Statistical Methodology for Deformations

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1 Introduction

This paper is concerned with changes of shape for objects in $\mathbb{R}^d$, typically with $d = 2$ or 3. Information about shape typically arises from landmark locations or images. In this paper we review the use of deformations to describe shape change. The review is selective and makes to claim to be comprehensive. Further development of some of the material can be found in Kent and Mardia (1994b), Mardia et al. (1995), and Glasbey and Mardia (1998, 2001).

Several important issues include the following:

1. What to deform: points, curves, surfaces or solid space.
2. Magnitude of deformation — small-scale or large-scale.
3. How to regularize deformations — different roughness penalties.
4. Numerical tractability — analytic or numerically intensive solutions.
5. Bijectivity – explicit or implicit.
6. Why deform.

2 What to deform

Consider a solid object in $\mathbb{R}^d$. Depending on the circumstances we may view the information about the object in different ways:

1. a set of labelled landmarks (e.g. Dryden and Mardia, 1998)
2. a continuous boundary; i.e. a curve in $\mathbb{R}^2$ or a surface in $\mathbb{R}^3$. Early work involving "snakes" was done by Kass et al. (1987). Later work on deformable templates can be found in e.g. Grenander et al. (1991), Grenander and Miller (1994), Cootes et al. (1992, 1994), Kent et al. (1996), and Kent et al. (2000).
3. the set of points inside the object (and maybe outside as well). Bookstein (1989, 1991) developed the use of thin-plate splines, and Miller and his group applied models from continuum mechanics (e.g. Christensen et al., 1996, Grenander and Miller, 1998, and Joshi and Miller, 2000).

The term *deformation* suggests the final interpretation, but it can be extended to the earlier interpretations as well.

The data can take three mains forms: (i) a set of labelled landmark locations, (ii) surface measurements, or (iii) a colour or grey-level image. In each case the aim it to deform one object to closely match another after deformation. For surfaces and images, the matching or labelling between corresponding pixels in the two surfaces or images is typically unknown.

3 Magnitude of deformation

Here the key distinction is between small-scale and large-scale deformation. In the former case we assume the deformation is close to an identity mapping (or at least an affine mapping), so that any mapping will be automatically bijective. However, bijectivity is not enforced by the mathematical formulation. Examples include thin-plate splines (Bookstein, 1989, 1991), clamped-plate splines (Marsland and Twining, 2002), and axis-preserving splines (Walker, 1999).

Let us consider the scale issue for each of the items in the previous section. Shape space for landmark data forms a (curved) manifold. For small-scale changes in landmarks, we are effectively looking at a tangent plane to this manifold where conventional multivariate techniques can be applied. For large-scale changes, it is necessary to accommodate the curvature of shape space. Similar issues arise in directional data analysis.

For small-scale changes in outlines, surfaces or solid objects, it is similarly unnecessary to worry explicitly about bijectivity. For large-scale deformation, a powerful general approach is to build up a full deformation out of a composition of small-scale changes. This forms the basis of the continuum mechanics approach of Miller and his co-authors.

The space of large-scale deformations subject to some boundary conditions (e.g. being an identity map on the boundary of a rectangular region) forms a group. Recent work has emphasized the construction of metrics on this group (e.g. Miller et al, 2002; Marsland and Twining, 2002).

4 Penalties

For continuous objects various penalties have been proposed based on integrated squared first and second order derivatives. It is convenient to categorize penalties on several criteria:

1. whether or not the penalty is separable. A separable penalty splits into a sum of terms, one for each component of the deformation. Typically the penalties arising from continuum mechanics are not separable, whereas the penalties for thin-plate spline type deformations are.

2. region of deformation, e.g. all of $\mathbb{R}^d$ or some compact region such as the interior of a rectangle or sphere.

3. whether similarity transformations have zero penalty and hence are automatically included within this framework, or whether similarity transformations need to be added explicitly.

For the most part the exact choice does not seem to matter, though more research is needed. In particular, Godwin (2000) showed that extreme versions of elastic penalties can lead to distorted fits when interpolating a deformation for a disk-like object in $\mathbb{R}^2$ given its behaviour on the boundary.

Penalties fit naturally into a nonparametric Bayesian paradigm, where minus the deformation penalty forms a log prior density for a Gaussian random field (typically intrinsic), and where a (possibly iid Gaussian) likelihood is formed from a pixel-wise comparison between two images. The images may be either raw images or may have been processed to highlight features such as edges. A deformation is sought which matches the two images as closely as possible subject to the deformation being a smooth as possible. Kent and Mardia (1994a) explore the link between prediction for intrinsic random fields (Kriging) and thin-plate splines.

5 Numerical tractability

If the data arise in the form of n landmarks, then for certain penalties there is an analytic solution for the deformation in terms of a linear combination of about n basis functions.

On the other hand for landmark data with other penalties, or for image data with any penalty, it is necessary to use a numerically intensive method to fit a deformation. Such methods might involve large Fourier expansions or finite element methods.

6 Bijectivity

To some extent the discussion of bijectivity is determined by the small-scale vs large-scale question. Small-scale changes are automatically (locally) bijective. If a large-scale deformation is built out of a composition of small-scale changes (the continuum mechanics approach), then it too will automatically be locally bijective.

A mapping is locally bijective if its Jacobian is everywhere nonzero. However, to be globally bijective, there is the additional requirement that distant parts of the image should not fold over one another after deformation.

Kent, Mardia and de Souza in unpublished work developed a multi-resolution approach to modelling a deformation based on a a composition of piecewise linear mappings on a set of triangular grids of increasing resolution. This approach has the advantage that bijectivity can be checked directly at each resolution.

7 Why deform?

This is an important question. From a statistical point of view, there are several main answers:

1. If the deformations themselves are of interest, then we need to model them in some way. The nonparametric approaches here give representations which can be decomposed into, e.g., principal components, giving the important parts of the deformations. Further, this way of thinking enables us to tackle spatial-temporal settings, as in growth models, where the shape of an object changes simultaneously in several different spatial directions, but at different rates in time.

2. Alternatively, the deformations between objects may be a nuisance feature which needs to be removed before comparing the objects in more detail. By deforming a set of objects to a common registration system, we can then compare them pixel by pixel, and thus look for fine-scale differences.

3. Identifying and tracking objects in images. This topic will not be covered here.

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