-tests on each sex separately, using Bonferroni correction for multiple comparisons. In each case, we found several statistically significant LoCA components with corrected $p$-values at or below 0.05.

One branch is shown in Fig. 6. We examined the males from two groups, with the first group consisting of *Presbytis melalophos*, *Presbytis potenziani*, and *Presbytis rubicunda* specimens, and the second group consisting of *Semnopithecus entellus* and *Trachypithecus johnii* specimens. Each group is visually represented by the average male of each species, alongside the three basis vectors with the lowest $p$-values for both PCA and LoCA. LoCA vector 1 represents lengthening of the face, which is shorter for the *Presbytis* group (see Fig. 7). Vector 11 captures the width of the nasal bone, which tends to be narrower for the *Presbytis* group.

Vector 8 shows a deformation of the sphenoid bone, internal to the zygomatic arch (cheekbone) and just behind the tooth row.

Two of the three most significant PCA vectors shown in Fig. 6 include local deformations identified by significant LoCA vectors. PCA vector 1 affects face length (like LoCA vector 1), and also includes other deformations. Similarly, PCA vector 11 combines the nasal bone deformation of LoCA vector 11 with a complex change to the back of the cranium. The other, PCA vector 3, shows a global change that focuses on the length of the nasal bone, and also deforms the zygomatic arches and affects the cranium’s width. Table 2 shows that both the PCA and LoCA vectors have similar $p$-values, showing that in this example, the increased locality of the LoCA vectors does not come at the cost of discriminating power.

## 5 Discussion

The LoCA components spread the shape variation in the ensemble across more significant components than does PCA, with each component optimized for spatial locality. These components isolate the shape variation of specific parts of the object. Because we often understand shape variation in terms of spatially localized object parts, this decomposition is useful in the analysis and interpretation of shape differences between groups. Also, we found that representing the shape of single, rather than multiple, object regions in a single shape parameter helped to prevent the obfuscation of relationships between individual regions and auxiliary variables.

We found that LoCA is broadly applicable to a variety of data sets despite differences in dimension, shape representation, and the density, accuracy, and source of the point-to-point correspondences.

### Table 2

Results of the $t$-Tests Performed in Fig. 6

<table>
<thead>
<tr>
<th></th>
<th>Vector</th>
<th>$E_{loc}$</th>
<th>$t(41)$</th>
<th>$p$-value</th>
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</thead>
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<td>PCA</td>
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<td>10.530</td>
<td>4.667609e-07</td>
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<tr>
<td></td>
<td>3</td>
<td>0.175157</td>
<td>6.3989</td>
<td>6.336334e-05</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>0.223596</td>
<td>-5.7523</td>
<td>1.576577e-04</td>
</tr>
<tr>
<td>Symmetric LoCA</td>
<td>1</td>
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<td>10.2211</td>
<td>2.324091e-06</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>0.00808553</td>
<td>7.1989</td>
<td>2.204578e-05</td>
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<tr>
<td></td>
<td>8</td>
<td>0.0179966</td>
<td>6.763</td>
<td>3.088845e-04</td>
</tr>
</tbody>
</table>

The shown $p$-values are Bonferroni-corrected. Note that the Symmetric LoCA vectors are both local and find statistically-significant differences between the branching groups.
This flexibility suggests that it might be applied even more broadly, particularly to articulated forms. The method is also flexible with respect to the definition of compatibility between surface points; the incorporation of symmetry that we used here is just one example. Another appealing possibility would be somehow combining geodesic distance with curvature change, to encourage vectors affecting regions of similar curvature (e.g., the ridges of the ventricles).

In our formulation, pairs of points are more compatible if the geodesic distance between them is lower. Hence, we implicitly encouraged a fixed neighborhood size for our localized basis vectors. It may be more natural to encourage shape basis vectors in which all of the points in a particular surface neighborhood deform in concert, regardless of the size of the neighborhood. Future work will also address the problem of how to construct shape bases whose basis vectors are spatially localized in this scale-invariant fashion.

It is unclear whether we would generate shape parameterizations that are more spatially localized, or more useful for making shape-based inferences, if we dropped the orthogonality constraint from LoCA or added other constraints to the optimization; for example, we could seek shape components that are both spatially localized and statistically independent, as in ICA. Future work will address this variant of our current method.

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REFERENCES


