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

Now consider a sample of N DT's \mathbf{D}_1 , ..., \mathbf{D}_N . To ensure the positive definiteness of DT's, a reparameterization is used, i.e., $\mathbf{D}_i = \mathbf{Q}_i \mathbf{Q}_i^T$, where $\mathbf{Q}_i \in \mathbb{R}^{3\times3}$. For example, $\mathbf{Q}_i = chol(\mathbf{D}_i)$ is the *Cholesky decomposition*, where \mathbf{Q}_i is lower triangular with positive diagonal elements. Note that \mathbf{Q}_i and any rotation and reflection of it $\mathbf{Q}_i \mathbf{R}_i$ ($\mathbf{R}_i \in O(3)$) can 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, ..., N.

The weighted Fréchet sample mean of $D_1, ..., D_N$ at N voxels with a certain distance function dist is defined by:

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

where the weights w_i are proportional to a function of the Euclidean distance between locations of the tensors (voxels), $0 \le w_i \le 1$ and $\sum_{i=1}^{N} w_i = 1$.

Weighted generalized Procrustes analysis (WGPA) is proposed to obtain the weighted mean of D_1 , ..., D_N . The objective of WGPA under rotation and reflection is to minimise a sum of weighted squared Euclidean norms S_{WGPA} which is given by

$$S_{WGPA}(\mathbf{D}_{1},...,\mathbf{D}_{N}) = \inf_{\mathbf{R}_{1},...,\mathbf{R}_{N}} \sum_{i=1}^{N} w_{i} \parallel \mathbf{Q}_{i}\mathbf{R}_{i} - \sum_{j=1}^{n} w_{j}\mathbf{Q}_{j}\mathbf{R}_{j} \parallel^{2}$$
$$= \inf_{\mathbf{R}_{1},...,\mathbf{R}_{N}} \sum_{i=1}^{N} w_{i} \parallel (1-w_{i})\mathbf{Q}_{i}\mathbf{R}_{i} - \sum_{j\neq i} w_{j}\mathbf{Q}_{j}\mathbf{R}_{j} \parallel^{2}$$
$$= \inf_{\mathbf{R}_{1},...,\mathbf{R}_{N}} \sum_{i=1}^{n} \frac{w_{i}}{(1-w_{i})^{2}} \parallel \mathbf{Q}_{i}\mathbf{R}_{i} - \frac{1}{(1-w_{i})} \sum_{j\neq i} w_{j}\mathbf{Q}_{j}\mathbf{R}_{j} \parallel^{2}.$$
(2)

Let $\hat{\mathbf{R}}_i, i = 1, ..., N$ be the estimates of the rotation matrices. Then, the WGPA mean tensor is given by

$$\bar{\mathbf{D}}_{WGPA} = \bar{\mathbf{Q}}_{WGPA} \bar{\mathbf{Q}}_{WGPA}^T,\tag{3}$$

where $\bar{\mathbf{Q}}_{WGPA} = \sum_{i=1}^{N} w_i \mathbf{Q}_i \hat{\mathbf{R}}_i$. We give Algorithm 1 for estimating $\hat{\mathbf{R}}_i, i = 1, ..., N$.

Algorithm 1 Weighted Generalised Procrustes Method

- 1: **Initial setting:** $Q_i^P \leftarrow chol(D_i), i = 1, ..., N$ 2: S_{WGPA} from previous iteration: $S_p \leftarrow 0$ 3: S_{WGPA} from current iteration: $S_c \leftarrow \sum_{i=1}^N w_i \parallel Q_i^P - \sum_{i=1}^N w_j Q_j^P \parallel^2$ 4: while $|S_p - S_c| >$ tolerance do
- for i = 1 to N do $\bar{Q}_i = \frac{1}{1 w_i} \sum_{j \neq i} w_j Q_j^P$ 5: 6:
- Calculate the rotation matrix R_i which minimises $\| \bar{Q}_i Q_i^P R_i \|$ with partial ordinary 7: Procrustes analysis O^{P}

8:
$$Q_i^P \leftarrow Q_i^P R_i$$

9: end for
10: $S_p \leftarrow S_c$
11: $S_c \leftarrow \sum_{i=1}^N w_i \parallel Q_i^P - \sum_{j=1}^N w_j Q_j^P \parallel^2$
12: end while

13: $\bar{Q}_{WGPA} \leftarrow \sum_{i=1}^{N} w_i Q_i^P$ 14: return 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 repectively. There is a clear swelling effect in Euclidean case. However, Procrustes, Log-Euclidean and Riemannian means provide more reasonable interpolations.

| d _E | | | | | | Ø | 0 |
|----------------|---|---|---|---|---|---|---|
| d _s | 0 | 0 | | | Ø | Ø | 0 |
| d∟ | 0 | 0 | ٥ | | Ø | Ø | 0 |
| d _R | 0 | 0 | 0 | ● | e | 0 | / |

Figure 1: Geodesic interpolations between two anisotropic diffusion tensors (in red) with Euclidean d_E , Procrustes d_S , Log-Euclidean d_L and Riemannian d_R methods from top to bottom.

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 than those without processing in Figure 2.



Figure 2: Smoothing and interpolation of the diffusion tensor data from human brain. a: FA map from Bayesian tensor field. c: FA map from processed tensor field. b and d: Zoomed inset regions. Green arrows: the cingulum. Light blue arrows: the corpus callosum.



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

Initial results of fibre tractographies of the brain stem in a healthy human brain have been shown in Figure 3. Tractography from WGPA processed tensor field is different from the other methods, and work is currently underway to assess whether WGPA is preferable.

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