Cortical surface reconstruction based on MEG data and spherical harmonics

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Abstract— Estimates of coefficients of a spherical harmonic Fourier decomposition of the cortical surface can be obtained solely using MEG/EEG data and free energy as objective function. A stochastic methodology based on a Metropolis Search followed by a Bayesian Model Averaging is proposed to reconstruct cortical anatomy based functional information.

I. INTRODUCTION

MEG/EEG brain imaging estimates neuronal activity based on magnetic or electrical fields due to neuronal activity measured outside the head. The non-invasive acquisition is a highly desirable characteristic of both MEG and EEG, but it complicates the reconstruction because of the resultant ill-posed inverse problem. Nowadays a large number of approaches are intended to reduce the uncertainty of the problem by defining it as linear, relating the neural activity and the data with a lead-field or propagation matrix [1], [2], commonly generated with a Structural Magnetic Resonance Image (sMRI) [3].

The use of a lead-field matrix introduces several extra challenges, especially because it has model reductions and linearisations that may affect the accuracy of the algorithms [3]. However this sensitivity to the underlying source model can be exploited. In a previous work we presented the possibility of using MEG data to reducing the uncertainty on the location of the brain due to co-registration error [4]. There, the location of the head inside the MEG helmet was unknown, and using the free energy value [5] as cost function (obtained with the Multiple Sparse Priors algorithm –MSP–, see [6]), it was possible to determine the most probable location of the head. In this paper we extent this idea and show how this approach can be extended to other characteristics of the brain such as its size and shape.

Several anatomical parameters such as the brain location, its size and shape can be related in a single mathematical model using a Fourier harmonic decomposition of the brain structure [7]–[9]. It consists of representing the cortical surface with a weighted sum of spherical harmonics. This Spherical Harmonic Representation (SPHARM) has several

advantages: (*i*) It is a tractable mathematical model of the cortical surface structure; (*ii*) it allows reducing the complexity of the brain structure whilst maintaining the topology of the surface (*iii*) it is a Fourier coefficient decomposition so different spatial scales are quantified in different harmonic components.

In this paper, an optimisation procedure for recovering the spherical harmonic coefficients of a subject specific cortical model using only functional MEG data is proposed, using the free energy for model selection as in [4]. Due to the non-linear relation between the free energy and the spherical harmonic coefficients, a Metropolis search [10] followed by a Bayesian Model Averaging stage [11] are used for recovering the structure of the cortical surface.

This paper is presented as follows, in Section II the SPHARM representation is introduced together with the effects of varying the coefficients, the use of free energy for model selection, and the estimation procedure used. In Section III synthetic MEG data generated with a realistic Boundary Elements Method (BEM) head model was used for recovering the SPHARM coefficients with no prior information. Finally, in Section IV concluding remarks are presented.

II. THEORY

In this section the spherical harmonic representation (SPHARM) is introduced in order to provide a mathematical model of the structure of the cortical surface. Then, using the negative variational free energy as a cost function, the parameters of this mathematical model will be adjusted to the best fitted model for a given MEG dataset, i.e., solely using MEG data it will be possible to recover structural characteristics.

A. Spherical harmonic representation of the cortical surface

Pial surface meshes can be extracted from sMRI using FreeSurfer [12] software package, and a weighted Fourier series (WFS) representation of the pial surface computed as in [8], allowing the surface to be expressed as a weighted linear combination of spherical harmonics. The WFS can be expressed as a kernel smoothing technique described by

$$
F_{\sigma}^{k}[f](p) = \sum_{l=0}^{k} \sum_{m=-l}^{l} e^{-l(l+1)\sigma} f_{lm} H_{lm}(p) \qquad (1)
$$

where σ is the bandwidth of the kernel, H_{lm} is the spherical harmonic of degree l and order m , and the Fourier coefficients are given by $f_{lm} = \langle f, H_{lm} \rangle$ where f is determined

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by solving a system of linear equations. p is the spherical parametrisation of a unit sphere, given in terms of the polar angle θ and azimuthal angle ϕ , as

$$
p = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))
$$
 (2)

with $p = (\theta, \phi) \in [0, \pi] \otimes [0, 2\pi]$. For this study, the Fourier series expansion bandwidth $\sigma = 0.001$, used for reconstruction of the pial surface, was selected based on a previous study [7].

Each spherical harmonic H_{lm} is related to a structural characteristic of the cortical surface, for example, as shown in Figure 1(b) the first harmonic (harmonic zero) of the original brain of Figure 1(a) is responsible of the location of the head inside the MEG helmet (co-registration). Each coefficient f_{lm} is formed by six parameters corresponding to the three Cartesian coordinates for each hemisphere. Figures $1(c)$ and $1(d)$ show variations in the y-axis parameters of several coefficients, controlling the size of the brain and the shape of the sulci. Note that all variations in the coefficients of Figure 1 were only performed over the left hemisphere, i.e., both hemispheres can be controlled independently.

Fig. 1. Figs. (b), (c) and (d) show different variations in the coefficients of the SPHARM of the brain of Fig. (a); note how they allow moving, resizing and modifying the shape of each hemisphere separately.

B. Free energy for model selection

The use of spherical harmonics gives the possibility to determine the best fitted structure of the cortical surface for a given MEG/EEG dataset. It can be achieved by determining the higher free energy value among several inverse solutions. The free energy [5] is a trade-off between the accuracy of the inverse solution and the complexity needed for obtaining it [13]. It approximates the log of the model evidence when the estimation of the neural activity approximates the truth.

Figure 2 shows the free energy for an increasing degree k of the Fourier series expansion, note that, for this simulated dataset, the free energy saturates at around $k = 20$ coefficients. In this example synthetic MEG data was used (see Section III for details).

Fig. 2. The number of harmonics used in the SPHARM directly affects the quality of the solution. A minimum of 20 harmonics provides stable free energy values when solving the MEG inverse problem.

The procedure to obtain the free energy value for each degree k in Figure 2 was the following: (*i*) Synthetic data were generated from 3 sources on a cortical surface formed from 42 harmonics (iii) After selecting the k value a new brain structure was obtained as proposed in [7], [8]; ((*iii*)) A lead-field matrix was generated for the new brain structure; $((iv))$ an inverse solution was obtained with the MSP algorithm using the new cortical surface and the original synthetic MEG data, and (v)) the free energy value of the solution was computed. All these stages were implemented within the SPM8 software package (http://www.fil.ion.ucl.ac.uk/spm/), including the lead-field computation with a 3-layers BEM head model.

The use of MEG data for recovering structural information has some constraints that must be accounted for. The anatomy can only be recovered if there is enough neural activity on it. Figure 3(a) shows simulated neural activity over the left hemisphere (the full experiment is explained in Section III), Figure 3(b) shows the free energy for the x -axis parameter of the first coefficient (head location) in the left hemisphere, a global maximum over the true value of the parameter is clear, but free energy landscape for variations in the parameters of the right hemisphere (where no source were simulated) is flat.

The translucent glass brains of Figure 3(a) show the frontal, lateral and superior views of the 512 dipoles with highest variance during the time windows of interest.

(a) Simulated neural activity in (b) Free energy for variations in SPHARM a single hemisphere coefficients

Fig. 3. (a) Synthetic MEG data from three sources of neural activity were simulated. (b) the free energy was used for determining the actual value of the parameters in the left hemisphere, right hemisphere parameters did not achieve a global maximum because of lack of information.

C. Metropolis search plus Bayesian Model Averaging for estimating the Fourier coefficients

Due to the high non-linearity of the parameters of each coefficient with respect to the free energy, added to noise issues and a large number of parameters (18 for the first three harmonics), it is necessary to implement a robust optimisation algorithm in order to recovery the actual values of the SPHARM coefficients. In this paper the same procedure proposed in [4] was implemented. It consists in a Metropolis search followed by a Bayesian Model Averaging (BMA) stage.

The metropolis search used consists in the following algorithm [4], [10]:

- 1) Select a random sample from the set of parameters that construct the coefficients of the spherical harmonics, solve the MSP algorithm and compute its free energy value.
- 2) Use a Gaussian proposal distribution to obtain a new set of parameters near their previous values. Perform the MSP reconstruction for the new head model and compute its free energy value.
- 3) Take a decision: if the free energy is higher than the previous iteration, accept it; if it is lower only accept it if compared with a random value it has higher probability (the free energy corresponds to a probability value).

4) Return to the second step and repeat until convergence. The algorithm converges once the mean and variance of the solution remain stable. The convergence criterion used here was the same of [4].

Once the Metropolis search has converged, a burn in of the first half of accepted values is performed in order to avoid dependency on the seed; then, a Bayesian Model Averaging is performed over the second half of accepted values. The BMA consists in averaging all the solutions based on their own probability, as follows:

- 1) Generate a posterior probability distribution of the solutions based on their approximated evidence (computed with the free energy).
- 2) Pick a set of parameters from this posterior probability distribution.
- 3) Obtain a normal random variable using the mean and covariance of the selected solution.
- 4) Iterate steps 2 and 3 at least 1000 times. The BMA is not computationally intensive, this stage can take less than 5 seconds.
- 5) Obtain a mean of the random variables.

These two stages will provide a mean and a interval of confidence of the set of parameters. This solution is not optimal but it is robust.

III. SIMULATION RESULTS

Several simulations with different configurations of sources of neural activity were performed to test the proposed approach. For each test a single trial dataset of 161 samples over 274 MEG sensors was generated by projecting the known neural source distribution into the sensor space. These neural sources consisted on pure sinusoidal signals. Gaussian white noise was added to the data to give a sensor level Signal to Noise Ratio (SNR) of zero decibels (same signal and noise power).

For each variation in the coefficients a new lead-field matrix was computed. The inverse solution used for each configuration was the MSP algorithm, it requires a distributed set of dipoles covering the cortical surface. For this experiment 8192 dipoles with fixed orientation perpendicular to the cortical surface were used, their location in the head was interpolated for each variation in the coefficients.

A. Metropolis search

For the example shown here, MEG data from three simulated sources of neural activity inside the left hemisphere (See Figure $3(a)$) were used. The three left hemisphere parameters of the first coefficient in the SPHARM were used for the optimisation, none prior information was used for recovering them (seeds from uniform distributions were selected, see their ranges in Table I). Due to the non-linearity of the free energy evolution, ten seeds were used and a Metropolis search was performed for each of them, Figure 4 shows the free energy values of 100 iterations of the selected chain of the Metropolis search.

B. Bayesian Model Averaging

Due to the non-linearity of the problem and the potentially large number of unknowns (although only three for this example) the Metropolis search may have accepted values at noisy local maxima, these effects can be mitigated using Bayesian Model Averaging. Also, the first half of accepted values must be burned out in order to avoid dependency on the seed. Then, the BMA stage was performed over the second half of accepted values of the selected chain (red circles in Figure 4).

The Table I shows the actual values of the three parameters, the seed of the selected chain and the final values of the parameters after the BMA stage. Note how large errors in the parameters were reduced to an average error of less

Fig. 4. Free energy evolution after 100 iterations of the Metropolis search, the red circles show the second half of accepted values used in the BMA stage.

than 1 %. The randomly selected seed had a L2-norm error of 62.2. The final value of the BMA over the second half of accepted values was accurate, with a norm error of 0.47.

TABLE I ERROR IN THE LEFT HEMISPHERE PARAMETERS OF THE FIRST HARMONIC COEFFICIENT.

	x parameter	$u parameter$	z parameter
true values	-113.89	-22.92	35.71
prior ranges	$[-2000]$	$[-100 100]$	$[-100 100]$
seeds	-105.61	-84.59	63.62
Initial error $(\%)$	7.27	269.05	78.15
Final values	-113.55	-22.61	35.61
Final error $(\%)$	0.30	1.37	0.29
Posterior variance	1.7	62	2.9

IV. CONCLUSIONS

In this paper a procedure to reconstruct the cortical surface with a spherical harmonic Fourier representation and MEG/EEG data was presented. It consists in recovering the parameters of the coefficients that weight the spherical harmonics, using the free energy for model comparison. Due to noise effects and high non-linearities, a Metropolis search followed by a Bayesian Model Averaging were used for providing a robust solution. This procedure allows reducing uncertainties in the forward modelling, and in future work we will look at the possibility of recovering a subject's cortical anatomys based on MEG data.

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