SPATIALLY LOCAL AND TEMPORALLY SMOOTH PCA FOR FMRI

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ABSTRACT

PCA has found use as an exploratory technique for fMRI analysis. However, underlying it is an implicit model that while allowing temporal non-stationary covariance assumes the same covariance structure for all voxels. Here we relax this assumption for the first time by developing a version of PCA that allows the covariance structure to vary spatially. The new method is applied to real data and provides interesting new insight.

Index Terms—Biomedical Imaging, Magnetic Resonance Imaging

1. INTRODUCTION

Functional Magnetic Resonance Imaging (fMRI) is the dominant method for non-invasive dynamical analysis of brain function. It involves the use of Magnetic Resonance (MR) scanner to rapidly obtain images of brain state. fMRI allows the researcher to observe brain activity of a subject for example while it is performing some task and therefore better understand brain organization and function.

fMRI depends on the ability of MR scanners to detect regional changes in oxygenation level of the blood following neural activity [1]. That is, it indirectly observes brain activity on the neuronal level. The blood oxygen level dependency (BOLD) response to stimulus is often modelled as a hump like function that reaches maximum in about 5 seconds and dies out after about 10 seconds [2]. In practice it is usually assumed that the BOLD response is linearly related to the stimulus; [3] shows that this assumption is correct to the first order.

In a typical experiment an MRI scanner is used to record signals that can be used to construct a sequence of brain activation images with a typical sampling time 2-5 sec while the subject reacts to a stimulus, e.g., auditory, visual, motor, etc. A typical blocked experiment usually consists of two states; the control state and a functional state. The functional state could for example involve finger tapping or a visual fixation on a flickering image and the rest state involves no motor action or visual fixation on non-flickering image.

An fMRI experiment yields spatiotemporal data. The data can be represented as a $T \times M$ matrix $Y = [y_{t,v}]$ where $T$ is the number of time points and $M$ is the number of voxels (3D analogue of pixel). The $T \times 1$ column vector $y_{v}$ represents a voxel $v$ and its associated time series. The $1 \times M$ row vector $y_{v}^{T}(t)$ represents a brain image scanned at time $t$.

It is possible to classify methods to extract information from fMRI data sets in either univoxel or multivoxel methods. Univoxel methods [4] focus on one voxel at a time and model it as a sum of BOLD response, noise and possible some nuisance signals. Then an inference is made to determine if it is activated or not. An activation map is then constructed which is a binary map that can be overlayed on a brain map for interpretation. Multivoxel methods do not need information about the stimulus. They use all the voxels to find spatial or temporal components that are in some way representative of the data. The researcher hopes that the temporal/spatial components can be associated to some physiological effects of interest that are due to motion, activation etc. These components can then be used for modelling purposes or visualized for interpretation.

Although multivoxel methods are traditionally used as an exploratory tool they effectively assume a single (non-stationary) covariance structure for all voxels. The two most common multivoxel methods in fMRI research are Principal component analysis (PCA) [5] that finds temporal/spatial components of maximal variance and Independent component analysis (ICA) [6], [7] that finds spatial/temporal components that are as independent as possible.

This paper presents a spatially local version of the smooth PCA introduced in [8]. We hope to combine the spatial locality of univoxel methods and the ability of multivoxel methods to deal with non-stationary noise to build better models.

The proposed approach falls into the category of local likelihood methods [9] where each observation within the region of interest gets equal weight. The local PCA model relates to the maximum likelihood (ML) based noisy PCA model of Tipping et al [10], but further extended to allow for the temporal smoothness of the BOLD response by using basis expansion of the PCA loading matrix. This smoothness idea is not new in fMRI research. It was employed in different settings in [11] et al who used global PCA and controlled

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smoothness by regularization and in a earlier work [12] by
the second author who used the smoothness idea in a multi
subject setting. The ML framework allows use of the AIC
criteria to select two tuning parameter; the number of basis
functions and the number of principal components. Another
example of this is [13].

The paper is organized as follows. In Section 2 the stan-
dard univoxel method is discussed. In Section 3 we discuss
the multivoxel method. Section 4 discusses the proposed lo-
cal PCA model and section 5 details the associated model se-
lection problem. In section 6 results are given and finally in
section 7 conclusions are drawn.

2. STANDARD UNIVOXEL METHOD

In the standard univoxel approach hypothesis testing gener-
ates activation map. A test statistic is constructed to test the
null hypothesis that the activation coefficients \( \beta_v \) are zero. It
is then plotted spatially to provide the activation map. The
standard model for observed voxel time series is given by

\[ y_v = X\beta_v + \eta_v, \quad v = 1, ..., M, \]

where the prediction matrix \( X \) is a \( T \times p \) matrix of the BOLD
response along with nuisance signals such as drift and \( \eta_v \)
is an \( T \times 1 \) zero mean noise signal with covariance \( \Sigma_{\eta_v} \).

Generalized least squares gives an estimate of \( \hat{\beta}_v \)

\[ \hat{\beta}_v = (X^T \Sigma_{\eta_v}^{-1} X)^{-1} X^T \Sigma_{\eta_v}^{-1} y_v, \quad v = 1, ..., M. \]

The standard F or t test statistic is constructed to test the null
hypothesis and generate activation map. In practice the noise
covariance is unknown so \( \beta_v \) and \( \Sigma_{\eta_v} \) have to be estimated
jointly. To do that the structure of the noise covariance has
to be assumed. Conventionally it is assumed to be stationary.
An example is given in [14] for the ARMA(1) case.

3. MULTIVOXEL METHOD

The most common multivoxel methods in use in fMRI are
PCA and ICA. Traditional use is exploratory but [10] pro-
vides statistical model for PCA which enables much greater
insight and sets the stage for generalizations. The multivoxel
model is given by

\[ y_v = F \delta_v + \epsilon_v, \quad v = 1, ..., M, \]

where \( F \) is a \( T \times r \) loading matrix, \( \epsilon_v \sim N(0, \sigma^2 I_T) \) and \( \delta_v \)
is a random vector with zero mean and covariance equal to the
identity matrix. In the PCA case \( \delta_v \) is assumed to be Gaussian
but in the ICA case it is as far from Gaussian as possible. The
covariance matrix for the multivariate model is given by

\[ C = FF^T + \sigma^2 I_T \]

That is unlike the univoxel method the Noise covariance is
the same for all voxels. Also note that the covariance is non-
stationary. Due to the fact that the same model is used for all
voxels it is not obvious how to construct an activation map.

4. LOCAL PCA MODEL

In the multivoxel method described above the loading matrix
is the same for all voxels. Here we propose to relax that
by developing a spatial local approach to PCA. In this case
the model for voxel time series is given by

\[ y_v = \Phi_v B_v \delta_v + \epsilon_v, \quad v = 1, ..., M, \]

where \( \Phi_v \) is a \( T \times m_v \) matrix of pre-specified basis func-
tions for example Fourier or B-splines, \( B_v \) is a \( m_v \times r_v \) ma-
trix, \( B_v^T B_v = \Delta_{B_v} \) is diagonal, \( \delta_v \sim N(0, I_{r_v}) \) and \( \epsilon_v \sim N(0, \sigma^2 I_T) \). The parameters are estimated locally, i.e., the
data to estimate at voxel \( v \) comes from a \( k \times k \) window \( L_v \)
centered at voxel \( v \). Inside a local \( k \times k \) window \( L_v \) the model induces a distribution on the voxel time series, i.e.,

\[ y_v \sim N(0, C_v) \]

where \( C_v = \Phi_v B_v B_v^T \Phi_v^T + \sigma_v^2 I_T \). The local
log-likelihood is given by

\[ l_v(y_v \in L_v; \theta_v) = -\frac{k^2}{2} \text{trace}(C_v^{-1} S_{y_v}) - \frac{k^2}{2} \log |C_v| \]

where \( S_{y_v} = \frac{1}{k^2} \sum_{u \in L_v} y_u y_u^T \) is the sample covariance and \( \theta_v \) is a vector of the parameters to be estimated, which are \( \sigma^2_v \) and the elements of \( B_v \). Note that \( v \) refers to the location
in the neighborhood of \( v \). The local likelihood is maximized
when

\[ \hat{B}_v = K_v (D_v - \sigma^2_v I_{m_v})^{1/2} \]

where \( K_v \) is the \( m_v \times r_v \) matrix of unit eigenvectors of \( S_{\Phi_v} = (\Phi_v^T \Phi_v)^{-1/2} \Phi_v^T S_{y_v} \Phi_v (\Phi_v^T \Phi_v)^{-1/2} \) estimated at location \( v \)
and \( D_v \) is a \( r_v \times r_v \) diagonal matrix that contains the cor-
responding eigenvalues. When \( B_v = \hat{B}_v \) the maximum like-
lihood for \( \sigma^2_v \) is given by

\[ \sigma^2_v = \frac{\text{trace}(S_{y_v}) - \text{trace}(D_v)}{T - r} \]

The significance of the \( \Phi_v \) matrix is that it allows us to put
a smoothness constraint on the loading matrix by controlling
the number of basis functions. Note that when \( m_v = T \) the
columns \( \Phi_v B_v \) are simply the principal components. We have
here used uniform weighting within the window but other
weighting are possible.

5. MODEL SELECTION

The log-likelihood framework allows to use the AIC criteri-
unbiased esti-
mean Kullback-Liebler distance between mod-
eled density and the estimated density provided that the modelled density belongs to the same family of probability densities as the density that truly generated the data. This is probably not the case for fMRI but as pointed in [16] it is a good approximation provided that the true density and the modelled density are not grossly different. The usage is slightly unconventional in this case as we are selecting two tuning parameters, i.e., the number of basis functions and the number of principal components. The AIC at voxel $v$ is given by

$$AIC_v(m, r) = -2l_v(y_u \in L_v; \hat{\theta}_v) + 2 \text{dim(}\hat{\theta}_v),$$

where $\hat{\theta}_v$ is the maximum likelihood estimate of the parameter vector $\theta_v$, and $\text{dim}(\hat{\theta}_v)$ is the number of free parameters given by $\text{dim}(\hat{\theta}_v) = mr - r(r - 1)/2 + r + 1$. The parameters $m_v$ and $r_v$ are chosen so that they correspond to the minimum of the AIC.

6. RESULTS

The data comes from a combined visual/motor experiment where a human subject performed right hand finger-thumb opposition and watched a flickering annual checkerboard. Fig. 1 shows the stimulus signals for the finger-thumb opposition and the flickering checkerboard. When the signal is high the subject performs the task when it is low it rests. This data set is available on the AFNI homepage. The data was obtained from a 3T MRI scanner with 2 sec TR. Two brain slices are investigated one where motor response is expected and another where visual response is expected.

Fig. 2 shows activation maps for the brain slices using a simple model [17] for the BOLD response using the standard univoxel method and assuming that the noise is white. The data consisted of $T=100$ time points and each slice has $M = 4096 = 64^2$ voxels. The conventional spatial smoothing and temporal filtering were not done. A spatial plot of the data that shows a cross-section of the brain at particular time is given on Fig. 3. The front of the brain is in the upper portion of the image. The time series associated with two voxels are displayed on Fig. 4.

The model was fitted where for each voxel $\Phi_v$ was a basis of $m_v$ Fourier basis functions and the region of interest was

**Fig. 1.** The stimulus signals. Left: Motor stimulus. Right: Visual stimulus

**Fig. 2.** Left: Motor activation. Right: Visual activation

**Fig. 3.** An example of fMRI image slice.

**Fig. 4.** Examples of fMRI timeseries

**Fig. 5.** A spatial plot of the optimal number of principal components and basis functions for the motor slice.

**Fig. 6.** A spatial plot of the optimal number of principal components and basis functions for the visual slice.
9 \times 9. For each voxel the AIC was calculated for \( m = 0, \ldots, T \) and \( r < m \). Then the number of PCs \( r_v \) and the number of Fourier basis functions \( m_v \) were determined as the values that gave minimum AIC. Fig. 5 and 6 give a spatial map of the optimal \( m \) and \( r \) for the motor and visual slice respectively. We see that for both slices especially the motor slice the degree of smoothness (number of basis functions) is not uniform. This could indicate the presence of smooth biological processes like the BOLD response. The number of PCs for both slices is also not uniform. We see that the number of PCs near the superior sagittal sinus (back of the brain) is much greater than for other regions for the motor slice. This suggests that the PCA dimension in a traditional global model may be dominated by noise and that PCA dimension in activation region is much less. This suggests there may be possible to build non-stationary model which could be superior to traditional statistical model in activated regions.

7. CONCLUSION

We presented a spatially local and temporally smooth PCA method that combines the spatial locality of the univoxel method with the ability of PCA to deal with non-stationary noise. The method also allows to select the degree of smoothness and the number of principal components automatically with the AIC criterium. In experiments we demonstrated the non-stationary spatially varying nature of the covariance structure. This suggests that there may be possible to build non-stationary model which could be superior to traditional statistical model. In future work we aim to extend our model to include the BOLD response, i.e.,

\[
y_v = X \beta_v + \Phi v B_v \delta_v + \epsilon_v, \quad v = 1, \ldots, M
\]

where the prediction matrix \( X \) is \( T \times p \) containing the BOLD response. Note that this model extends the standard univoxel method by allowing for non-stationary noise. Work is also underway extending this method to use ICA instead of PCA.

8. REFERENCES


