Non-singular spherical harmonic expressions of geomagnetic vector and gradient tensor fields in the local north-oriented reference frame

By

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Abstract

General expressions of magnetic vector (MV) and magnetic gradient tensor (MGT) in terms of the first- and second-order derivatives of spherical harmonics at different degrees/orders, are relatively complicated and singular at the poles. In this paper, we derived alternative non-singular expressions for the MV, the MGT and also the third-order partial derivatives of the magnetic potential field in local north-oriented reference frame. Using our newly derived formulae, the magnetic potential, vector and gradient tensor fields and also the third-order partial derivatives of the magnetic potential field at an altitude of 300 km are calculated based on a global lithospheric magnetic field model GRIMM_L120 (version 0.0) with spherical harmonic degrees 16–90. The corresponding results at the poles are discussed and the validity of the derived formulas is verified using the Laplace equation of the magnetic potential field.

1 Introduction

Compared to the magnetic vector and scalar measurements, magnetic gradients lead to more robust models of the lithospheric magnetic field. The ongoing Swarm mission of the European
Space Agency (ESA) provides measurements not only of the vector and scalar data but also an estimate of their east-west gradients (e.g. Olsen et al., 2004, 2015; Friis-Christensen et al., 2006). Kotsiaros and Olsen (2012, 2014) proposed to recover the lithospheric magnetic field through Magnetic Space Gradiometry in the same way that has been done for modeling the gravitational potential field from the satellite gravity gradient tensor measurements by the Gravity field and steady-state Ocean Circulation Explorer (GOCE). Purucker et al. (2005, 2007), Sabaka et al. (2015) and Kotsiaros et al. (2015) also reported efforts to model the lithospheric magnetic field using magnetic gradient information from the satellite constellation. Their results showed that by using gradients data, the modeled lithospheric magnetic anomaly field has enhanced shorter wavelength content and has a much higher quality compared to models built from vector field data. This is because the gradients data can remove the highly time-dependant contributions of the magnetosphere and ionosphere that are correlated between two side-by-side satellites.

The order-2 magnetic gradient tensor consists of spatial derivatives highlighting certain structures of the magnetic field (e.g. Schmidt and Clark, 2000, 2006). It can be used to detect the hidden and small-scale magnetized sources (e.g. Pedersen and Rasmussen, 1990; Harrison and Southam, 1991) and to investigate the orientation of the lineated magnetic anomalies (e.g. Blakely and Simpson, 1986). Quantitative magnetic interpretation methods such as the analytic signal, edge detection, spatial derivatives, Euler deconvolution, and transforms, all set in Cartesian coordinate system (e.g. Blakely, 1995; Purucker and Whaler, 2007; Taylor et al., 2014) also require calculating the higher-order derivatives of the magnetic anomaly field and need to be extended to regional and global scales to handle the curvature of the Earth and other planets. Ravat et al. (2002) and Ravat (2011) utilized the analytic signal method and the total gradient to interpret...
the satellite-altitude magnetic anomaly data. Therefore, both the magnetic field modeling and also the geological interpretations require the calculation for the partial derivatives of the magnetic field, possibly at the poles for specific systems of coordinates. Spherical harmonic analysis, established originally by Gauss (1839), is generally used to model the global magnetic internal fields of the Earth and other terrestrial planets (e.g. Maus et al., 2008; Langlais et al., 2009; Thébault et al., 2010, Finlay et al., 2010; Lesur et al., 2013, Sabaka et al., 2013; Olsen et al., 2014). Series of spherical harmonic functions themselves made of Schmidt semi-normalized associated Legendre functions (SSALFs) (e.g. Blakely, 1995; Langel and Hinze, 1998), are fitted by least-squares to magnetic measurements, giving the spherical harmonic coefficients (i.e. the Gaussian coefficients) defining the model. Kotsiaros and Olsen (2012, 2014) presented the MV and the MGT using a spherical harmonic representation and, of course, their expressions are singular as they approach the poles. Even if there are satellite data gaps around the poles, it is advisable to use non-singular spherical harmonic expressions for the MV and the MGT in case airborne or shipborne magnetic data are utilized (e.g. Golynsky et al., 2013; Maus, 2010). A rotation of the coordinate system is always possible to avoid the polar singularity, but this solution is very ineffective for large data sets.

In this paper, following Petrovskaya and Vershkov (2006) and Eshagh (2008, 2009) for the gravitational gradient tensor in the local north oriented, orbital reference and geocentric spherical frames, the non-singular expressions in terms of spherical harmonics for the MV, the MGT and the third-order derivatives of the magnetic potential field in the specially defined local-north-oriented reference frame (LNORF) are presented. In the next section, the traditional expressions of the MV and the MGT are first stated, then some necessary propositions are proved and at last new
non-singular expressions are derived. In Section 3, the new formulae are tested using the global lithospheric magnetic field model GRIMM_L120 (version 0.0) (Lesur et al., 2013) and compared with the results by traditional formulae. Finally, some conclusions are drawn and further applications are also discussed.

2 Methodology

In this section, the traditional expressions of MV and MGT are presented, and their numerical problems are stated. Then based on some necessary mathematical derivations, new expressions are given.

2.1 Traditional expressions

The scalar potential $V$ of the Earth’s magnetic field in a source-free region can be expanded in the truncated series of spherical harmonics at the point $P(r, \theta, \phi)$ with the geocentric distance $r$, co-latitude $\theta$ and longitude $\phi$ (e.g. Backus et al., 1996):

$$V(r, \theta, \phi) = a \sum_{l=1}^{L} \sum_{m=-l}^{l} \frac{1}{r^{l+1}} \left( g_l^m \cos m\phi + h_l^m \sin m\phi \right) \tilde{P}_l^m \left( \cos \theta \right),$$  

(1)

where $a=6371.2$ km is the radius of the Earth’s magnetic reference sphere; $\tilde{P}_l^m \left( \cos \theta \right)$ (or $\tilde{D}_l^m$ for simplification) is the SSALF of degree $l$ and order $m$; $L$ is the maximum spherical harmonic degree; $g_l^m$ and $h_l^m$ are the geomagnetic harmonic coefficients describing internal sources of the Earth.

If considered in the LNORF $\{x, y, z\}$ (e.g. Olsen et al., 2010), where $z$-axis points downward in geocentric radial direction, $x$-axis points to the north, and $y$-axis towards the east (that is, a right-handed system). At the poles, we define that the $x$-axis points to the meridian of $180^\circ$ E (or
three components of the MV can be expressed as:

\[
B_x(r, \theta, \varphi) = \frac{1}{r} \frac{\partial}{\partial(-\varphi)} V(r, \theta, \varphi) \\
= \sum_{l=1}^{l+2} \left( \sum_{m=0}^{l} \frac{a}{r} \right) g^m \cos m \varphi + h^m \sin m \varphi \left[ \frac{d}{d\theta} \tilde{P}_l^m(\cos \theta) \right],
\]

(2a)

\[
B_y(r, \theta, \varphi) = -\frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} V(r, \theta, \varphi) \\
= \sum_{l=1}^{l+2} \left( \sum_{m=0}^{l} \frac{a}{r} \right) m g^m \sin m \varphi - h^m \cos m \varphi \left[ \frac{1}{\sin \theta} \tilde{P}_l^m(\cos \theta) \right],
\]

(2b)

\[
B_z(r, \theta, \varphi) = -\frac{\partial}{\partial(-r)} V(r, \theta, \varphi) \\
= -\sum_{l=1}^{l+2} \left( \sum_{m=0}^{l+1} \right) \left( g^m \cos m \varphi + h^m \sin m \varphi \right) \tilde{P}_l^m(\cos \theta).
\]

(2c)

The MGT can be written as (e.g. Kotsiaros and Olsen, 2012)

\[
\nabla B = \begin{pmatrix} B_{xx} & B_{xy} & B_{xz} \\ B_{yx} & B_{yy} & B_{yz} \\ B_{zx} & B_{zy} & B_{zz} \end{pmatrix} = \begin{pmatrix} \partial B_x / \partial x & \partial B_x / \partial y & \partial B_x / \partial z \\ \partial B_y / \partial x & \partial B_y / \partial y & \partial B_y / \partial z \\ \partial B_z / \partial x & \partial B_z / \partial y & \partial B_z / \partial z \end{pmatrix}
\]

(3)

where nine elements are expressed respectively as:

\[
B_{xx} = \frac{1}{a} \sum_{l=1}^{l+2} \left( \sum_{m=0}^{l} \frac{a}{r} \right) g^m \cos m \varphi + h^m \sin m \varphi \\
\times \left[ -\frac{d^2}{d\theta^2} \tilde{P}_l^m(\cos \theta) + (l+1) \tilde{P}_l^m(\cos \theta) \right],
\]

(4a)

\[
B_{xy} = B_{yx} = \frac{1}{a} \sum_{l=1}^{l+2} \left( \sum_{m=0}^{l} \frac{a}{r} \right) m g^m \sin m \varphi - h^m \cos m \varphi \\
\times \left[ -\frac{1}{\sin \theta} \frac{d}{d\theta} \tilde{P}_l^m(\cos \theta) + \frac{\cos \theta}{\sin^2 \theta} \tilde{P}_l^m(\cos \theta) \right],
\]

(4b)

\[
B_{xz} = B_{zx} = \frac{1}{a} \sum_{l=1}^{l+2} \left( \sum_{m=0}^{l} \frac{a}{r} \right) (l+2) g^m \cos m \varphi + h^m \sin m \varphi \left[ \frac{d}{d\theta} \tilde{P}_l^m(\cos \theta) \right],
\]

(4c)
The expressions for $V$, $B_z$, and $B_{zz}$ can be calculated stably even for very high spherical harmonic degrees and orders by using the Holmes and Featherstone (2002a) scheme. However, there exist the singular terms of $1/\sin \theta$ and $1/\sin^2 \theta$ in Eq. (2b), Eq. (4b), Eq. (4d) and Eq. (4e) when the computing point approaches to the poles. Besides, some expressions contain the terms of first- and second-order derivatives of SSALFs, such as Eq. (2a) and Eq. (4a) ~ (4d). Nevertheless, the derivatives up to second-order for very high degree and orders of SSALFs can be recursively calculated by the Horner algorithm (Holmes and Featherstone, 2002b). These algorithms are relatively complicated and thus we want to use alternative expressions to avoid the singular terms and also the partial derivatives of SSALFs. It should be stated that our work differs from those presented by Petrovskaya and Vershkov (2006) and Eshagh (2009) in the LNORF and also the associated Legendre functions (ALFs). Nonetheless, the following mathematical derivations are carried out based on their studies in gravity field.

### 2.2 Mathematical derivations

To deal with the singular terms and first- and second-order derivatives of the SSALFs, some useful mathematical derivations are introduced and proved in the following.

1. **Derivation of $d \tilde{P}^m_l / d \theta$:**
Based on Eq. (Z.1.44) in Ilk (1983)

\[
\frac{dP_i^m}{d\theta} = 0.5\left[(l + m)(l - m + 1)P_i^{m-1} - P_i^{m+1}\right], 
\]
(5)

and the relation between the ALFs and the SSALFs as

\[
\tilde{P}_i^m = \sqrt{C_m(l - m)l(l + m)}P_i^m,
\]
(6)

thus the first-order derivative of the SSALFs can be deduced as:

\[
\frac{d\tilde{P}_i^m}{d\theta} = a_{i,m}\tilde{P}_i^{m-1} + b_{i,m}\tilde{P}_i^{m+1},
\]
(7a)

\[
a_{i,m} = 0.5\sqrt{l + m}\sqrt{l - m + 1}\sqrt{C_m/C_{m-1}},
\]
(7b)

\[
b_{i,m} = -0.5\sqrt{l + m + 1}\sqrt{l - m}\sqrt{C_m/C_{m+1}},
\]
(7c)

where \( C_m = 2 - \delta_{m,0} \) and \( \delta \) is the Kronecker delta.

2 - Derivation of \( \frac{d^2\tilde{P}_i^m}{d\theta^2} \):

According to Eq. (23) in Eshagh (2008) as

\[
\frac{d^2P_i^m}{d\theta^2} = 0.25(l + m)(l - m + 1)(l + m - 1)P_i^{m-2}
\]

\[
- 0.25[(l + m)(l - m + 1) + (l - m)(l + m + 1)]P_i^m,
\]
\[
+ 0.25P_i^{m+2}
\]
(8)

the second-order derivative of the SSALFs can be written as:

\[
\frac{d^2\tilde{P}_i^m}{d\theta^2} = c_{i,m}\tilde{P}_i^{m-2} + d_{i,m}\tilde{P}_i^m + e_{i,m}\tilde{P}_i^{m+2},
\]
(9a)

\[
c_{i,m} = 0.25\sqrt{l + m}\sqrt{l + m - 1}\sqrt{l - m + 2}\sqrt{l - m + 1}\sqrt{C_m/C_{m-2}},
\]
(9b)

\[
d_{i,m} = -0.25[(l + m)(l - m + 1) + (l - m)(l + m + 1)],
\]
(9c)

\[
e_{i,m} = 0.25\sqrt{l + m + 2}\sqrt{l + m + 1}\sqrt{l - m}\sqrt{l - m - 1}\sqrt{C_m/C_{m+2}}.
\]
(9d)

3 - Derivation of \( \frac{P_i^m}{\sin \theta} \):

Using Eq. (Z.1.42) in Ilk (1983)

\[
\frac{P_i^m}{\sin \theta} = 0.5\left[(l + m)(l + m - 1)P_i^{m-1} + P_i^{m+1}\right]/m, \quad m \geq 1,
\]
(10)

and Eq. (6), we can obtain that
\[ \frac{\tilde{P}^n_i}{\sin \theta} = f_{l,m} \tilde{P}^{m-1}_{l-1} + g_{l,m} \tilde{P}^{m+1}_{l-1}, \quad m \geq 1, \]  
\[ f_{l,m} = 0.5 \sqrt{l + m + 1} \sqrt{l + m - 1} \frac{C_m}{C_{m-1}} \frac{m}{m}, \quad m \geq 1, \]  
\[ g_{l,m} = 0.5 \sqrt{l - m + 1} \sqrt{l - m - 1} \frac{C_m}{C_{m+1}} \frac{m}{m}, \quad m \geq 1, \]  
\[ 4 - \text{Derivation of } \frac{\tilde{P}^n_i}{\sin^2 \theta}: \]

Employing Eq. (31) in Eshagh (2008) as

\[ P^m_i / \sin^2 \theta = \left[ (l + m)(l + m - 1)(l - m + 1)(l - m + 2)/(m - 1)P^{m-2}_i \right. \]
\[ + \left[ (l + m)(l + m - 1)/(m - 1) + (l - m)(l - m - 1)/(m + 1) \right] P^m_i \]
\[ + 1/(m + 1)P^{m+2}_i \right] / (4m), \quad m \geq 2, \]  
\[ \text{and Eq. (6), we have} \]

\[ \tilde{P}^n_i / \sin^2 \theta = h_{l,m} \tilde{P}^{m-2}_i + k_{l,m} \tilde{P}^m_i + n_{l,m} \tilde{P}^{m+2}_i, \quad m \geq 2, \]  
\[ h_{l,m} = 0.25 \sqrt{l + m + 1} \sqrt{l - m + 1} \sqrt{l + m + 2} \frac{C_m}{C_{m-2}} \frac{m}{m(m - 1)}, \quad m \geq 2, \]  
\[ k_{l,m} = 0.25 \left[ (l + m)(l + m - 1)/(m - 1) + (l - m)(l - m - 1)/(m + 1) \right] / m, \quad m \geq 2, \]  
\[ n_{l,m} = 0.25 \sqrt{l - m + 1} \sqrt{l - m - 1} \sqrt{l + m + 2} \frac{C_m}{C_{m+2}} \frac{m}{m(m + 1)}, \quad m \geq 1. \]  
\[ 5 - \text{Derivation of } d\tilde{P}^n_i / (\sin \theta \theta) : \]

Using Eq. (36) in Eshagh (2008) as

\[ dP^m_i / (\sin \theta \theta) = \frac{0.25 \left[ (l + m)(l + m - 1)(l - m - 1)/(m - 1)P^{m-2}_i \right. \]
\[ + \left[ (l + m)(l - m + 1)/(m - 1) - (l + m + 1)(l + m)/(m + 1) \right] P^m_i \]
\[ - 1/(m + 1)P^{m+2}_i \right] } / (4m), \quad m \geq 2, \]
\[ \text{and Eq. (6), we can derive} \]

\[ d\tilde{P}^n_i / (\sin \theta \theta) = o_{l,m} \tilde{P}^{m-2}_i + q_{l,m} \tilde{P}^m_i + x_{l,m} \tilde{P}^{m+2}_i, \quad m \geq 2, \]  
\[ o_{l,m} = 0.25 \sqrt{l + m + 1} \sqrt{l + m + 2} \frac{C_m}{C_{m-2}} \frac{m}{m}, \quad m \geq 2, \]  
\[ q_{l,m} = 0.25 \sqrt{l - m + 1} \sqrt{l - m + 2} \frac{C_m}{C_{m+2}} \frac{m}{m}, \quad m \geq 2, \]  
\[ x_{l,m} = -0.25 \sqrt{l + m + 1} \sqrt{l - m - 1} \sqrt{l - m - 2} \frac{C_m}{C_{m+2}} \frac{m}{m + 1}. \]  
\[ 6 - \text{Derivation of } d\tilde{P}^n_i / (\sin \theta \theta) - \tilde{P}^n_i \cos \theta / \sin^2 \theta : \]
According to Petrovskaya and Vershkov (2006) and Eshagh (2009), we can write
\[
\frac{dP_i^m}{(\sin \theta d\theta)} - P_i^m \cos \theta / \sin^2 \theta = 0.5\left[ (m-1)(l+m)(l-m+1)P_{i-1}^{m-1} / \sin \theta - (m+1)P_i^{m+1} / \sin \theta \right] / m, \quad m \geq 1, \tag{16}
\]
and using Eq. (36) in Eshagh (2008), we can obtain
\[
P_i^{m-1} / \sin \theta = 0.5\left[ (l-m)(l-m+3)P_{i+1}^{m-2} + P_i^m \right] (m-1), \quad m \geq 2, \tag{17a}
\]
\[
P_i^{m+1} / \sin \theta = 0.5\left[ (l-m)(l-m+1)P_i^m + P_{i+1}^{m+2} \right] / (m+1). \tag{17b}
\]
Substituting Eq. (17) into the right hand side of Eq. (16) and after simplification, we can derive
\[
\frac{dP_i^m}{(\sin \theta d\theta)} - P_i^m \cos \theta / \sin^2 \theta = 0.25\left[ (l+m)(l-m+1)(l-m+3)P_{i+1}^{m-2}, \quad m \geq 1. \tag{18}
\right.\]
\[
+ 2m(l-m+1)P_i^m - P_{i+1}^{m+2} \right] / m
\]
And coming Eq. (6), we obtain that
\[
\frac{d\tilde{P}_i^m}{(\sin \theta d\theta)} - \tilde{P}_i^m \cos \theta / \sin^2 \theta = 0.25\left[ \sqrt{l+m}\sqrt{l-m+1}\sqrt{l-m+3}\sqrt{C_m} / C_{m-2} \tilde{P}_{i+1}^{m-2}
\right.\]
\[
+ 2m\sqrt{l-m+1}\sqrt{l+m+1}\tilde{P}_i^m
\]
\[
- \sqrt{l+m+1}\sqrt{l+m+2}\sqrt{l+m+3}\sqrt{l-m}\sqrt{C_m} / C_{m+2} \tilde{P}_{i+1}^{m+2} \right] / m, \quad m \geq 1. \tag{19}
\]
\[7\) - Derivation of \[\left[ (l+1)\sin^2 \theta \tilde{P}_i^m + m^2 \tilde{P}_i^m \sin \theta \cos \theta \tilde{P}_i^m / d\theta \right] / \sin^2 \theta :\]
\[
\sin \theta \cos \theta \d \tilde{P}_i^m / d\theta = m\tilde{P}_i^m + (l+1)\sin^2 \theta \partial \tilde{P}_i^m - \sin \theta \tilde{P}_{i+1}^{m+1}. \tag{20}
\]
we can derive
\[
\left[ (l+1)\sin^2 \theta \tilde{P}_i^m + m^2 \tilde{P}_i^m - \sin \theta \cos \theta \tilde{P}_i^m / d\theta \right] / \sin^2 \theta
\]
\[
= m(m-1)\tilde{P}_i^m / \sin^2 \theta + \tilde{P}_{i+1}^{m+1} / \sin \theta \tag{21}
\]
According to Eq. (10), we can write
\[
P_{i+1}^{m+1} / \sin \theta = 0.5\left[ (l+m+2)(l+m+1)P_i^m + P_{i+1}^{m+2} \right] / (m+1). \tag{22}
\]
Inserting Eq. (12) and Eq. (22) into Eq. (21), and after some simplifications, we obtain that
\[ (l + 1) \sin^2 \theta P_l^m + m^2 P_l^m - \sin \theta \cos \theta \partial \tilde{P}_l^m / \partial \theta \] / \sin^2 \theta \\
= 0.25(l + m)(l + m - 1)(l + m + 1)(l + m + 2)P_l^{m-2} \\
+ 0.25[l + m(l + m - 1) + (l - m)(l - m - 1)(m - 1)/(m + 1)]P_l^m \\
+ 2(l + m + 2)(l + m + 1)/(m + 1)\tilde{P}_l^m + 0.25P_l^{m+2} \quad (23)

And combing with Eq. (6), we can derive
\[ (l + 1) \sin^2 \theta \tilde{P}_l^m + m^2 \tilde{P}_l^m - \sin \theta \cos \theta \partial \tilde{P}_l^m / \partial \theta \] / \sin^2 \theta \\
= 0.25 \sqrt{l + m - 1} \sqrt{l + m - 1} \sqrt{l - m + 1} \sqrt{l - m + 2} \sqrt{C_m / C_{m-2}} \tilde{P}_l^{m-2} \\
+ 0.25[l + m(l + m - 1) + (l - m)(l - m - 1)(m - 1)/(m + 1)]\tilde{P}_l^m \\
+ 2(l + m + 2)(l + m + 1)/(m + 1)\tilde{P}_l^m \\
+ 0.25 \sqrt{l + m + 1} \sqrt{l + m + 2} \sqrt{l - m} \sqrt{l - m - 1} \sqrt{C_m / C_{m+2}} \tilde{P}_l^{m+2} \quad (24)

2.3 New expressions

Inserting the corresponding mathematical derivations in the last section into Eq. (2) and Eq. (4)

and after some simplifications, the new expressions for MV and MGT can be written as:

\[ B_x = \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+2} (g_l^m \cos m \phi - h_l^m \sin m \phi) (a_{l,m}^{x} \tilde{P}_l^{m-1} + b_{l,m}^{x} \tilde{P}_l^{m+1}) \], \quad (25a)

\[ B_y = \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+2} (g_l^m \sin m \phi + h_l^m \cos m \phi) (a_{l,m}^{y} \tilde{P}_l^{m-1} + b_{l,m}^{y} \tilde{P}_l^{m+1}) \], \quad (25b)

\[ B_z = \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+2} (g_l^m \cos m \phi + h_l^m \sin m \phi) (a_{l,m}^{z} \tilde{P}_l^{m}) \], \quad (25c)

\[ B_{xx} = \frac{1}{a} \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+3} (g_l^m \cos m \phi + h_l^m \sin m \phi) (a_{l,m}^{xx} \tilde{P}_l^{m-2} + b_{l,m}^{xx} \tilde{P}_l^{m} + c_{l,m}^{xx} \tilde{P}_l^{m+2}) \], \quad (26a)

\[ B_{xy} = \frac{1}{a} \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+3} (g_l^m \sin m \phi - h_l^m \cos m \phi) (a_{l,m}^{xy} \tilde{P}_l^{m-2} + b_{l,m}^{xy} \tilde{P}_l^{m} + c_{l,m}^{xy} \tilde{P}_l^{m+2}) \], \quad (26b)

\[ B_{xz} = \frac{1}{a} \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+3} (g_l^m \cos m \phi - h_l^m \sin m \phi) (a_{l,m}^{xz} \tilde{P}_l^{m-2} + b_{l,m}^{xz} \tilde{P}_l^{m} + c_{l,m}^{xz} \tilde{P}_l^{m+2}) \], \quad (26c)

\[ B_{yx} = \frac{1}{a} \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+3} (g_l^m \sin m \phi + h_l^m \cos m \phi) (a_{l,m}^{yx} \tilde{P}_l^{m-2} + b_{l,m}^{yx} \tilde{P}_l^{m} + c_{l,m}^{yx} \tilde{P}_l^{m+2}) \], \quad (26d)

\[ B_{yz} = \frac{1}{a} \sum_{l=1}^{l} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+3} (g_l^m \sin m \phi - h_l^m \cos m \phi) (a_{l,m}^{yz} \tilde{P}_l^{m-2} + b_{l,m}^{yz} \tilde{P}_l^{m} + c_{l,m}^{yz} \tilde{P}_l^{m+2}) \], \quad (26e)
where the corresponding coefficients of the SSALFs are given as following:

\[
\begin{align*}
\mathbf{a}^x_{i,m} & = 0.5\sqrt{l + m + 1} + \sqrt{C_m / C_{m-1}} \\
\mathbf{b}^x_{i,m} & = -0.5\sqrt{l + m + 1} \sqrt{l - m} \sqrt{C_m / C_{m+1}}, \\
\mathbf{a}^y_{i,m} & = 0.5\sqrt{l + m + 1} \sqrt{l - m} \sqrt{C_m / C_{m-1}} \\
\mathbf{b}^y_{i,m} & = 0.5\sqrt{l - m + 1} \sqrt{l - m} \sqrt{C_m / C_{m+1}}, \\
\mathbf{a}^{z+}_{i,m} & = -(l + 1), \\
\mathbf{a}^{z-}_{i,m} & = -(l + 1)(l + 2) = (l + 2)\mathbf{a}^{z+}_{i,m}.
\end{align*}
\]  

Furthermore, some other higher-order partial derivatives and their transforms are usually used to image geologic boundaries in magnetic prospecting, such as the higher-order enhanced analytic signal (e.g. Hsu et al., 1996). Therefore, we also give the third-order partial derivatives of the magnetic potential field as:
\[ B_{xzz} = \frac{\partial B_{zz}}{\partial z} = \frac{\partial^2 B_{zz}}{\partial x^2} = \frac{\partial^2 B_{z}}{\partial z \partial x} \]
\[ = \frac{1}{a^2} \sum_{l=1}^{L} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+4} \left( g_i^m \cos m\phi + h_i^m \sin m\phi \right) \left( a_{i,m}^{xzz} \bar{p}_{l}^{m-2} + b_{l,m}^{xzz} \bar{P}_{l}^{m} + c_{i,m}^{xzz} \bar{P}_{l}^{m+2} \right) , \] (28a)

\[ B_{xy} = \frac{\partial B_{x}}{\partial y} = \frac{\partial^2 B_{x}}{\partial y \partial z} = \frac{\partial^2 B_{y}}{\partial x \partial z} = \frac{\partial^2 B_{y}}{\partial z \partial x} \]
\[ = \frac{1}{a^2} \sum_{l=1}^{L} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+4} \left( g_i^m \sin m\phi - h_i^m \cos m\phi \right) \left( a_{i,m}^{xy} \bar{p}_{l}^{m-2} + b_{l,m}^{xy} \bar{P}_{l}^{m} + c_{i,m}^{xy} \bar{P}_{l}^{m+2} \right) , \] (28b)

\[ B_{z} = \frac{\partial^2 B_{z}}{\partial z^2} = \frac{\partial^2 B_{z}}{\partial x \partial z} = \frac{\partial^2 B_{z}}{\partial z \partial x} \]
\[ = \frac{1}{a^2} \sum_{l=1}^{L} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+4} \left( g_i^m \cos m\phi + h_i^m \sin m\phi \right) \left( a_{i,m}^{z} \bar{P}_{l}^{m-1} + b_{l,m}^{z} \bar{P}_{l}^{m} + c_{i,m}^{z} \bar{P}_{l}^{m+1} \right) , \] (28c)

\[ B_{y} = \frac{\partial^2 B_{y}}{\partial z^2} = \frac{\partial^2 B_{y}}{\partial x \partial z} = \frac{\partial^2 B_{y}}{\partial z \partial x} \]
\[ = \frac{1}{a^2} \sum_{l=1}^{L} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+4} \left( g_i^m \cos m\phi + h_i^m \sin m\phi \right) \left( a_{i,m}^{y} \bar{P}_{l}^{m-1} + b_{l,m}^{y} \bar{P}_{l}^{m} + c_{i,m}^{y} \bar{P}_{l}^{m+1} \right) , \] (28d)

\[ B_{xx} = \frac{\partial^2 B_{x}}{\partial z^2} = \frac{\partial^2 B_{x}}{\partial x \partial z} = \frac{\partial^2 B_{x}}{\partial z \partial x} \]
\[ = \frac{1}{a^2} \sum_{l=1}^{L} \sum_{m=0}^{l} \left( \frac{a}{r} \right)^{l+4} \left( g_i^m \cos m\phi + h_i^m \sin m\phi \right) \left( a_{i,m}^{xx} \bar{P}_{l}^{m} \right) , \] (28e)

where the corresponding coefficients of the SSALFs are presented as:

\[
\begin{align*}
a_{i,m}^{xx} &= (l + 3)a_{i,m}^{xx} \\
b_{i,m}^{xx} &= (l + 3)b_{i,m}^{xx} \\
c_{i,m}^{xx} &= (l + 3)c_{i,m}^{xx} \\
\end{align*}
\]
\[ , \] (29a)

\[
\begin{align*}
a_{i,m}^{xy} &= (l + 3)a_{i,m}^{xy} \\
b_{i,m}^{xy} &= (l + 3)b_{i,m}^{xy} \\
c_{i,m}^{xy} &= (l + 3)c_{i,m}^{xy} \\
\end{align*}
\]
\[ , \] (29b)
\[
\begin{align*}
    a_{i,m}^{xx} &= 0.5(l + 2)(l + 3)\sqrt{l + m} \sqrt{l - m + 1} C_m / C_{m-1} \\
    &= (l + 2)(l + 3)a_{l,m}^{xx} = (l + 3)a_{l,m}^{x-z} \\
    b_{i,m}^{xx} &= -0.5(l + 2)(l + 3)\sqrt{l + m} \sqrt{l - m - 1} C_m / C_{m+1} \\
    &= (l + 2)(l + 3)b_{l,m}^{x-x} = (l + 3)b_{l,m}^{x-z} \\
    c_{i,m}^{yy} &= (l + 3)c_{l,m}^{yy} \\
    a_{i,m}^{yy} &= 0.5(l + 2)(l + 3)\sqrt{l + m} \sqrt{l + m - 1} C_m / C_{m-1} \\
    &= (l + 2)(l + 3)a_{l,m}^{yy} = (l + 3)a_{l,m}^{y-z} \\
    b_{i,m}^{yy} &= 0.5(l + 2)(l + 3)\sqrt{l - m} \sqrt{l - m - 1} C_m / C_{m+1} \\
    &= (l + 2)(l + 3)b_{l,m}^{y-y} = (l + 3)b_{l,m}^{y-z} \\
    c_{i,m}^{zz} &= (l + 3)c_{l,m}^{zz} \\
    a_{i,m}^{zz} &= -(l + 1)(l + 2)(l + 3) = (l + 3)a_{l,m}^{z-z} = (l + 2)(l + 3)a_{l,m}^{z-z}.
\end{align*}
\]

(29c) \hspace{1cm} (29d) \hspace{1cm} (29e) \hspace{1cm} (29f)

In this way, we avoid computing recursively the SSALFs with singular terms, their first- and second-order derivatives as in the traditional formulae. The cost is only to calculate two additional degrees and orders for the SSALFs at most. It should be mentioned that, in this study, we use the conventional form of SSALF that if \( m < 0 \), then \( \tilde{P}_l^m = (\text{-}1)^{|m|} P_l^{|m|} \) and if \( m > l \), then \( \tilde{P}_l^m = 0 \).

3 Numerical investigation and discussion

We test the derived expressions and the numerical implementation in C/C++, by calculating the magnetic potential, vector and its gradients and also the third-order partial derivatives of the magnetic potential field on a grid with 0.125° × 0.125° cell size at the altitude of 300 km relative to the Earth’s magnetic reference sphere using the lithospheric magnetic field model GRIMM_L120 (version 0.0) defined by Lesur et al. (2013). The magnetic potential, MV, MGT and the third-order partial derivatives of the magnetic potential field in the two polar regions mapped by the lithospheric field model with spherical harmonic degrees/orders 16–90 are shown in Fig. 1 and Fig.
2, respectively. The corresponding statistics around the north and south poles are, respectively, presented in Table 1 and Table 2. A simple test is that the MGT meets the Laplace's equation of the potential field, that is, the trace of the MGT should be equal to zero. Our numerical results show that the amplitudes of $B_{xx} + B_{yy} + B_{zz}$ in the north and south polar regions are in the range of $[-2.012 \times 10^{-15} \, \text{pT/m} : +2.026 \times 10^{-15} \, \text{pT/m}]$ (1 Tesla = $10^3$ mT = $10^9$ nT = $10^{12}$ pT = $10^{18}$ aT), respectively. The relative error is almost equal the machine accuracy. Therefore, this feature proves the validity of our derived formulae. In addition, as shown in Fig. 1 and Fig. 2, it is obvious that the MGT and also the third-order partial derivatives of the magnetic potential field enhance the lineation and contacts at the satellite altitude. It also reveals some small-scale anomalies, which is very helpful for the further geological interpretation. A core field model with spherical harmonic degrees/orders 1~15 is also used to test and the results not shown here indicate the correctness of the formulae in the full range of the spherical harmonic degrees/orders, where the computational stability of the Legendre function with ultrahigh-order is not considered.

Furthermore, the computed magnetic fields are smooth near the poles and don’t have the singularities but some components have the dependence on the direction of reference frame at the poles. As shown in Fig. 3, the magnetic potential $V$, $B_z$, $B_{zz}$ and $B_{zzz}$ components at the poles are independent of the direction of the $x_P$ and $y_P$ axes, while changing with the direction of the $x_P$ and $y_P$ axes at the poles, the $B_x$, $B_y$, $B_{xz}$, $B_{yz}$, $B_{xzz}$ and $B_{yzz}$ components have a period of 360° and the $B_{xxx}$, $B_{xxy}$, $B_{xyz}$, $B_{yxx}$, $B_{yxy}$ and $B_{yyz}$ components have a period of 180°. These variations can be accurately described by a sine or cosine function relating to the horizontal rotation of the reference frame and the differences among these magnetic effects are magnitude, period and initial phase. Therefore, $B_x$, $B_y$, $B_{xz}$, $B_{yz}$, $B_{xzz}$, $B_{yzz}$, $B_{xxz}$, $B_{xyz}$ and $B_{yyz}$ components are not smooth at/cross the
poles. Therefore, to determine the single value at the poles (Fig. 1 and Fig. 2) we specially define
that the x-axis points to the meridian of 180° E (or 180° W) at north pole and of 0° at south pole,
that is, the LNORF moving from Greenwich meridian to the poles.

Compared with the traditional formulae in Section 2.1, there are two advantages of our derived
formulae in Section 2.3. On the one hand, the traditional derivatives up to second-order are
removed in the new formulae; therefore, the relatively complicated method by the Horner's
recursive algorithm (Holmes and Featherstone, 2002b) can be avoided. On the other hand, the
singular terms of 1/sinθ and 1/ sin²θ are removed in the new formulae; consequently, the scale
factor of e.g. 10^-280 (Holmes and Featherstone, 2002a,b) is not required when the computing point
approaches to the poles and the magnetic fields at the poles can also be calculated in the defined
reference frame. In fact, there are differences between the results by our expressions and those by
the Horner's recursive algorithm, for instance, if using the same model and the parameters as those
in Fig. 1 and Fig. 2, the differences of the three components Bx, By and Bz are at a level of [-3×10^-11
nT : +3×10^-11 nT].

4 Conclusions

We develop in this paper the new expressions for the MV, the MGT and the third-order partial
derivatives of the magnetic potential field in terms of spherical harmonics. The traditional
expressions have complicated forms involving first- and second-order derivatives of the SSALFs
and are singular when approaching to the poles. Our newly derived formulae don't contain the
first- and second-order derivatives of the SSALFs and remove the singularities at the poles.
However, our formulae are derived in the spherical LNORF with specific definition at the poles.
For an application to the magnetic data of a satellite gradiometry mission in the future (e.g. Kotsiaros and Olsen, 2014), it is necessary to describe the MV and the MGT in the local orbital or other reference frame, where the new MV and MGT are the linear functions of the MV and the MGT in the LNORF with coefficients related to the satellite track azimuth (e.g. Petrovskaya and Vershkov, 2006) or other rotation angles. The other main purpose of this paper is in the future to contribute to the signal processing and the geophysical & geological interpretation of global lithospheric magnetic field model, especially near polar areas.

Supplementary software implementation is performed by the programming language C/C++. The source code and input data presented in this paper can be obtained by contacting the lead author via email.

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### Tables and figures

**Table 1.** Statistics of the magnetic potential, MV, MGT and third-order partial derivatives of the magnetic potential field around the north pole (0° ≤ θ ≤ 30°) at the altitude of 300 km using the lithospheric magnetic field model GRIMM_L120 (version 0.0) (Lesur et al., 2013) for spherical harmonic degrees 16–90.

<table>
<thead>
<tr>
<th>Magnetic effects</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V$ [mT×m]</td>
<td>-5.1554771</td>
<td>+4.7867519</td>
<td>+0.0828017</td>
<td>±1.7377648</td>
</tr>
<tr>
<td>$B_x$ [nT]</td>
<td>-14.7389250</td>
<td>+17.6917740</td>
<td>-0.0890689</td>
<td>±4.9797007</td>
</tr>
<tr>
<td>$B_y$ [nT]</td>
<td>-15.1297000</td>
<td>+13.6053000</td>
<td>+0.0010738</td>
<td>±4.8239313</td>
</tr>
<tr>
<td>$B_z$ [nT]</td>
<td>-19.8715270</td>
<td>+25.3666030</td>
<td>-0.198845</td>
<td>±6.7066701</td>
</tr>
<tr>
<td>$B_{xx}$ [pT/m]</td>
<td>-0.1054684</td>
<td>+0.0621351</td>
<td>+0.0001872</td>
<td>±0.0215871</td>
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<tr>
<td>$B_{xy}$ [pT/m]</td>
<td>-0.0410371</td>
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<td>±0.0115018</td>
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<tr>
<td>$B_{xz}$ [pT/m]</td>
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<td>±0.0247522</td>
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<td>$B_{yy}$ [pT/m]</td>
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<td>±0.0186580</td>
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<td>$B_{yz}$ [pT/m]</td>
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<td>±0.0228174</td>
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<td>$B_{zz}$ [pT/m]</td>
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<td>+0.0002917</td>
<td>±0.0336965</td>
</tr>
<tr>
<td>$B_{xx}+B_{yy}+B_{zz}$ [pT/m]</td>
<td>-2.012×10⁻¹⁵</td>
<td>+2.026×10⁻¹⁵</td>
<td>+8.085×10⁻¹⁹</td>
<td>±5.101×10⁻¹⁶</td>
</tr>
<tr>
<td>$B_{xx}$ [aT/m²]</td>
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<td>$B_{xy}$ [aT/m²]</td>
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<tr>
<td>$B_{xz}$ [aT/m²]</td>
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<td>$B_{yy}$ [aT/m²]</td>
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<td>+1.1697371</td>
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<td>±0.2421663</td>
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Table 2. Statistics of the magnetic potential, MV, MGT and third-order partial derivatives of the magnetic potential field around the south pole (150° ≤ θ ≤ 180°) at the altitude of 300 km using the lithospheric magnetic field model GRIMM_L120 (version 0.0) (Lesur et al., 2013) for spherical harmonic degrees 16–90.

<table>
<thead>
<tr>
<th>Magnetic effects</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V ) [mT×m]</td>
<td>-3.3267455</td>
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<tr>
<td>( B_x ) [nT]</td>
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</tr>
<tr>
<td>( B_y ) [nT]</td>
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<tr>
<td>( B_z ) [nT]</td>
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<tr>
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<td>±0.0166266</td>
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<tr>
<td>( B_{yy} ) [pT/m]</td>
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<tr>
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<td>±0.0154623</td>
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<td>( B_{yz} ) [pT/m]</td>
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<td>-0.0019900</td>
<td>±0.0258066</td>
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<tr>
<td>( B_{xx} + B_{yy} + B_{zz} ) [pT/m]</td>
<td>-1.027×10^{-15}</td>
<td>+2.012×10^{-15}</td>
<td>+1.113×10^{-18}</td>
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<tr>
<td>( B_{xx} ) [nT/m²]</td>
<td>-0.4605216</td>
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<tr>
<td>( B_{yy} ) [nT/m²]</td>
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<td>+0.2947601</td>
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<td>( B_{zz} ) [nT/m²]</td>
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<td>( B_{xy} ) [nT/m²]</td>
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<td>±0.2084566</td>
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</table>
Figure 1. Lithospheric magnetic potential, vector and its gradients fields and third-order partial derivatives of the magnetic potential field around the north pole (0°≤θ≤30°) at the altitude of 300 km as defined by the lithospheric magnetic field model GRIMM_L120 (version 0.0) (Lesur et al., 2013) for spherical harmonic degrees 16–90. (a) is magnetic potential (V), (b) (c) and (d) are three components (B_x, B_y and B_z) of magnetic vector, (e), (f), (g), (h), (i) and (j) are six elements (B_{xx}, B_{xy}, B_{xz}, B_{yy}, B_{yz} and B_{zz}) of magnetic gradient tensor, (k), (l), (m), (n), (o) and (p) are six elements (B_{xxx}, B_{xxy}, B_{xxz}, B_{yxx}, B_{yzy} and B_{zzz}) of third-order partial derivatives of the magnetic potential field, respectively. The dark green lines are the plate boundaries by Bird (2003). All maps are shown by Polar Stereographic projections.
Figure 2. Lithospheric magnetic potential, vector and its gradients fields and third-order partial derivatives of the magnetic potential field around the south pole ($150^\circ \leq \theta \leq 180^\circ$) at the altitude of 300 km as defined by the lithospheric magnetic field model GRIMM_L120 (version 0.0) (Lesur et al., 2013) for spherical harmonic degrees 16–90. (a) is magnetic potential ($V$), (b) (c) and (d) are three components ($B_x$, $B_y$ and $B_z$) of magnetic vector, (e), (f), (g), (h), (i) and (j) are six elements ($B_{xx}$, $B_{xy}$, $B_{xz}$, $B_{yy}$, $B_{yz}$ and $B_{zz}$) of magnetic gradient tensor, (k), (l), (m), (n), (o) and (p) are six elements ($B_{xxx}$, $B_{xyy}$, $B_{xz}z$, $B_{yyz}$, $B_{yz}z$ and $B_{zzz}$) of third-order partial derivatives of the magnetic potential field, respectively. The dark green lines are the plate boundaries by Bird (2003). All maps are shown by Polar Stereographic projections.
Figure 3. Limit values of magnetic potential ($V$), vector ($B_x$, $B_y$ and $B_z$) and its gradients ($B_{xx}$, $B_{xy}$, $B_{xz}$, $B_{yy}$, $B_{yz}$ and $B_{zz}$) and third-order partial derivatives of the magnetic potential field ($B_{xxy}$, $B_{xzx}$, $B_{yzz}$, $B_{yzy}$, $B_{zzx}$ and $B_{zzz}$) at the poles when the local reference frames vary from different meridians (the direction of $x_P$ axe changing from different meridian to the poles). Red and blue lines indicate the magnetic effects at north-pole and at south-pole, respectively. The reference frame is specially defined that the $x_P$-axis points to the meridian of 180° E (or 180° W) at north pole and 0° at south pole and the $y_P$-axis points to the meridian of 90° E at two poles. The values at two poles showed by black dashed arrows are used to plot the maps in Fig. 1 and Fig. 2.