Weighted generalised Procrustes analysis of diffusion tensors

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1 Introduction

Diffusion tensor imaging (DTI) is a specific MRI modality which provides a unique insight into tissue structure and organisation *in vivo*. In DTI, displacement of water molecules over time is modelled by a zero-mean trivariate Gaussian distribution (Alexander, 2005) with covariance matrix evolving linearly with time and determined by the diffusion tensor (DT), a 3×3 symmetric positive-definite matrix. DT inference from observed diffusion MRI data has been commonly carried out using least squares (Koay *et al.*, 2006) and Bayesian (Behrens *et al.*, 2007, Zhou *et al.*, 2008) methods. At each location (voxel) of interest, the principal eigenvector of the tensor estimates the dominant fibre orientation whereas various tensor-derived diffusion anisotropy indices measure local anisotropy. White matter tractography attempts to integrate local estimates into brain connectivity maps which are of interest in neuroscience. In particular, DTI has been used to study stroke (Le Bihan *et al.*, 2001) and a wide range of neurological disorders such as multiple sclerosis, Alzheimer's and Parkinson's disease, and schizophrenia (Lenglet *et al.*, 2009).

Since diffusion MRI is a relatively low resolution modality, advanced tensor processing methods such as non-Euclidean interpolation, have been considered. Yet, reliable and accurate estimation of the highly complex white matter architecture of the brain remains a challenge despite the many advances in modelling, processing, and analysis of diffusion MRI data (Lenglet *et al.*, 2009). Moreover, further inference, e.g. analysis of variance across groups, depends critically on tensor processing methods such as interpolation (Chao *et al.*, 2008). At the same time, the recently introduced DT processing methods based on Procrustes analysis (Dryden *et al.*, 2009) have shown promising performance and deserve further investigation. Thus, this paper explores *weighted generalized Procrustes analysis (WGPA)* in which an arbitrary number of tensors can be interpolated or smoothed efficiently with the additional flexibility of controlling their individual contributions. The approach is illustrated through synthetic examples as well as white matter tractography of a healthy human brain.

2 Weighted Generalised Procrustes Analysis

Consider a sample of N DT's $\mathbf{D}_1, \ldots, \mathbf{D}_N$. To ensure their non-negative definiteness (and symmetry), we use the reparameterisation $\mathbf{D}_i = \mathbf{Q}_i \mathbf{Q}_i^T$, where $\mathbf{Q}_i \in \mathbb{R}^{3\times3}$. For example, $\mathbf{Q}_i = chol(\mathbf{D}_i)$ can be the *Cholesky decomposition,* in which case $\mathbf{Q}_i$ is lower triangular with non-negative diagonal elements. Note that $\mathbf{Q}_i$ and any of its "rotation and reflection" $\mathbf{Q}_i\mathbf{R}_i$ ($\mathbf{R}_i \in O(3)$) result in the same $\mathbf{D}_i$, i.e. $\mathbf{D}_i = \mathbf{Q}_i\mathbf{Q}_i^T = \mathbf{Q}_i\mathbf{R}_i(\mathbf{Q}_i\mathbf{R}_i)^T, i = 1, \ldots, N$.

Given a suitable distance function dist, the weighted Fréchet sample mean of $\mathbf{D}_1, \ldots, \mathbf{D}_N$ is defined by:

$$\bar{\mathbf{D}} \quad = \quad \arg\inf_{\mathbf{D}} \sum_{i=1}^{N} w_i \mathrm{dist}(\mathbf{D}_i, \mathbf{D})^2, \tag{1}$$

where the weights w_i satisfy $w_i \geq 0$ and $\sum_{i=1}^{N} w_i = 1$, and in applications can be, for example, a function of the Euclidean distance from the location of interest to the sampling locations (e.g. voxels).

Weighted generalized Procrustes analysis (WGPA) is proposed to estimate $\bar{\mathbf{D}}$ when $\mathrm{dist} = d_S$ is the size-and-shape distance (cf. (6) in (Dryden *et al.*, 2009)). It can then be shown that the *WGPA mean tensor* is given by

$$\bar{\mathbf{D}}_{WGPA} = \bar{\mathbf{Q}}_{WGPA} \bar{\mathbf{Q}}_{WGPA}^T, \tag{2}$$

where $\bar{\mathbf{Q}}_{WGPA} = \sum_{i=1}^{N} w_i \mathbf{Q}_i \hat{\mathbf{R}}_i$ and the orthogonal matrices $\hat{\mathbf{R}}_i, i = 1, \ldots, N$ minimize S_{WGPA}, the sum of weighted squared Euclidean norms which is given by

$$\begin{aligned} S_{WGPA}(\mathbf{D}_1, ..., \mathbf{D}_N) &= \inf_{\mathbf{R}_1,...,\mathbf{R}_N} \sum_{i=1}^{N} w_i \parallel \mathbf{Q}_i \mathbf{R}_i - \sum_{j=1}^{n} w_j \mathbf{Q}_j \mathbf{R}_j \parallel^2 \\ &= \inf_{\mathbf{R}_1,...,\mathbf{R}_N} \sum_{i=1}^{N} w_i \parallel (1 - w_i) \mathbf{Q}_i \mathbf{R}_i - \sum_{j \neq i} w_j \mathbf{Q}_j \mathbf{R}_j \parallel^2 \\ &= \inf_{\mathbf{R}_1,...,\mathbf{R}_N} \sum_{i=1}^{n} \frac{w_i}{(1 - w_i)^2} \parallel \mathbf{Q}_i \mathbf{R}_i - \frac{1}{(1 - w_i)} \sum_{j \neq i} w_j \mathbf{Q}_j \mathbf{R}_j \parallel^2 . \end{aligned} \tag{3}$$

Below we give Algorithm 1 for computing $\bar{\mathbf{Q}}_{WGPA}$:

Algorithm 1 Weighted Generalised Procrustes Method

Initial setting: $\mathbf{Q}_i^P \leftarrow chol(\mathbf{D}_i)$, $i = 1, ..., N$
S_{WGPA} from previous iteration: $S_p \leftarrow 0$
S_{WGPA} from current iteration: $S_c \leftarrow \sum_{i=1}^{N} w_i \parallel \mathbf{Q}_i^P - \sum_{j=1}^{N} w_j \mathbf{Q}_j^P \parallel^2$
while $|S_p - S_c| >$ tolerance **do**
  for $i = 1$ to N **do**
    $\bar{\mathbf{Q}}_i = \frac{1}{1-w_i} \sum_{j \neq i} w_j \mathbf{Q}_j^P$
    Calculate the $\hat{\mathbf{R}}_i$ minimising $\parallel \bar{\mathbf{Q}}_i - \mathbf{Q}_i^P \mathbf{R}_i \parallel$ (partial ordinary Procrustes analysis)
    $\mathbf{Q}_i^P \leftarrow \mathbf{Q}_i^P \hat{\mathbf{R}}_i$
  end for
  $S_p \leftarrow S_c$
  $S_c \leftarrow \sum_{i=1}^{N} w_i \parallel \mathbf{Q}_i^P - \sum_{j=1}^{N} w_j \mathbf{Q}_j^P \parallel^2$
end while
$\bar{\mathbf{Q}}_{WGPA} \leftarrow \sum_{i=1}^{N} w_i \mathbf{Q}_i^P$
return $\bar{\mathbf{Q}}_{WGPA}$

3 Results

3.1 Geodesic interpolation

Figure 1 presents geodesic interpolations of two synthetic DT's (in red) with Euclidean (d_E), Procrustes (d_S), Log-Euclidean (d_L) and Riemannian (d_R) metrics respectively. There is a clear swelling effect in the Euclidean case. However, Procrustes, Log-Euclidean and Riemannian means provide more reasonable interpolations.

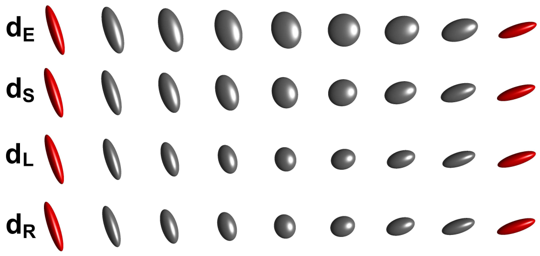

Figure 1: Geodesic interpolations between two anisotropic diffusion tensors (in red) with (top down) Euclidean d_E, Procrustes d_S, Log-Euclidean d_L and Riemannian d_R methods. (Colour figures will be included in the proceedings available online).

3.2 Applications to real data

A tensor field from a healthy human brain has been smoothed and interpolated (with 2 interpolations between each pair of original voxels). The Fractional Anisotropy (FA) maps from the processed tensors are shown in Figure 2. Obviously, the FA map from the processed tensor data is much smoother than the one without processing. The feature that the cingulum is distinct from the corpus callosum is clearer in the anisotropy map from the processed data (c,d) than in the unprocessed originals (a,b). Initial fibre tractography results for the brain stem of a healthy human have been shown in Figure 3. Evidently, the tractography based on the WGPA processed tensor field is different from the tractography based on the other methods, and work is currently underway to assess whether WGPA is preferable.

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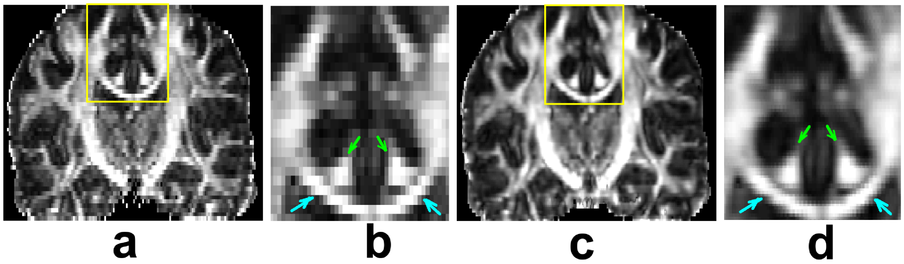

Figure 2: Smoothing and interpolation of the diffusion tensor data from a human brain. a: FA map from Bayesian estimate of the tensor field. c: FA map from processed tensor field. b and d: Zoomed inset regions. Green arrows: the cingulum. Cyan arrows: the corpus callosum. (Colour figures will be included in the proceedings available online)

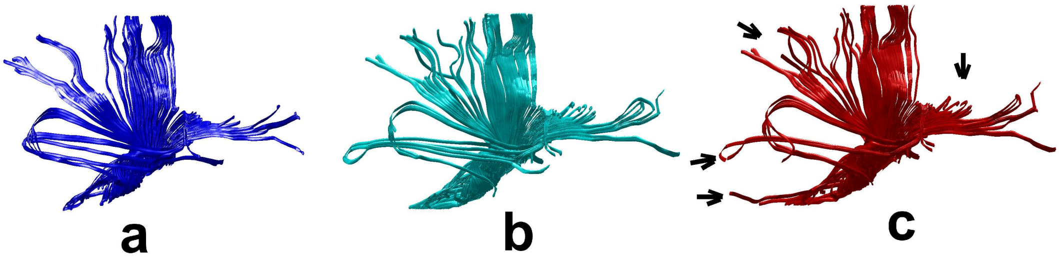

Figure 3: Fibre tractograhpies using the Bayesian estimates (a), Euclidean smoothing (b) and WGPA smoothing (c). Black arrows point out some obvious differences when the WGPA tracts are compared with the other methods.

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