

Measurement-Based Shape Analysis

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Abstract

Conventional methods for shape analysis, based upon Procrustes and PCA, seem incapable of dealing with ‘non-landmark’ features, meaning measured positions not associated with well defined locations. This is due to an assumption of homogeneous errors, associated with an attempt to extract linear models with biologically meaningful descriptions. We propose a shape analysis system based upon the description of landmarks with measurement covariance which will extend the modelling process to ‘pseudo-landmarks’ such as boundaries and surfaces. We discuss the properties of our approach and how these covariances can be considered characteristic of the local shape. The method has been implemented and tested on measurements from fly wing, hand and face data. We use these data to explore possible advantages and disadvantages over the use of Procrustes/PCA.

1 Introduction

Over a decade during 70’s, bio-mathematical and biometrical aspects of biological shape studies were treated separately. This early work was later criticised during 80’s by Bookstein [4], Goodall [9] and Kendall [11]. Later Bookstein [5] worked towards converging notations from Goodall, Kendall and himself, for the biometric analysis of landmark data in a bio-mathematically interpretable framework of shape. As a consequence of these efforts, the standard method for analysis of variation in landmark position is generally regarded as “Procrustes”. It comprises a least squares alignment of a set of landmark features to a mean shape, and this is often followed by eigen-vector analysis of the linear correlations in variation around that mean. While the technique is now very popular the approach has several limitations with regard to the types of variation with which it can deal. One of these limitations is due to the assumption associated with taking least-squares differences and eigen vector summaries of distributions. Though many regard these as simply definitional, and in particular associated with shape, any statistical interpretation suggests that data are measures with homogeneous noise. It is this statistical interpretation we intend to investigate here.

Although landmarks are generally carefully chosen in order to allow accurate measurements of position within the image, problems will occur if ‘pseudo landmarks’, measured from smooth curves (and only accurately localised in one dimension 1D), are input to the analysis. Landmarks with a high degree of variability can act as outliers in the alignment stage, generating correlated compensating shifts and rotations of the other points. As PCA aims to describe the main sources of variation, high levels of such correlated movement will then necessarily contaminate the extraction of eigen-vectors. This contamination cannot be considered a genuine biological variation, as it has occurred purely due to the uncertainty in the measurement. This in turn follows from the subjective definition of the landmark leading to the view that problems can be avoided via appropriate definition. The mathematical

concept of homology (and mapping) underlies many of the considerations behind much theoretical work which is described with the mathematical formalisms of iso-morphism. Because of such restrictions on the definition of landmarks, semi-landmarks were introduced in order to allow inclusion of other points which are not homologous among the specimens, where a unique corresponding location can not be uniquely defined. Measurement at these locations must be augmented by a constraint, such as bending energy [6, 13], in order to recover the information missing due to the nature of local structure. However, it is easy to construct examples where such resolution of corresponding locations is not biologically meaningful.

From a statistical perspective a homology must be augmented by distributions indicative of the extent to which a correspondence can be established. The standard way to deal with inappropriate weighting of data in a least-squares fit is to introduce weighting, or more generally to generalise the least-squares cost to a Mahalanobis distance, computed using measurement covariances. By avoiding the requirement of specifying a unique homologous location, this has the advantage of accommodating varying information in measured data without having to re-create missing data or to reject some points as outliers.

There have been several attempts in the literature to include measurement errors for landmark points. Fitzpatrick et al [10] worked on the relationship between localization error and registration error in rigid-body, point-based registration. Chui and Rangarajan [7] proposed a general framework for non-rigid point matching where outliers are effectively rejected. Goodall [8] suggested a method which assumed a single covariance for all landmark perturbation. It has been noted that such a matrix is inestimable [12]. Goodall himself acknowledged that “as a model of measurement error this is a drawback, as the direction of greatest variation may vary considerably between landmarks”. Despite this problem, later work [14] generalised this idea to a Bayesian framework. Instead, we suggest an approach which can support the process of landmark location as measurement, with a covariance describing the localisation of each landmark separately. For example, Rohr et al [15] used such covariance matrices in a Mahalanobis distance form for non-isotropic data. This was, however, for the purpose of image registration using splines. As we believe this to be the correct statistical form for this problem, we investigate possible generalisations of Procrustes along these lines, and show one of several ways that measurement covariance can be reliably estimated.

2 The Method

Suppose that there are K shapes (2D) in our data-set and each shape vector \mathbf{w}_k contains N landmark points, i.e. $\mathbf{w}_k = [w_{1x}, w_{1y}, w_{2x}, w_{2y}, \dots, w_{Nx}, w_{Ny}]$. We apply a scale s_k , a rotation R_k and a translation \mathbf{t}_k to the original data to get an aligned version of the data called \mathbf{z}_k ; $\mathbf{z}_{kn} = s_k R_k (\mathbf{w}_{kn} - \mathbf{t}_k)$. The mathematical description of the model so far can accommodate any value of scale or orientation for the definition of mean model. We hence define the orientation of mean shape so that the line between a specified pair of points is horizontal. This also has the benefit that initial estimates of alignment for sample k can be set according to the relative positions of these points. We use the average distance between these landmarks to rescale the mean shape at each iteration so that scale remains numerically defined.

We assume a common, fixed, 2×2 covariance for each landmark derived from the measurement process. These are composed into the matrix C . This is a tri-diagonal matrix, the diagonal line of which contains data for individual landmarks. Outside of the 2×2 covariances, the off diagonal elements of C are zero, i.e. there are no correlations between landmark measurements (biological correlations are however to be modelled by the PCA process). The use of a fixed data covariance cancels out when taking the weighted mean to regenerate the conventional formula $\mathbf{m} = (1/K) \sum_{k=1}^K \mathbf{z}_k$, where $\mathbf{z}_k = [\mathbf{z}_{k1}, \mathbf{z}_{k2}, \dots, \mathbf{z}_{kN}]$.

In order to apply the PCA as a standard statistical tool and obtain a model, we introduce ghost points. Ghost points $\mathbf{g}_k^T = W(\mathbf{z}_k - \mathbf{m})^T$ are defined in the original coordinate system and, being scaled projections relative to the shape centroid, are an alternative way to summarise the original measurement. Projection to ghost points amplifies the spatial variation in directions which are well measured relative to those which are not so that the resulting locations have isotropic errors. In turn, this allows accurately measured structure to be encoded in the most significant eigen vectors of the linear model. The whitening matrix W is computed by applying singular value decomposition to C^{-1} ; $C^{-1} = U^T V U$. By making $W^T I W$ equivalent to C^{-1} we find that $W = V^{1/2} U$.

Application of PCA to \mathbf{g}_k follows for construction of the shape covariance, giving the eigen vectors \mathbf{e}_j and values μ_j for the whitened space of ghost points as those which minimise the unexplained variance for fixed $J < N$. For any specific shape example k , linear factors λ_{jk} can be computed to best approximate \mathbf{z}_k with the model \mathbf{z}'_k as follows.

$$F = \sum_{k=1}^K \mathbf{g}_k^T \mathbf{g}_k \approx \sum_{j=1}^J \mu_j \mathbf{e}_j^T \mathbf{e}_j \quad , \quad \mathbf{z}'_k = \mathbf{m} + W^{-1} \sum_{j=1}^J \lambda_{jk} \mathbf{e}_j \quad (1)$$

Here J parameter is the number of eigen vectors used in the model and $\lambda_{jk} = \mathbf{e}_j \cdot \mathbf{g}_k$. In order to find the best R_k, \mathbf{t}_k, s_k parameters for each k , the cost function we would expect to be minimised (e.g. using simplex) is a Mahalanobis distance. A genuine Likelihood should be based upon the variation of the data around the assumed model. Failure to do this results in only partial registration and residual distributions which cannot be meaningfully interpreted. Using this argument, if we wish to align to the mean shape we should use a covariance B consistent with the distribution around this mean. It therefore quantifies the entire variation of the sample as opposed to the noise in the measurement. The Likelihood function is

$$\log(P_k) = (\mathbf{m} - \mathbf{z}_k)^T B^{-1} (\mathbf{m} - \mathbf{z}_k) \quad , \quad B = \frac{1}{K} \sum_{k=1}^K (\mathbf{m} - \mathbf{z}_k)(\mathbf{m} - \mathbf{z}_k)^T \quad (2)$$

This also stabilises the alignment process with respect to poorly localised landmarks, but unlike C , B is independent of eigen vector estimation. We can therefore iteratively compute the best alignment and B prior to construction of the linear shape model. As an initial estimate of the model and transformed data is required, it makes sense to start from the Procrustes result. To reach the best possible alignment we should iteratively estimate R_k, \mathbf{t}_k and s_k using the assumed $\mathbf{e}_j, \mathbf{m}, C^{-1}$ (or B^{-1}) and W^{-1} . This gives us a new \mathbf{z}_k , and so, a new \mathbf{m} and F for construction of \mathbf{e}_j . For fixed covariances, convergence can be monitored via construction of the total Likelihood $\log(P) = \sum_k \log(P_k)$. The measurement covariance may be computed using the final estimates of \mathbf{z}_k and \mathbf{z}'_k either as a new estimate of the assumed C , or as a consistency check;

$$C = \frac{1}{K} \sum_{k=1}^K (\mathbf{z}'_k - \mathbf{z}_k)(\mathbf{z}'_k - \mathbf{z}_k)^T \quad (3)$$

When attempting to estimate C , the use of free parameters during model fitting reduces the sample covariance obtained from residuals. A possible outcome of this is the over weighting of landmarks leading to a runaway convergence on one landmark, during iterative estimation. For an eigen vector \mathbf{e} defined in the ghost space, the total correction would be

$$\Delta C = \frac{W^{-1} \mathbf{e}^T \otimes W^{-1} \mathbf{e}}{W^{-1} \mathbf{e}^T C^{-1} W^{-1} \mathbf{e}} = W^{-1} \mathbf{e}^T \otimes W^{-1} \mathbf{e} \quad (4)$$

This is correct for the tri-diagonal components, and is added to the sample covariance. The known structure of covariances is enforced by zeroing relevant off-diagonal terms.

3 Experiments

Our first set of data corresponds to left-hand images (40 samples, 56 landmarks) of 4 individual hands with various angles between fingers [1]. The second set corresponds to face images (200 samples, 68 landmarks) taken from video frames of talking faces of 3 individuals [2]. Finally we test the stability of our method using 4 sets of repeat mark-up data (200 samples per set, 15 landmarks) from fly wings [3]. We choose the minimum number of linear components which gives a ratio χ^2/DoF (degrees of freedom) about unity (3 for fly wings, 9 for hands, and 11 for faces).



Figure 1: Aligned points using Procrustes (left) and our method (middle); error bars (scaled by 20) estimated using our method (right).



Figure 2: Aligned points using Procrustes (left) and our method (middle); error bars (scaled by 20) estimated using our method (right).

We show the results in Figs. 1-3. Here sub-figures on the left column (except for Fig. 3) correspond to the aligned data using Procrustes, while sub-figures on the middle column correspond to those using our method. Further, sub-figures on the right column show the error bars computed using the eigen vectors and values of the 2×2 covariance matrices. Error bars for each landmark show the extent of an elliptical (non-isotropic) distribution around the corresponding point in the mean shape showing why we can not assume isotropic measurement distributions. It is clear from Fig. 1 that compared to Procrustes our method results in tighter groupings. The largest variances correspond to the landmark points which are not well constrained or unstable to some extent. They are either defined mathematically (based on two neighbouring landmarks) or pseudo landmarks with high variations in one direction. Most points on the sides of fingers have their largest variation in the directions tangent to the boundary curves. From the error bars in Fig. 2, it is clear that points at symmetrical locations on face data have similar variances, with those on the symmetry line being almost vertical. Similarly in Fig. 3, the error bars are oriented in the directions we expect based on the structures observed on fly wings. The values of standard deviations estimated vary between half a pixel and a few pixels (4.4 for fly wings, 8.7 for hands, and 4.0 for faces).

Finally, we investigate the stability of our method. There are four datasets available from left and right wings (L and R) of 200 female flies (L1, L2, R1 and R2) [3]. We perform

a simple χ^2 test based upon the construction of corrected covariances on one data set and then used for the calculation of χ^2 for a second set. We set the statistical test for significant difference on the basis of an allowable range of χ^2/DoF corresponding to $\pm 4 S.D.$, i.e. [0.72, 1.28] for 200 samples. The corresponding plot in Fig. 3 confirms the stability of our method, as almost all χ^2/DoF values fall in the range expected. Further χ^2 tests (not shown here) with different numbers of data samples and combinations of datasets indicate the appropriateness of the assumed linear model for the fixed number of components.



Figure 3: The χ^2/DoF ratios (left) when our method is applied to 3 sets of repeat fly wing data (L2, R1, R2) using fixed covariances (right; scaled by 30) estimated earlier using L1 set (middle).

4 Conclusions

In order to remove the theoretical difficulties associated with conventional approaches to morphometric shape analysis [8], we have implemented a method which takes appropriate account of measurement and landmark localisation stability to obtain a new form of analysis which is consistent with a Likelihood based definition of the alignment and model building tasks. Our results indicate that measurement covariances can be reliably estimated in our data even for small sample sizes, contradicting the common view that this should be impossible. This may be the result of using a corrected estimate rather than the conventional sample covariance.

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