

3D Magnetic modelling of ellipsoidal bodies

Diego Takahashi Tomazella¹ and Vanderlei C. Oliveira Jr¹

¹Department of Geophysics, Observatório Nacional, Rio de Janeiro, Brazil

Correspondence to: Diego Takahashi Tomazella (diego.takahashi@gmail.com)

Abstract.

TEXT

1 Introduction

Based on the mathematical theory of the magnetic induction developed by Poisson (1824), Maxwell (1873) affirmed that, if U is the gravitational potential produced by any body with uniform density ρ and arbitrary shape at a point (x, y, z) , then $-\frac{\partial U}{\partial x}$ is the magnetic scalar potential produced at the same point by the same body if it has a uniform magnetization oriented along x with intensity ρ . Maxwell (1873) generalized this idea as a way of determining the magnetic scalar potential produced by any body uniformly magnetized in a given direction. By presuming that this uniform magnetization is due to induction, he postulated that the resulting magnetic field (intensity) at all points within the body must also be uniform and parallel to the magnetization. As a consequence, the gravitational potential U at points within the body must be a quadratic function of the spatial coordinates. Apparently, Maxwell (1873) was the first one to postulate that ellipsoids are the only finite bodies having a gravitational potential which satisfies this property and hence can be uniformly magnetized in the presence of a uniform magnetic field.

This property can be extended to other bodies whose shape derives from an ellipsoid (e.g., spheres, elliptic cylinders), however all the remaining non-ellipsoidal bodies cannot be uniformly magnetized in the presence of a uniform inducing field (Jahren, 1963; Joseph and Schlömann, 1965; Clark and Emerson, 1999).

Self-demagnetization demagnetization gives rise to shape anisotropy.

Self-demagnetization is a function of the shape of the body.

The self-demagnetization contributes to decrease the magnitude of the magnetization along the shortest dimensions of a body.

Ellipsoids are the only bodies which enable an analytical computation of its self-demagnetization.

Ellipsoids can assume a wide range of shapes and therefore can be used to represent different geological bodies.

It is well-known by that the self-demagnetization can be neglected if the body has a susceptibility lower than 0.1 SI (Austin et al., 2014; Clark, 2014; Clark et al., 1986; Emerson et al., 1985; Eskola and Tervo, 1980; Guo et al., 1998, 2001; Purss and Cull, 2005; Hillan and Foss, 2013).

However, neglecting the self-demagnetization in geological bodies with high susceptibilities (> 0.1 SI) may strongly mislead the results obtained from magnetic methods.

Farrar (1979) demonstrated the importance of the ellipsoidal model in taking into account the self-demagnetization and determining reliable drilling directions on the Tennant Creek field, Australia.

5 Posteriorly, Hoschke (1991) also showed how the ellipsoidal model proved to be highly successful in locating and defining ironstone bodies in the Tennant Creek field.

Clark (2000) provides a good discussion about the influence of the self-demagnetization in magnetic interpretation of the Osborne copper-gold deposit, Australia. This deposit is hosted by ironstone bodies that have very high susceptibility. According to Clark (2000), neglecting the effects of self-demagnetisation led errors of $\approx 55^\circ$ in the interpreted dip.

10 Based on magnetic modelling and rock property measurements, Austin et al. (2014) showed that, contrary to previous interpretations, the magnetization of the Candelaria iron oxide copper-gold deposit, Chile, is not dominated by the induced component. Rather, the deposit has a relatively weak remanent magnetization and is strongly affected by self-demagnetization.

These examples show the practical importance of self-demagnetization for the correct interpretation of magnetic data produced by geological bodies having high susceptibilities.

15 These examples also show the importance of the ellipsoidal model in producing trustworthy geological models of orebodies, which may save significant cost associated with drilling.

2 Methodology

2.1 Geometrical parameters and coordinate systems

Let (x, y, z) be a point referred to a Cartesian coordinate system with axes x , y and z pointing to, respectively, North, East and down. For convenience, we denominate this coordinate system as *main coordinate system*. Let us consider an ellipsoidal body with centre at the point (x_c, y_c, z_c) , semi-axes defined by positive constants a , b , c , where $a > b > c$, and orientation defined by three angles α , β , and γ . The points (x, y, z) located on the surface of this ellipsoidal body satisfy the following equation:

$$(\mathbf{r} - \mathbf{r}_c)^T \mathbf{A} (\mathbf{r} - \mathbf{r}_c) = 1, \quad (1)$$

where $\mathbf{r} = [x \ y \ z]^T$, $\mathbf{r}_c = [x_c \ y_c \ z_c]^T$, \mathbf{A} is a positive definite matrix given by

$$25 \quad \mathbf{A} = \mathbf{V} \begin{bmatrix} a^{-2} & 0 & 0 \\ 0 & b^{-2} & 0 \\ 0 & 0 & c^{-2} \end{bmatrix} \mathbf{V}^T, \quad (2)$$

and \mathbf{V} is an orthogonal matrix whose columns are defined by unit vectors \mathbf{v}_1 , \mathbf{v}_2 , and \mathbf{v}_3 .

The vectors \mathbf{v}_1 , \mathbf{v}_2 , and \mathbf{v}_3 depend on the orientation angles α , β , γ and are defined as follows (Clark et al., 1986):

$$\mathbf{v}_1 = \begin{bmatrix} -\cos \alpha \cos \delta \\ -\sin \alpha \cos \delta \\ -\sin \delta \end{bmatrix}, \quad (3)$$

$$\mathbf{v}_2 = \begin{bmatrix} \cos \alpha \cos \gamma \sin \delta + \sin \alpha \sin \gamma \\ \sin \alpha \cos \gamma \sin \delta - \cos \alpha \sin \gamma \\ -\cos \gamma \cos \delta \end{bmatrix}, \quad (4)$$

$$\mathbf{v}_3 = \begin{bmatrix} \sin \alpha \cos \gamma - \cos \alpha \sin \gamma \sin \delta \\ -\cos \alpha \cos \gamma - \sin \alpha \sin \gamma \sin \delta \\ \sin \gamma \cos \delta \end{bmatrix}. \quad (5)$$

For triaxial ellipsoids (i.e., $a > b > c$), the orthogonal matrix \mathbf{V} (Eq. 2) is calculated by using Eqs. 3, 4, and 5 as follows:

$$\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 \end{bmatrix}. \quad (6)$$

Similarly, the matrix \mathbf{V} (Eq. 2) for prolate ellipsoids (i.e., $a > b = c$) is calculated according to Eq. 6 by using Eqs. 3, 4, and 5, but with $\gamma = 0^\circ$ (Emerson et al., 1985). Finally, the matrix \mathbf{V} (Eq. 2) for oblate ellipsoids (i.e., $a < b = c$) is calculated by using Eqs. 3, 4, and 5, with $\gamma = 0^\circ$, as follows (Emerson et al., 1985):

$$\mathbf{V} = \begin{bmatrix} \mathbf{v}_2 & \mathbf{v}_1 & -\mathbf{v}_3 \end{bmatrix}. \quad (7)$$

The orientation of the semi-axes a , b , and c are defined by the first, second, and third columns of the matrix \mathbf{V} given by Eq. 6, in the case of a triaxial or prolate ellipsoid, or the matrix \mathbf{V} given by Eq. 7, in the case of an oblate ellipsoid.

The magnetic modelling of an ellipsoidal body is commonly performed in a particular Cartesian coordinate system that is aligned with the body semi-axes and has the origin coincident with the body centre. For convenience, we denominate this particular coordinate system as *local coordinate system*. The relationship between the Cartesian coordinates $(\tilde{x}, \tilde{y}, \tilde{z})$ of a point in a local coordinate system and the Cartesian coordinates (x, y, z) of the same point in the main system is given by:

$$\tilde{\mathbf{r}} = \mathbf{V}^\top (\mathbf{r} - \mathbf{r}_c), \quad (8)$$

where $\tilde{\mathbf{r}} = [\tilde{x} \ \tilde{y} \ \tilde{z}]^\top$, \mathbf{r} and \mathbf{r}_c are defined in Eq. 1 and the matrix \mathbf{V} is defined according to Eqs. 6 or 7, depending on the ellipsoid type.

2.2 Theoretical background

Consider a magnetized ellipsoid immersed in a uniform magnetic field \mathbf{H}_0 (in Am^{-1}). This uniform field can be, for example, the main component of the Earth's magnetic field, which is usually assumed to be generated by the Earth's liquid core. In the

absence of conduction currents, the total magnetic field $\mathbf{H}(\mathbf{r})$ at the position \mathbf{r} (Eqs. 2 and 8) of a point referred to the main coordinate system is defined as follows (Sharma, 1966; Eskola and Tervo, 1980; Reitz et al., 1992; Stratton, 2007):

$$\mathbf{H}(\mathbf{r}) = \mathbf{H}_0 - \nabla V(\mathbf{r}), \quad (9)$$

where the second term is the negative gradient of the magnetic scalar potential $V(\mathbf{r})$ given by:

$$5 \quad V(\mathbf{r}) = -\frac{1}{4\pi} \iiint_{\vartheta} \mathbf{M}(\mathbf{r}')^\top \nabla \left(\frac{1}{\|\mathbf{r} - \mathbf{r}'\|} \right) dx' dy' dz'. \quad (10)$$

In this equation, $\mathbf{r}' = [x' \ y' \ z']^\top$ is the position vector of a point located within the volume ϑ , the integral is conducted over the variables x' , y' and z' representing the coordinates of a point located within the volume ϑ of the ellipsoid, $\|\cdot\|$ denotes the Euclidean norm and $\mathbf{M}(\mathbf{r}')$ is the magnetization vector (in Am^{-1}). Eq. 10 is valid anywhere, independently if the position vector \mathbf{r} represents a point located inside or outside the magnetized body (DuBois, 1896).

10 Based on Maxwell's postulate, let us assume that the body has a uniform magnetization given by

$$\mathbf{M} = \mathbf{K} \mathbf{H}^\dagger, \quad (11)$$

where \mathbf{H}^\dagger is the resultant uniform magnetic field at any point within the body and \mathbf{K} is a constant and symmetrical 2nd-order tensor representing the magnetic susceptibility of the body. In this case, Equation 9 can be rewritten as follows:

$$\mathbf{H}(\mathbf{r}) = \mathbf{H}_0 - \mathbf{N}(\mathbf{r}) \mathbf{K} \mathbf{H}^\dagger, \quad (12)$$

15 where $\mathbf{N}(\mathbf{r})$ is a symmetrical matrix whose ij -element $n_{ij}(\mathbf{r})$ is given by

$$n_{ij}(\mathbf{r}) = -\frac{1}{4\pi} \frac{\partial^2 f(\mathbf{r})}{\partial r_i \partial r_j}, \quad i = 1, 2, 3, \quad j = 1, 2, 3, \quad (13)$$

$r_1 = x$, $r_2 = y$, $r_3 = z$ are the elements of the position vector \mathbf{r} (Eq. 1), and

$$f(\mathbf{r}) = \iiint_{\vartheta} \frac{1}{\|\mathbf{r} - \mathbf{r}'\|} dx' dy' dz'. \quad (14)$$

Notice that the scalar function $f(\mathbf{r})$ (Eq. 14) is proportional to the gravitational potential that would be produced by the ellipsoidal body with volume ϑ if it had a uniform density equal to the inverse of the gravitational constant. It can be shown that the elements $n_{ij}(\mathbf{r})$ are finite whether \mathbf{r} is a point within or without the volume ϑ (Peirce, 1902; Webster, 1904). The matrix $\mathbf{N}(\mathbf{r})$ (Eq. 12) is called *depolarization tensor* (Soliv  rez, 1981, 2008).

The following part of this paper moves on to describe the magnetic field $\mathbf{H}(\mathbf{r})$ (Eq. 12) at points located both within and without the volume ϑ of the ellipsoidal body. However, the mathematical developments are conveniently performed in the local coordinate system related to the respective ellipsoidal body.

2.3 Coordinate transformation

To continue our description of the magnetic modelling of ellipsoidal bodies, it is convenient to perform two important coordinate transformations. The first one transforms the scalar function $f(\mathbf{r})$ (Eq. 14) from the main coordinate system into a new scalar function $\tilde{f}(\tilde{\mathbf{r}})$ referred to the local coordinate system. The function $\tilde{f}(\tilde{\mathbf{r}})$ was first presented by Dirichlet (1839) to describe the gravitational potential produced by homogeneous ellipsoids. Posteriorly, several authors also deduced and used this function for describing the magnetic and gravitational fields produced by triaxial, prolate, and oblate ellipsoids (Maxwell, 1873; Thomson and Tait, 1879; DuBois, 1896; Peirce, 1902; Webster, 1904; Kellogg, 1929; Stoner, 1945; Osborn, 1945; Lowes, 1974; Peake and Davy, 1953; Chang, 1961; Clark et al., 1986; Tejedor et al., 1995; Stratton, 2007). It is convenient to use $\tilde{f}^\dagger(\tilde{\mathbf{r}})$ and $\tilde{f}^\ddagger(\tilde{\mathbf{r}})$ to define the function $\tilde{f}(\tilde{\mathbf{r}})$ evaluated, respectively, at points $\tilde{\mathbf{r}}$ inside and outside the volume ϑ of the ellipsoidal body.

The scalar function $\tilde{f}^\dagger(\tilde{\mathbf{r}})$ is given by

$$\tilde{f}^\dagger(\tilde{\mathbf{r}}) = \pi abc \int_0^\infty \left(1 - \frac{\tilde{x}^2}{a^2 + u} - \frac{\tilde{y}^2}{b^2 + u} - \frac{\tilde{z}^2}{c^2 + u} \right) \frac{1}{R(u)} du, \quad \tilde{\mathbf{r}} \in V, \quad (15)$$

where

$$R(u) = \sqrt{(a^2 + u)(b^2 + u)(c^2 + u)}. \quad (16)$$

This function represents the gravitational potential that would be produced by the ellipsoidal body at points located within its volume ϑ if it had a uniform density equal to the inverse of the gravitational constant. Notice that, in this case, the gravitational potential is a quadratic function of the spatial coordinates \tilde{x} , \tilde{y} , and \tilde{z} , which supported the Maxwell's (1873) postulate about uniformly magnetized ellipsoids. In a similar way, the function $\tilde{f}^\ddagger(\tilde{\mathbf{r}})$ is given by

$$\tilde{f}^\ddagger(\tilde{\mathbf{r}}) = \pi abc \int_\lambda^\infty \left(1 - \frac{\tilde{x}^2}{a^2 + u} - \frac{\tilde{y}^2}{b^2 + u} - \frac{\tilde{z}^2}{c^2 + u} \right) \frac{1}{R(u)} du, \quad \tilde{\mathbf{r}} \notin V, \quad (17)$$

where $R(u)$ is defined by Eq. 16 and the parameter λ is defined according to the ellipsoid type as a function of the spatial coordinates \tilde{x} , \tilde{y} , and \tilde{z} (see Appendix B). For readers interested in additional information about the parameter λ , we recommend Webster (1904, p. 234), Kellogg (1929, p. 184) and Clark et al. (1986).

The second important coordinate transformation is defined with respect to Eq. 12. By properly using the orthogonality of matrix \mathbf{V} (Eqs. 6 and 7), the magnetic field $\mathbf{H}(\mathbf{r})$ (Eq. 12) can be transformed from the main coordinate system to a local coordinate system as follows:

$$\underbrace{\mathbf{V}^\top \mathbf{H}(\mathbf{r})}_{\tilde{\mathbf{H}}(\tilde{\mathbf{r}})} = \underbrace{\mathbf{V}^\top \mathbf{H}_0}_{\tilde{\mathbf{H}}_0} - \underbrace{\mathbf{V}^\top \mathbf{N}(\mathbf{r}) \mathbf{V}}_{\tilde{\mathbf{N}}(\tilde{\mathbf{r}})} \underbrace{\mathbf{V}^\top \mathbf{K} \mathbf{V}}_{\tilde{\mathbf{K}}} \underbrace{\mathbf{V}^\top \mathbf{H}^\dagger}_{\tilde{\mathbf{H}}^\dagger}, \quad (18)$$

where the superscript " \sim " denotes quantities referred to the respective local coordinate system.

In Eq. 18, the transformed depolarization tensor $\tilde{\mathbf{N}}(\tilde{\mathbf{r}})$ is calculated as a function of the original depolarization tensor $\mathbf{N}(\mathbf{r})$ (Eq. 12). In this case, the elements of $\tilde{\mathbf{N}}(\tilde{\mathbf{r}})$ are calculated as a function of the second derivatives of the function $f(\mathbf{r})$ (Eq. 14),

which is defined in the main coordinate system. It can be shown (Appendix A), however, that the elements $\tilde{n}_{ij}(\tilde{\mathbf{r}})$ of $\tilde{\mathbf{N}}(\tilde{\mathbf{r}})$ can also be calculated as follows:

$$\tilde{n}_{ij}(\tilde{\mathbf{r}}) = -\frac{1}{4\pi} \frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_i \partial \tilde{r}_j}, \quad i = 1, 2, 3, \quad j = 1, 2, 3, \quad (19)$$

where $\tilde{r}_1 = \tilde{x}$, $\tilde{r}_2 = \tilde{y}$, and $\tilde{r}_3 = \tilde{z}$ are the elements of the transformed vector $\tilde{\mathbf{r}}$ (Eq. 8) and $\tilde{f}(\tilde{\mathbf{r}})$ is given by Eq. 15 or 17,

5 depending if $\tilde{\mathbf{r}}$ represents a point located within or without the volume ϑ of the ellipsoidal body.

2.4 Internal magnetic field and magnetization

By considering $\tilde{\mathbf{r}}$ as a point within the volume ϑ of the ellipsoid and using the Maxwell's postulate about the uniformity of the magnetic field $\mathbf{H}(\mathbf{r})$ inside ellipsoidal bodies, we can use Eq. 18 for defining the resultant uniform magnetic field $\tilde{\mathbf{H}}^\dagger$ inside the ellipsoidal body as follows:

$$10 \quad \tilde{\mathbf{H}}^\dagger = \left(\mathbf{I} - \tilde{\mathbf{N}}^\dagger \tilde{\mathbf{K}} \right)^{-1} \tilde{\mathbf{H}}_0, \quad (20)$$

where \mathbf{I} is the identity matrix and $\tilde{\mathbf{N}}^\dagger$ represents the transformed depolarization tensor evaluated within the volume ϑ of the ellipsoidal body. The elements of $\tilde{\mathbf{N}}^\dagger$ will be presented in a latter section.

Let us pre-multiply the uniform internal field $\tilde{\mathbf{H}}^\dagger$ (Eq. 20) by the transformed susceptibility tensor $\tilde{\mathbf{K}}$ (Eq. 18) to obtain

$$\begin{aligned} \tilde{\mathbf{M}} &= \tilde{\mathbf{K}} \left(\mathbf{I} - \tilde{\mathbf{N}}^\dagger \tilde{\mathbf{K}} \right)^{-1} \tilde{\mathbf{H}}_0 \\ &= \left(\mathbf{I} - \tilde{\mathbf{K}} \tilde{\mathbf{N}}^\dagger \right)^{-1} \tilde{\mathbf{K}} \tilde{\mathbf{H}}_0, \end{aligned} \quad (21)$$

15 where $\tilde{\mathbf{M}}$ represents the transformed magnetization, as can be easily verified by using Eqs. 11 and 18. The matrix identity used for obtaining the second line of Eq. 21 is given by Searle (1982, p. 151).

Equation 21 can be easily generalized for the case in which the ellipsoid has also a uniform remanent magnetization $\tilde{\mathbf{M}}_R$. Let us first consider that the uniform remanent magnetization satisfies the condition $\tilde{\mathbf{H}}_A = \tilde{\mathbf{K}}^{-1} \tilde{\mathbf{M}}_R$, where $\tilde{\mathbf{H}}_A$ represents a hypothetical uniform ancient field. Then, if we assume that $\tilde{\mathbf{H}}_0$, in Eqs. 20 and 21, is in fact the sum of the uniform magnetic

20 field $\tilde{\mathbf{H}}_0$ and the hypothetical ancient field $\tilde{\mathbf{H}}_A$, we obtain the following generalized equation

$$\tilde{\mathbf{M}} = \left(\mathbf{I} - \tilde{\mathbf{K}} \tilde{\mathbf{N}}^\dagger \right)^{-1} \left(\tilde{\mathbf{K}} \tilde{\mathbf{H}}_0 + \tilde{\mathbf{M}}_R \right). \quad (22)$$

Equation 22 is consistent with that given by Clark et al. (1986, Eq. 38).

2.5 External magnetic field and total-field anomaly

The magnetic field $\Delta \tilde{\mathbf{H}}(\tilde{\mathbf{r}})$ produced by an ellipsoid at external points is calculated from Eqs. 18 and 22 as the difference

25 between the resultant field $\tilde{\mathbf{H}}(\tilde{\mathbf{r}})$ and the uniform field $\tilde{\mathbf{H}}_0$:

$$\Delta \tilde{\mathbf{H}}(\tilde{\mathbf{r}}) = -\tilde{\mathbf{N}}^\dagger(\tilde{\mathbf{r}}) \tilde{\mathbf{M}}. \quad (23)$$

The elements of the transformed depolarization tensor $\tilde{\mathbf{N}}^\dagger(\tilde{\mathbf{r}})$ used in Eq. 23 will be presented in the following section.

The $\Delta\tilde{\mathbf{H}}(\tilde{\mathbf{r}})$ can be interpreted as a uniformly magnetized body located in the crust while the uniform field $\tilde{\mathbf{H}}_0$ can be interpreted as the main component of the geomagnetic field on the study area, which is commonly assumed to be generated at the liquid part of the Earth's core. Equation 23 gives the magnetic field (in A m^{-1}) produced by an ellipsoid. However, in geophysics, the most widely used field is the magnetic induction (in nT). Fortunately, this conversion can be easily done by multiplying Eq. 23 by $k_m = 10^9 \mu_0$, where μ_0 represents the magnetic constant (in H m^{-1}).

For geophysical applications, it is preferable to calculate the total-field anomaly produced by the magnetic sources. This scalar quantity is defined as follows (Blakely, 1996):

$$\Delta\tilde{T}(\tilde{\mathbf{r}}) = \|\tilde{\mathbf{B}}_0 + \Delta\tilde{\mathbf{B}}(\tilde{\mathbf{r}})\| - \|\tilde{\mathbf{B}}_0\|, \quad (24)$$

where $\tilde{\mathbf{B}}_0 = k_m \tilde{\mathbf{H}}_0$ and $\Delta\tilde{\mathbf{B}}(\tilde{\mathbf{r}}) = k_m \Delta\tilde{\mathbf{H}}(\tilde{\mathbf{r}})$ (Eq. 23). In practical situations, however, $\|\tilde{\mathbf{B}}_0\| \gg \|\Delta\tilde{\mathbf{B}}(\tilde{\mathbf{r}})\|$ and, consequently, the following approximation is valid (Blakely, 1996):

$$\Delta\tilde{T}(\tilde{\mathbf{r}}) \approx \frac{\tilde{\mathbf{B}}_0^\top \Delta\tilde{\mathbf{B}}(\tilde{\mathbf{r}})}{\|\tilde{\mathbf{B}}_0\|}. \quad (25)$$

2.6 Transformed depolarization tensors $\tilde{\mathbf{N}}(\tilde{\mathbf{r}})$

2.6.1 Depolarization tensor $\tilde{\mathbf{N}}^\dagger$

The elements of the transformed depolarization tensor $\tilde{\mathbf{N}}^\dagger$ used to compute the uniform magnetic field $\tilde{\mathbf{H}}^\dagger$ (Eq. 20) and the magnetization $\tilde{\mathbf{M}}$ (Eqs. 21 and 22) are calculated according to Eq. 19, with $\tilde{f}(\tilde{\mathbf{r}})$ given by $\tilde{f}^\dagger(\tilde{\mathbf{r}})$ (Eq. 15). As we have already pointed out, the $\tilde{f}^\dagger(\tilde{\mathbf{r}})$ (Eq. 15) is a quadratic function of the spatial coordinates \tilde{x} , \tilde{y} and \tilde{z} . Consequently, the elements \tilde{n}_{ij}^\dagger , $i = 1, 2, 3, j = 1, 2, 3$, of $\tilde{\mathbf{N}}^\dagger$ do not depend on the transformed position vector $\tilde{\mathbf{r}}$ (equation 8). Besides, the off-diagonal elements are zero and the diagonal elements are given by (Stoner, 1945):

$$\tilde{n}_{ii}^\dagger = \frac{abc}{2} \int_0^\infty \frac{1}{(e_i^2 + u) R(u)} du, \quad i = 1, 2, 3, \quad (26)$$

where $R(u)$ is defined by Eq. 16 and $e_1 = a$, $e_2 = b$, and $e_3 = c$. These elements are commonly known as *demagnetizing factors* and are defined according to the ellipsoid type. Notice that, according to Eqs. 18 and A7,

$$\mathbf{N}(\mathbf{r}) = \mathbf{V} \tilde{\mathbf{N}}^\dagger \mathbf{V}^\top, \quad (27)$$

where $\tilde{\mathbf{N}}^\dagger$ (Eqs. 20, 21 and 22) is a diagonal matrix and \mathbf{V} (Eqs. 6 and 7) is an orthogonal matrix. This equation shows that, for the particular case in which \mathbf{r} and consequently $\tilde{\mathbf{r}}$ represent a point inside the volume ϑ of the ellipsoid, the elements \tilde{n}_{ii}^\dagger (Eq. 36) of $\tilde{\mathbf{N}}^\dagger$ represent the eigenvalues while the columns of \mathbf{V} represent the eigenvectors of the original depolarization tensor $\mathbf{N}(\mathbf{r})$.

Triaxial ellipsoids

For triaxial ellipsoids (e.g., $a > b > c$), the demagnetization factors obtained by solving Eq. 36 are given by:

$$\tilde{n}_{11}^{\dagger} = \frac{abc}{(a^2 - c^2)^{\frac{1}{2}} (a^2 - b^2)} [F(\kappa, \phi) - E(\kappa, \phi)] , \quad (28)$$

$$5 \quad \tilde{n}_{22}^{\dagger} = -\frac{abc}{(a^2 - c^2)^{\frac{1}{2}} (a^2 - b^2)} [F(\kappa, \phi) - E(\kappa, \phi)] + \frac{abc}{(a^2 - c^2)^{\frac{1}{2}} (b^2 - c^2)} E(\kappa, \phi) - \frac{c^2}{b^2 - c^2} \quad (29)$$

and

$$\tilde{n}_{33}^{\dagger} = -\frac{abc}{(a^2 - c^2)^{\frac{1}{2}} (b^2 - c^2)} E(\kappa, \phi) + \frac{b^2}{b^2 - c^2} , \quad (30)$$

where

$$F(\kappa, \phi) = \int_0^{\phi} \frac{1}{(1 - \kappa^2 \sin^2 \psi)^{\frac{1}{2}}} d\psi , \quad (31)$$

10 and

$$E(\kappa, \phi) = \int_0^{\phi} (1 - \kappa^2 \sin^2 \psi)^{\frac{1}{2}} d\psi , \quad (32)$$

with $\kappa = [(a^2 - b^2) / (a^2 - c^2)]^{\frac{1}{2}}$ and $\cos \phi = c/a$. The functions $F(\kappa, \phi)$ (Eq. 31) and $E(\kappa, \phi)$ (Eq. 32) are called Legendre's normal elliptic integrals of the first and second kind, respectively. Stoner (1945) presented a detailed deduction of the demagnetization factors \tilde{n}_{11}^{\dagger} (Eq. 28), \tilde{n}_{22}^{\dagger} (Eq. 29) and \tilde{n}_{33}^{\dagger} (Eq. 30). Clark et al. (1986) presented similar formulas, but without any

15 proof.

Prolate ellipsoids

For prolate ellipsoids (e.g., $a > b = c$), the demagnetization factors obtained by solving Eq. 36 are given by:

$$\tilde{n}_{11}^{\dagger} = \frac{1}{m^2 - 1} \left\{ \frac{m}{(m^2 - 1)^{\frac{1}{2}}} \ln \left[m + (m^2 - 1)^{\frac{1}{2}} \right] - 1 \right\} \quad (33)$$

and

$$20 \quad \tilde{n}_{22}^{\dagger} = \frac{1}{2} (1 - \tilde{n}_{11}^{\dagger}) , \quad (34)$$

where $\tilde{n}_{33}^{\dagger} = \tilde{n}_{22}^{\dagger}$, which uses the \tilde{n}_{11}^{\dagger} defined in Eq. 33, and $m = a/b$. The detailed deduction of the demagnetization factors \tilde{n}_{11}^{\dagger} (Eq. 33) and \tilde{n}_{22}^{\dagger} (Eq. 34) can be found, for example, in Stoner (1945). These formulas were posteriorly presented by Emerson et al. (1985), but without any mathematical proof.

Oblate ellipsoids

For oblate ellipsoids (e.g., $a < b = c$), the demagnetization factors obtained by solving Eq. 36 are given by:

$$\tilde{n}_{11}^\dagger = \frac{1}{1-m^2} \left[1 - \frac{m}{(1-m^2)^{\frac{1}{2}}} \cos^{-1} m \right], \quad (35)$$

where \tilde{n}_{22}^\dagger and \tilde{n}_{33}^\dagger are calculated according to Eq. 34, but with \tilde{n}_{11}^\dagger defined in Equation 35, and $m = a/b$. The detailed deduction of these demagnetization factors can be found, for example, in Stoner (1945). These formulas can also be found in Emerson et al. (1985), but without any mathematical proof. The only difference, however, is that Emerson et al. (1985) replaced the term \cos^{-1} by a term \tan^{-1} , according to the trigonometric identity $\tan^{-1} x = \cos^{-1}(1/\sqrt{x^2+1})$, $x > 0$.

2.6.2 Depolarization tensor $\tilde{\mathbf{N}}^\dagger(\tilde{\mathbf{r}})$

The elements $\tilde{n}_{ij}^\dagger(\tilde{\mathbf{r}})$, $i = 1, 2, 3$, $j = 1, 2, 3$, of the transformed depolarization tensor $\tilde{\mathbf{N}}^\dagger(\tilde{\mathbf{r}})$ used to compute the magnetic field $\Delta\tilde{\mathbf{H}}(\tilde{\mathbf{r}})$ (Eq. 23) and the total-field anomaly $\Delta\tilde{T}(\tilde{\mathbf{r}})$ (Eqs. 24 and 25) are calculated according to Eq. 19, with $\tilde{f}(\tilde{\mathbf{r}})$ given by $\tilde{f}^\dagger(\tilde{\mathbf{r}})$ (Eq. 17). By following Clark et al. (1986), the diagonal elements \tilde{n}_{ii}^\dagger and the off-diagonal elements \tilde{n}_{ij}^\dagger , $i = 1, 2, 3$, $j = 1, 2, 3$, are given by

$$\tilde{n}_{ii}^\dagger(\tilde{\mathbf{r}}) = \frac{abc}{2} \left(\frac{\partial\lambda}{\partial\tilde{r}_i} h_i \tilde{r}_i - g_i \right) \quad (36)$$

and

$$\tilde{n}_{ij}^\dagger(\tilde{\mathbf{r}}) = \frac{abc}{2} \left(\frac{\partial\lambda}{\partial\tilde{r}_i} h_j \tilde{r}_j \right), \quad (37)$$

where

$$h_i = \frac{1}{(e_i^2 + \lambda) R(\lambda)}, \quad (38)$$

$$g_i = \int_{\lambda}^{\infty} \frac{1}{(e_i^2 + u) R(u)} du, \quad (39)$$

$e_1 = a$, $e_2 = b$, $e_3 = c$, and $\frac{\partial\lambda}{\partial\tilde{r}_i}$ is defined in Appendix B (Eq. B22). The functions g_i (Eq. 39) are defined according to the ellipsoid type.

Triaxial ellipsoids

For triaxial ellipsoids (e.g., $a > b > c$), the functions g_i (Eq. 39) are defined as follows (Clark et al., 1986):

$$g_1 = \frac{2}{(a^2 - b^2)(a^2 - c^2)^{\frac{1}{2}}} [F(\kappa, \phi) - E(\kappa, \phi)], \quad (40)$$

$$g_2 = \tag{41}$$

and

$$g_3 = , \tag{42}$$

5 where $F(\kappa, \phi)$ and $E(\kappa, \phi)$ are defined by Eqs. 32 and 31, but with $\sin \phi = \sqrt{(a^2 - c^2) / (a^2 + \lambda)}$.

Prolate and oblate ellipsoids

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3 Numerical simulations

3.1 Demagnetization factors

10 Figure 1 TEXT TEXT TEXT Fig. 1 TEXT TEXT TEXT (Fig. 1)

3.2 Ellipsoidal models

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3.3 Susceptibility

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15 4 Conclusions

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5 Code availability

TEXT

Appendix A: Relationship between the derivatives of the functions $f(\mathbf{r})$ and $\tilde{f}(\tilde{\mathbf{r}})$

20 Let $\tilde{f}(\tilde{\mathbf{r}})$ be the scalar function obtained by transforming $f(\mathbf{r})$ (Eq. 14) from the main coordinate system to a local coordinate system. For convenience, let us rewrite Eq. 8 as follows:

$$\tilde{r}_k = v_{k1} r_1 + v_{k2} r_2 + v_{k3} r_3 + c_k , \tag{A1}$$

where \tilde{r}_k , $k = 1, 2, 3$, are the elements of the transformed position vector $\tilde{\mathbf{r}}$ (Eq. 8), r_j , $j = 1, 2, 3$, are the elements of the position vector \mathbf{r} (Eq. 1), v_{kj} , $j = 1, 2, 3$, are the elements of the matrix \mathbf{V} (Eq. 6 or 7), and c_k is a constant defined by the coordinates x_c , y_c , and z_c of the centre of the ellipsoidal body.

By considering the functions $f(\mathbf{r})$ (Eq. 14) and $\tilde{f}(\tilde{\mathbf{r}})$ evaluated at the same point, but on different coordinate systems, we have:

$$\frac{\partial f(\mathbf{r})}{\partial r_j} = \frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_1} \frac{\partial \tilde{r}_1}{\partial r_j} + \frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_2} \frac{\partial \tilde{r}_2}{\partial r_j} + \frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_3} \frac{\partial \tilde{r}_3}{\partial r_j}, \quad j = 1, 2, 3,$$

which, from Eq. A1, can be given by

$$\frac{\partial f(\mathbf{r})}{\partial r_j} = v_{j1} \frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_1} + v_{j2} \frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_2} + v_{j3} \frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_3}, \quad j = 1, 2, 3. \quad (\text{A2})$$

Now, by deriving $\frac{\partial f(\mathbf{r})}{\partial r_j}$ (Eq. A2) with respect to the i th element r_i of the position vector \mathbf{r} (Eq. 1), we obtain:

$$\begin{aligned} \frac{\partial^2 f(\mathbf{r})}{\partial r_i \partial r_j} &= v_{j1} \frac{\partial}{\partial r_i} \left(\frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_1} \right) + v_{j2} \frac{\partial}{\partial r_i} \left(\frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_2} \right) + v_{j3} \frac{\partial}{\partial r_i} \left(\frac{\partial \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_3} \right) \\ &= v_{j1} \left(\frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_1 \partial \tilde{r}_1} v_{i1} + \frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_2 \partial \tilde{r}_1} v_{i2} + \frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_3 \partial \tilde{r}_1} v_{i3} \right) + \\ &+ v_{j2} \left(\frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_1 \partial \tilde{r}_2} v_{i1} + \frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_2 \partial \tilde{r}_2} v_{i2} + \frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_3 \partial \tilde{r}_2} v_{i3} \right) + \\ &+ v_{j3} \left(\frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_1 \partial \tilde{r}_3} v_{i1} + \frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_2 \partial \tilde{r}_3} v_{i2} + \frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_3 \partial \tilde{r}_3} v_{i3} \right) \\ &= \begin{bmatrix} v_{j1} & v_{j2} & v_{j3} \end{bmatrix} \tilde{\mathbf{F}}(\tilde{\mathbf{r}}) \begin{bmatrix} v_{i1} \\ v_{i2} \\ v_{i3} \end{bmatrix}, \end{aligned} \quad (\text{A3})$$

where $\tilde{\mathbf{F}}(\tilde{\mathbf{r}})$ is a 3×3 matrix whose ij -th element is $\frac{\partial^2 \tilde{f}(\tilde{\mathbf{r}})}{\partial \tilde{r}_i \partial \tilde{r}_j}$. From Eq. A3, we obtain

$$\mathbf{F}(\mathbf{r}) = \mathbf{V} \tilde{\mathbf{F}}(\tilde{\mathbf{r}}) \mathbf{V}^\top, \quad (\text{A4})$$

where $\mathbf{F}(\mathbf{r})$ is a 3×3 matrix whose ij -th element is $\frac{\partial^2 f(\mathbf{r})}{\partial r_i \partial r_j}$ and \mathbf{V} is defined by Eqs. 6 or 7, depending on the ellipsoid type. As one may noticed, the matrices $\mathbf{F}(\mathbf{r})$ and $\tilde{\mathbf{F}}(\tilde{\mathbf{r}})$ represent the Hessians of the functions $f(\mathbf{r})$ (Eq. 14) and $\tilde{f}(\tilde{\mathbf{r}})$, respectively.

Besides, the depolarization tensor $\mathbf{N}(\mathbf{r})$ (Eq. 12) can be rewritten by using the matrix $\mathbf{F}(\mathbf{r})$ as follows

$$\mathbf{N}(\mathbf{r}) = -\frac{1}{4\pi} \mathbf{F}(\mathbf{r}). \quad (\text{A5})$$

By properly using the orthogonality of the matrix \mathbf{V} , we may rewrite Eq. A4 as follows:

$$\tilde{\mathbf{F}}(\tilde{\mathbf{r}}) = \mathbf{V}^\top \mathbf{F}(\mathbf{r}) \mathbf{V}. \quad (\text{A6})$$

Finally, by multiplying both sides of Eq. A6 by $-\frac{1}{4\pi}$ and using Eq. A5, we conclude that

$$\tilde{\mathbf{N}}(\tilde{\mathbf{r}}) = \mathbf{V}^\top \mathbf{N}(\mathbf{r}) \mathbf{V}. \quad (\text{A7})$$

Appendix B: Parameter λ and its spatial derivatives

Here, we follow the reasoning presented by Webster (1904) for analysing the parameter λ which defines triaxial, prolate and oblate ellipsoids.

B1 Parameter λ defining triaxial ellipsoids

- 5 Let us consider an ellipsoid with semi-axes a, b, c oriented along the \tilde{x} -, \tilde{y} -, and \tilde{z} -axis, respectively, of its local coordinate system, where $a > b > c > 0$. This ellipsoid is defined by the following equation:

$$\frac{\tilde{x}^2}{a^2} + \frac{\tilde{y}^2}{b^2} + \frac{\tilde{z}^2}{c^2} = 1. \quad (\text{B1})$$

A quadric surface (e.g., ellipsoid, hyperboloid of one sheet or hyperboloid of two sheets) which is confocal with the ellipsoid defined in Eq. B1 can be described as follows:

$$10 \quad \frac{\tilde{x}^2}{a^2 + u} + \frac{\tilde{y}^2}{b^2 + u} + \frac{\tilde{z}^2}{c^2 + u} = 1, \quad (\text{B2})$$

where u is a real number. Equation B2 represents an ellipsoid for u satisfying the condition

$$u + c^2 > 0. \quad (\text{B3})$$

Given a, b, c , and a u satisfying B3, we may use B2 for determining a set of points (x, y, z) lying on the surface of an ellipsoid which is confocal with that one defined in Eq. B1. Now, consider the problem of determining the ellipsoid which is

- 15 confocal with that one defined in B1 and pass through a particular point $(\tilde{x}, \tilde{y}, \tilde{z})$. This problem consists in determining the real number u that, given $a, b, c, \tilde{x}, \tilde{y}$, and \tilde{z} , satisfies Eq. B2 and the condition expressed by Eq. B3. By rearranging Eq. B2, we obtain the following cubic equation for u :

$$p(u) = (a^2 + u)(b^2 + u)(c^2 + u) - (b^2 + u)(c^2 + u)\tilde{x}^2 - (a^2 + u)(c^2 + u)\tilde{y}^2 - (a^2 + u)(b^2 + u)\tilde{z}^2. \quad (\text{B4})$$

This cubic equation shows that:

$$20 \quad u = \begin{cases} d \rightarrow \infty & , \quad p(u) > 0 \\ -c^2 & , \quad p(u) < 0 \\ -b^2 & , \quad p(u) > 0 \\ -a^2 & , \quad p(u) < 0 \end{cases}. \quad (\text{B5})$$

Notice that, according to B5, the smaller, intermediate and largest roots of the cubic equation $p(u)$ (Eq. B4) are located, respectively, in the intervals $[-a^2, -b^2]$, $[-b^2, -c^2]$ and $[-c^2, \infty[$. Remember that we are interested in a u satisfying the condition expressed by Eq. B3. Consequently, according to the signal analysis shown in Eq. B5, we are interested in the largest root λ of the cubic equation $p(u)$ (Eq. B4).

From Eq. B4, we obtain a simpler one given by

$$p(u) = u^u + p_2 u^2 + p_1 u + p_0 , \quad (\text{B6})$$

where

$$p_2 = a^2 + b^2 + c^2 - \tilde{x}^2 - \tilde{y}^2 - \tilde{z}^2 , \quad (\text{B7})$$

5

$$p_1 = b^2 c^2 + a^2 c^2 + a^2 b^2 - (b^2 + c^2) \tilde{x}^2 - (a^2 + c^2) \tilde{y}^2 - (a^2 + b^2) \tilde{z}^2 \quad (\text{B8})$$

and

$$p_0 = a^2 b^2 c^2 - b^2 c^2 \tilde{x}^2 - a^2 c^2 \tilde{y}^2 - a^2 b^2 \tilde{z}^2 . \quad (\text{B9})$$

Finally, from Eqs. B7, B8 and B9, the largest root λ of $p(u)$ (Eq. B6) can be calculated as follows (Weisstein, 2017):

$$10 \quad \lambda = 2 \sqrt{-Q} \cos\left(\frac{\theta}{3}\right) - \frac{p_2}{3} , \quad (\text{B10})$$

where

$$\theta = \cos^{-1}\left(\frac{R}{\sqrt{Q^3}}\right) , \quad (\text{B11})$$

$$Q = \frac{3p_1 - p_2^2}{9} \quad (\text{B12})$$

15 and

$$R = \frac{9p_1 p_2 - 27p_0 - 2p_2^3}{54} . \quad (\text{B13})$$

B2 Parameter λ defining prolate and oblate ellipsoids

Let us now consider a prolate ellipsoid with semi-axes a , b , c oriented along the \tilde{x} -, \tilde{y} -, and \tilde{z} -axis, respectively, of its local coordinate system, where $a > b = c > 0$. In this case, the Eq. defining the surface of the ellipsoid is obtained by substituting

20 $c = b$ in Eq. B1. Consequently, the equation defining the respective confocal quadric surface is given by

$$\frac{\tilde{x}^2}{a^2 + u} + \frac{\tilde{y}^2 + \tilde{z}^2}{b^2 + u} = 1 \quad (\text{B14})$$

and the new condition that must be fulfilled by the variable u so that Eq. B14 represent an ellipsoid is

$$u + b^2 > 0 . \quad (\text{B15})$$

Similarly to the case of a triaxial ellipsoid presented in the previous subsection, we are interested in determining the real number u that, given a , b , \tilde{x} , \tilde{y} , and \tilde{z} , satisfies Eq. B14 and the condition expressed by Eq. B15. From Eq. B14, we obtain the following quadratic equation for u :

$$p(u) = (a^2 + u)(b^2 + u) - (b^2 + u)\tilde{x}^2 - (a^2 + u)(\tilde{y}^2 + \tilde{z}^2). \quad (\text{B16})$$

5 This equation shows that

$$u = \begin{cases} d \rightarrow \infty & , \quad f(\rho) > 0 \\ -b^2 & , \quad f(\rho) < 0 \\ -a^2 & , \quad f(\rho) > 0 \end{cases} \quad (\text{B17})$$

and, consequently, that its two roots lie in the intervals $[-a^2, -b^2]$ and $[-b^2, \infty[$. Therefore, according to the condition established by Eq. B15 and the signal analysis shown in Eq. B17, we are interested in the largest root λ of the quadratic equation $p(u)$ (Eq. B16).

10 By properly manipulating Eq. B16, we obtain a simpler one given by

$$p(u) = u^2 + p_1 u + p_0, \quad (\text{B18})$$

where

$$p_1 = a^2 + b^2 - \tilde{x}^2 - \tilde{y}^2 - \tilde{z}^2 \quad (\text{B19})$$

and

$$15 \quad p_0 = a^2 b^2 - b^2 \tilde{x}^2 - a^2 (\tilde{y}^2 + \tilde{z}^2). \quad (\text{B20})$$

Finally, by using Eqs. B19 and B20, the largest root λ of $p(u)$ (Eq. B18) can be easily calculated as follows:

$$\lambda = \frac{-p_1 + \sqrt{p_1^2 - 4p_0}}{2}. \quad (\text{B21})$$

In the case of oblate ellipsoids, the procedure for determining the parameter λ is very similar to this one for prolate ellipsoids. The semi-axes a , b , c of oblate ellipsoids are defined so that $b = c > a > 0$ and the condition that must be fulfilled by the variable u is $u + a^2 > 0$. In this case, the two roots of the resulting quadratic equation lie in the intervals $[-b^2, -a^2]$ and $[-a^2, \infty[$. Consequently, we are still interested in the largest root of the quadratic equation for the variable u , which is also calculated by using Eq. B21.

B3 Spatial derivative of the parameter λ

The magnetic modelling of triaxial, prolate or oblate ellipsoids requires not only the parameter λ defined by Eqs. B10 and B21, but also its derivatives with respect to the spatial coordinates \tilde{x} , \tilde{y} , and \tilde{z} . Fortunately, the spatial derivatives of the parameter λ can be calculated in a very similar way for all ellipsoid types.

Let us first consider a triaxial ellipsoid. In this case, the spatial derivatives of λ are given by

$$\frac{\partial \lambda}{\partial \tilde{r}_j} = \frac{\frac{2\tilde{r}_j}{(e_j^2 + \lambda)}}{\left(\frac{\tilde{x}}{a^2 + \lambda}\right)^2 + \left(\frac{\tilde{y}}{b^2 + \lambda}\right)^2 + \left(\frac{\tilde{z}}{c^2 + \lambda}\right)^2}, \quad j = 1, 2, 3, \quad (\text{B22})$$

where $\tilde{r}_1 = \tilde{x}$, $\tilde{r}_2 = \tilde{y}$, $\tilde{r}_3 = \tilde{z}$, $e_1 = a$, $e_2 = b$, and $e_3 = c$. This equation can be determined directly from equation B2. The spatial derivatives of λ in the case of prolate or oblate ellipsoids can also be calculated by using Eq. B22 for the particular case

5 in with $b = c$.

Author contributions. TEXT

Acknowledgements. TEXT

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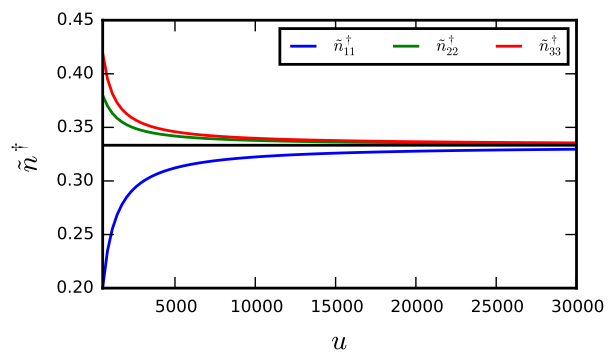


Figure 1. TEXT