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The use of the asymptotic expansion to speed up the computation of a series of spherical harmonics

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Abstract. When a function is expressed as an infinite series of spherical harmonics the convergence can be accelerated by subtracting its asymptotic expansion and adding it in analytically closed form. In the present article this technique is applied to two biophysical cases: to the potential distribution in a spherically symmetric volume conductor and to the covariance matrix of biomagnetic measurements.

1. Introduction

In biophysical modelling a function is sometimes expressed as an infinite series of spherical harmonics. An example is the potential caused by a current source in an inhomogeneous spherical volume conductor representing the head. When this model is used to estimate sources on the basis of the measured potential distribution on the scalp, it is important to compute the potential as quickly as possible, because the potential has to be calculated on each iteration. However, without special precautions, many terms of the spherical harmonics expansion are needed to obtain accurate results. This is true for superficial sources, in particular. The technique we propose is based on the derivation of an asymptotic approximation of the function, which is known both in closed form and as a series of spherical harmonics. This approximation is then subtracted from the function as a series expansion and added in closed form. The resulting series of differences converges much faster than the original series, provided that the asymptotic approximation is properly weighted. Another example of the use of a spherical harmonic expansion is the lead field covariance matrix, which is used for minimum norm estimation (Hämäläinen and Ilmoniemi 1991). With the same technique as for the potential distribution in a spherical model, the computation time of these matrix elements can be reduced substantially.

2. The potential in a spherical volume conductor

To show how the proposed technique works, we will apply it to the special case of a dipole source in a three-sphere model. The spheres represent the brain, the skull and the scalp and have outer radii r_1, r_2 and r_3, respectively. It will be assumed that the conductivities of the brain and the scalp are equal and that ξ denotes the ratio of the skull and the brain conductivities. The field point (r_e, θ_e, ϕ_e) is located on the surface of the outermost sphere. For a dipole on the z-axis, lying in the x-z plane, we have the following expression for the potential ψ (Geselowitz 1967):

$$\psi = \sum_{n=1}^{\infty} f_n \frac{r_0^{n-1}}{r_e^{n-1}} \left(Q_r n P_{n0}(\cos\theta_e) + Q_t P_{n1}(\cos\theta_e)\cos\phi_e \right) \tag{1}$$

with

$$f_n = \frac{\xi}{4\pi\sigma r_1^2} \frac{(2n+1)^3}{n(n+1)}$$
$$\times\left[[(n+1)\xi+n]\left(\frac{n\xi}{n+1}+1\right)+(1-\xi)[(n+1)\xi+n](g_1^{2n+1}-g_2^{2n+1})-n(1-\xi)^2\left(\frac{g_1}{g_2}\right)^{2n+1}\right]^{-1} \tag{2}$$

Here, r_0 is the radial coordinate of the dipole, and Q_r and Q_t are its radial and tangential component, respectively. Finally, $g_1 \equiv r_3/r_1$ and $g_2 \equiv r_2/r_1$, so that $g_1, g_2 < 1$.
To find the asymptotic approximation f_n is expanded as follows:

$$f_n = \sum_{k=1}^{\infty} n^{-k} f^{(k)} + O(n^{-\infty}) \tag{3}$$

The $O(n^{-\infty})$ result from terms with g_i^{2n+1}. These terms are of order infinity, because $\lim_{n\to\infty} g_i^{2n+1}/n^{-k} \doteq 0$, for any finite k, and therefore they only contribute to the first few terms of equation (2). The kth order asymptotic approximation is defined as

$$\phi^{(k)}(\Lambda) = \sum_{n=1}^{\infty} \frac{\Lambda^{n-1}}{n^k} \left(Q_r n P_{n0}(\cos\theta_e) + Q_t P_{n1}(\cos\theta_e)\cos\phi_e \right) \tag{4}$$

and $f^{(0)}\phi^{(0)} + f^{(1)}\phi^{(1)} + f^{(2)}\phi^{(2)} + \ldots\ldots$ is called asymptotic expansion of ψ. For $k = 0$, 1 we can express $\phi^{(k)}$ in a closed form by taking appropriately chosen partial derivatives of the infinite medium potential (see Appendix). We obtain,

$$\phi^{(0)} = (Q_r(\cos\theta_e - \Lambda) + Q_t \sin\theta_e \cos\phi_e)\, R^{-3} \tag{5}$$

$$\phi^{(1)} = Q_r\left(\frac{1}{\Lambda R} - \frac{1}{\Lambda}\right) + Q_t \sin\theta_e \cos\phi_e \frac{1 + R^{-1}}{1 - \Lambda\cos\theta_e + R} \tag{6}$$

where R is the distance between the electrode and the dipole,

$$R = (1 - 2\Lambda\cos\theta_e + \Lambda^2)^{1/2} \tag{7}$$

If Λ is chosen as r_0/r_e and the coefficients $f^{(0)}$ and $f^{(1)}$ are chosen as

$$f^{(0)} = \frac{8\xi}{4\pi\sigma(1+\xi)^2 r_e^2} \quad \text{and} \quad f^{(1)} = \frac{4\xi}{4\pi\sigma(1+\xi)^2 r_e^2} \tag{8}$$

the expansions (1) and (4) match. Now ψ is expressed as

$$\psi = f^{(0)}\phi^{(0)} + f^{(1)}\phi^{(1)}$$
$$+ \sum_{i=1}^{\infty} (f_n - f^{(0)} - n^{-1} f^{(1)})\, \Lambda^{n-1} [Q_r n P_{n0}(\cos\theta_e) + Q_t P_{n1}(\cos\theta_e)\cos\phi_e] \tag{9}$$

Since $(Q_r \; nP_{n0} \; (\cos\theta_e) + Q_t P_{n1} \; (\cos\theta_e) \; \cos\phi_e) = O(n)$, the series of differences converges as $\Sigma n^{-1}\Lambda^n$, instead of as $\Sigma n\Lambda^n$, which represents the convergence of the original series. Therefore, much fewer terms are necessary to compute (9) than (1), with the same precision. Note that for this three-sphere model, we have $f^{(0)} = 2f^{(1)}$ and, therefore, the sum $f^{(0)}\phi^{(0)} + f^{(1)}\phi^{(1)}$ has a clear physical interpretation: it is the potential caused by a dipole in a homogeneous sphere (substitute $\xi = 1$ into equation (2)). This is however not true for the general sphere model. With the formulae presented in De Munck (1988), the asymptotic expansion can be found for the potential in the general (anisotropic) concentric sphere model. In this model the field point is not restricted to the outer surface, which is useful for analysing recordings from patients with implanted electrodes. It can be shown that in this model the asymptotic expansion has the following properties (the derivation is given in De Munck and Peters (1991)):

1. When the layers are anisotropic, the weights $f^{(k)}$ and Λ only depend on the radii and conductivities of the layers between (and including) the electrode and the dipole.

2. When all layers between the source and the field point are isotropic then the matching Λ is given by r_0/r_e; if one (or more) of those layers are anisotropic then Λ is disturbed by that layer(s).

3. Under the conditions of (2), the parameters $f^{(k)}$ are independent of the radii, as is the case with the three-sphere model.

4. When the dipole is in an anisotropic layer, the weighing coefficients $f^{(k)}$ are different for a radial and a tangential dipole. Their ratio equals the ratio of the radial and tangential conductivity.

Since the asymptotic expansion $f^{(0)}\phi^{(0)} + f^{(1)}\phi^{(1)} + f^{(2)}\phi^{(2)}$ is devised as an approximation of the true potential, properties (1) - (4) shed some light on the dependence of the potential on the volume conductor. Note, however, that in this expansion the infinite order terms are omitted, whereas they do have an influence on the lower order terms of the spherical harmonic expansion (1).

3. The lead field covariance matrix

Hämäläinen and Ilmoniemi (1991) derived a method to interpolate electromagnetic data based on minimum norm estimates. Their method can be summarised with the following formula:

$$B_i' = \sum_{jk} C_{ij}' \; C_{jk}^{\text{inv}} B_k \tag{10}$$

where B_k are the measured magnetic fields, and B_i' are the interpolated values. C_{jk} is the lead field covariance matrix, defined by

$$C_{jk} = \int \mathrm{d}\boldsymbol{x} \, f(\boldsymbol{x}) \; \boldsymbol{L}(\boldsymbol{x};\boldsymbol{x}_j,\boldsymbol{n}_j)\cdot \boldsymbol{L}(\boldsymbol{x};\boldsymbol{x}_k,\boldsymbol{n}_k) \tag{11}$$

where $\boldsymbol{x}_j$ are the measurement points. Similarly, the C_{ji}' denote the covariance matrix for the combinations of the measurement points with the interpolation points. In equation (11) $\boldsymbol{L}(\boldsymbol{x};\boldsymbol{x},\boldsymbol{n}_j)$ is the lead field corresponding to B_j, i.e. if $\boldsymbol{B}(\boldsymbol{x};\boldsymbol{x}_j)\cdot\boldsymbol{n}_j$ is the magnetic field at the point $\boldsymbol{x}_j$, in the direction n_j, caused by a dipole $\boldsymbol{Q}$ at $\boldsymbol{x}$, then

$$\boldsymbol{B}(\boldsymbol{x};\boldsymbol{x}_j)\cdot\boldsymbol{n}_j = \boldsymbol{Q}\cdot\boldsymbol{L}(\boldsymbol{x};\boldsymbol{x}_j,\boldsymbol{n}_j). \tag{12}$$

In this formulation, the computation of each matrix element of C requires a three-dimensional integration and, therefore, the method is very time consuming. To speed up the computation using the asymptotic expansion, the integrals should first be expressed in a series of spherical harmonics. It can be shown (De Munck *et al* 1991) that, for $f(\mathbf{x}) = r^2\delta(r_0 - r)$, C_{jk} can be expressed as

$$C_{jk} = (\boldsymbol{n}_j \cdot \nabla_j)(\boldsymbol{n}_k \cdot \nabla_k)\frac{\mu_0^2}{4\pi}\sum_{n=1}^{\infty}\frac{n}{(n+1)(2n+1)}\frac{r_0^{2n+2}}{(r_j r_k)^{n+1}}P_{n0}(\cos\omega_{jk}) \tag{13}$$

where

$$\cos\omega_{jk} = \cos\theta_j\cos\theta_k + \sin\theta_j\sin\theta_k\cos(\phi_j - \phi_k) \tag{14}$$

is the angle between the positions of the magnetometers j and k. (r_j, θ_j, ϕ_j) are the spherical coordinates of the jth magnetometer, $\boldsymbol{n}_j \cdot \nabla_j$ is the corresponding directional derivative and r_0 denotes the dipole layer radius.

With equation (13) the computation time is already substantially reduced. Now Λ is defined as $r_0^2 r_j^{-1} r_k^{-1}$ and $n/[(n+1)(2n+1)]$ is expanded as $1/(2n) - 3/(2n^2) + O(n^{-3})$. When the first-order approximation is expressed in closed form we obtain:

$$\mu_0^2\sum_{n=1}^{\infty}\frac{1}{n}\Lambda^n P_{n0}(\cos\omega) = -\mu_0^2\ln\frac{1 - \Lambda\cos\omega + (1 - 2\Lambda\cos\omega + \Lambda^2)^{1/2}}{2} \tag{15}$$

The logarithm in equation (15) seems to spoil the advantages of the asymptotic expansion method. However, we still have to take the partial derivatives of equation (15) and then the logarithm will disappear.

When both gradiometers are radial, a simpler formula is obtained. After taking the partial derivatives with respect to r_j and r_k we obtain

$$C_{jk} = \frac{\mu_0^2}{16\pi}\sum_{n=1}^{\infty}\left(2n+1 - \frac{1}{2n+1}\right)\frac{r_0^{2n+2}}{(r_j r_k)^{n+2}}P_{n0}(\cos\omega_{jk}) \tag{16}$$

Here the sum of the terms with $2n+1$ is easily recognised as the potential of a radial dipole in a homogeneous conducting sphere, which can be expressed in closed form using equations (5) - (7).

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Appendix

In this appendix it is shown how an analytically closed expression can be derived for the zeroth and first-order approximation of ψ. The derivation is based on the expansion of the monopole potential in Legendre polynomials:

$$R^{-1} = \sum_{n=0}^{\infty} \Lambda^n P_{n0}(\cos\theta_e) \tag{A.1}$$

If we differentiate this equation with respect to Λ or to θ_e, we find equation (5). If the term with $n = 0$ in (A.1) is omitted, and the result is divided by Λ, we have the radial part of equation (6). If subsequently the radial part of equation (6) is integrated over Λ, equation (15) is obtained. Finally, if equation (15) is differentiated with respect to θ_e, we obtain the tangential part of equation (6).