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A uniqueness theorem for tomography-assisted potential-field inversion

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SUMMARY

Scanning magnetometers are increasingly used to characterize the magnetization of mineral grains in rock samples. Up-scaling this measurement technique to large numbers of individual particles is hampered by the intrinsic non-uniqueness of potential-field inversion. Here it is shown that this problem can be circumvented by adding tomographic information that determines the location of the possible field sources. Standard potential theory is used to prove a uniqueness theorem that completely characterizes the mathematical background of the corresponding source-localized inversion. It exactly resolves under which conditions a potential-field measurement on a surface can be uniquely decomposed into signals from the different source regions. The intrinsic non-uniqueness of potential-field inversion prevents that the source distribution inside the tomographically outlined regions can be recovered, but the potential field of each region is uniquely defined. For scanning magnetometers in rock magnetism, this result implies that magnetic dipole vectors of large numbers of individual magnetic particles can be reliably reconstructed from surface scans of the magnetic field, if the particle positions are independently determined. This provides an incentive to improve scanning methods for future palaeomagnetic applications.

Key words: Inverse theory; Joint inversion; Rock and mineral magnetism; Magnetic anomalies: modelling and interpretation.

1 INTRODUCTION

Recent developments in scanning magnetometers for rock magnetic purposes promise that this technique will be increasingly important for future rock magnetic studies from the millimetre scale down to the nanometre scale (Egli & Heller 2000; Uehara & Nakamura 2007; Weiss *et al.* 2007; Hankard *et al.* 2009; Lima & Weiss 2009; Lima *et al.* 2014; Glenn *et al.* 2017; de Groot *et al.* 2018). A general physical limitation of this method is the intrinsic non-uniqueness of potential-field inversion. This results from the fact that a charge distribution inside a sphere can be replaced by an equivalent surface charge distribution creating exactly the same outside potential (Kellogg 1929). Therefore, when inverting magnetic field surface measurements, all mathematical approaches have to make substantial additional assumptions about the source magnetization to achieve useful reconstructions (see, e.g. Baratchart *et al.* 2013; Zhdanov 2015). To remediate this problem, we previously suggested to constrain the location of the sources inside the investigated region Ω by adding independent tomographic information (de Groot *et al.* 2018). The corresponding tomography-assisted inversion algorithm turned out to be extremely successful and efficient, which seemed to deserve a mathematical underpinning. This led to the following new type of inversion problem:

When the potential field is known on the surface $\partial\Omega$ of a region Ω, and it is further known that all sources are inside some tomographically outlined regions $P_1, \ldots, P_N \not\subset \Omega$, is it possible to uniquely decompose the measured signal into signals assigned to $P_1, \ldots, P_N$?

For example, is it impossible that in Fig. 1(a) some non-vanishing charge distribution inside the particles P_1, P_2, P_4 and P_5 creates exactly the same measurement signal as some charge distribution inside the omitted particle P_3?

Here it will be shown that this is impossible if the regions $P_1, \ldots, P_N$ are pairwise disjoint, and the complement of the union of each subset is simply connected in $\mathbb{R}^3$. The latter requirement is always fulfilled for separate 'blob-shaped' particles, but excludes ring-shapes or particles that lie inside each other.

The intrinsic non-uniqueness of potential-field inversion turns out to be constrained to the uncertainty of the internal source distribution within the individual regions $P_1, \ldots, P_N$. In the practical application of a tomography-assisted scanning magnetometer, this means that one can uniquely determine which part of the measurement signal comes from which particle. From that one can exactly determine the magnetic dipole moments of the individual particles. If the signal-to-noise ratio allows, one can even determine higher multipole moments, but one cannot determine, for example, the

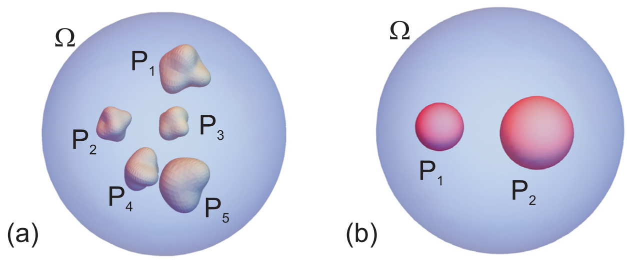

Figure 1. The geometric situation for the unique-source-assignment theorem. The idea is that one measures the normal derivative of a potential, for example, of the magnetic, electric or gravitational potential, on the surface $\partial\Omega$ of the region Ω. (a) The sketch for the general case shows several disjoint source regions $P_1, \ldots, P_5$, which are known beforehand, for example, by X-ray tomography. The new theorem guarantees that the measurement signal on $\partial\Omega$ can be uniquely decomposed into signals from the individual source regions if these have the No-Mutual-Annihilator property. (b) Sketch for the simplified case of two disjoint spherical source regions.

magnetization distribution inside the particles—this is impossible due to the intrinsic non-uniqueness.

The proof of this unexpectedly general result proceeds in three steps. First it is proved for two regions P_1, P_2 that a non-zero charge distribution in one region cannot annihilate the signal of a charge distribution in the other region. This is the content of the two-region No-Mutual-Annihilator (NMA) theorem in Section 2. This theorem encapsulates the main mathematical difficulty in that its proof requires facts from the theory of partial differential equations for potential fields and analytic continuation. The second step, its generalization to an arbitrary number N of regions, just proceeds by mathematical induction. Finally, the main theorem on unique source assignment in Section 3 also follows relatively easily from the general NMA theorem via the linearity of the von Neumann boundary-value problem for the Poisson equation.

The main mathematical idea is therefore contained in the two-region NMA theorem, that can be regarded as a substantial generalization of a theorem of Gauss about separating the internal and external components of the geomagnetic field (Gauss 1877; Backus *et al.* 1997). It essentially relies on the fact that harmonic functions are analytic and can be uniquely analytically continued on simply connected open sets (Axler *et al.* 2001, theorem 1.27).

In Section 3.1 it is shown that the inverse operator, which maps a full surface measurement to the contribution from an individual region, is continuous. This is of considerable practical importance because it implies that the inverse problem of determining individual particle magnetizations from a tomography-assisted surface scan is well posed in the sense of Hadamard (Zhdanov 2015), and can be efficiently solved if data quality allows it.

2 THE NO-MUTUAL-ANNIHILATOR THEOREM

Before continuing with the precise formulation of the results, the reader is kindly asked to recall some terminology from the theory of metric spaces as collected in the Appendix. Having done that, let $\Omega \subset \mathbb{R}^3$ be open and $\partial\Omega$ a non-empty, smooth manifold. For all practical purposes, Ω in the following is assumed to be bounded, although mathematically this is not strictly necessary. For an open bounded region G with $\overline{G} \subset \Omega$ the (von Neumann) annihilator of G in $\partial\Omega$ is defined as the vector space of charge distributions in G ,which create no measurement signal on the boundary $\partial\Omega$. To simplify the proofs, it is assumed that these charge distributions have some finite distance to the boundary of G. This can be formalized as

$$\begin{aligned}\mathrm{Ann}(G) := \Big\{&\rho \in L^1(G) : \operatorname{supp}\rho \subset G,\\ &\exists\Phi \in C^2(\Omega)\cap C^1(\overline{\Omega}) : \Delta\,\Phi = \rho \text{ and } \frac{\partial\Phi}{\partial n} = 0 \text{ on } \partial\Omega\Big\}.\end{aligned}$$

Because the measurement signal is the normal derivative of the potential, the potential itself is only defined up to a globally constant summand, and in the following this constant is chosen such that the analytic continuation of Φ to $\mathbb{R}^3$ vanishes at infinity. The corresponding potentials are called zero-gauged.

N pairwise disjoint compact sets $P_1, \ldots, P_N$ with $P_i \not\subset \Omega$ have the NMA property if,

$$\mathrm{Ann}\left(\bigcup_{i=1}^{N} P_i\right) = \bigoplus_{i=1}^{N} \mathrm{Ann}(P_i).$$

This NMA property is a central concept in the following proofs, and it is useful to visualize its physical meaning. In the above equation the '$\not\supset$' inclusion is always true because any element of the vector space spanned by the annihilators of the P_i is an annihilator of the union $\bigcup_{i=1}^{N} P_i$. This means that if each of some charge distributions ρ_k with support inside P_k creates no signal on $\partial\Omega$, then also any linear combination

$$\alpha_1\,\rho_1 + \ldots + \alpha_N\,\rho_N$$

with $\alpha_1, \ldots, \alpha_N \in \mathbb{R}$ creates no signal on $\partial\Omega$. The other inclusion '$\not\subset$' in the NMA property is the one which excludes mutual annihilators. For it implies, that every annihilator of the union is a linear combination of individual annihilators. It is thus impossible to have a charge distribution ρ within the union $\bigcup_{i=1}^{N} P_i$ of all particles, which generates a zero signal on the boundary, such that if the charge distribution is set to zero in some, but not all of the P_i, the resulting boundary signal is not zero.

An example of two sets that do not have the NMA property are two nested balls $P_1 = B(r)$ and $P_2 = B(R)\backslash B(r)$ for $0 < r < R$. A well-known annihilator in this case are constant non-zero charge distributions of opposite signs such that the integral over $B(R)$ is zero (Zhdanov 2015). Setting the charge distribution in one of P_1, P_2 to zero clearly generates a non-zero field on $\partial\Omega$. It is also known that the annihilator sets Ann(G) for $\overline{G} \subset \Omega$ contain a wide variety of other more complicated charge distributions. For example, if G is star-shaped, any charge distribution $\rho \in L^1(G)$ that for all harmonic functions $h \in C^2(\Omega) : \Delta\,h = 0$ fulfils

$$\int_G h(r)\,\rho(r)\,\mathrm{d}V = 0,$$

generates no field on $\partial\Omega$, and thus is a member of Ann(G) (Zhdanov 2015). This apparently bleak state of affairs with respect to unique-inversion results is emphasized by the fact that Zhdanov (2015) reports as the best uniqueness result so far that if a gravity field is known to be generated by a star-shaped body of constant density $\rho(r) = \rho_0$, the inverse problem to determine this shape from its gravitational field has a unique solution (Novikov 1938).

The above historical background, may lead to serious doubt as to whether a far-reaching uniqueness result, like the one presented here, is in conflict with the well-established non-uniqueness results. Yet, intuitively it also appears plausible that, for example, two point charges inside a sphere, which lie far apart from each other, but close to the surface of the sphere do have the NMA property. At least if the

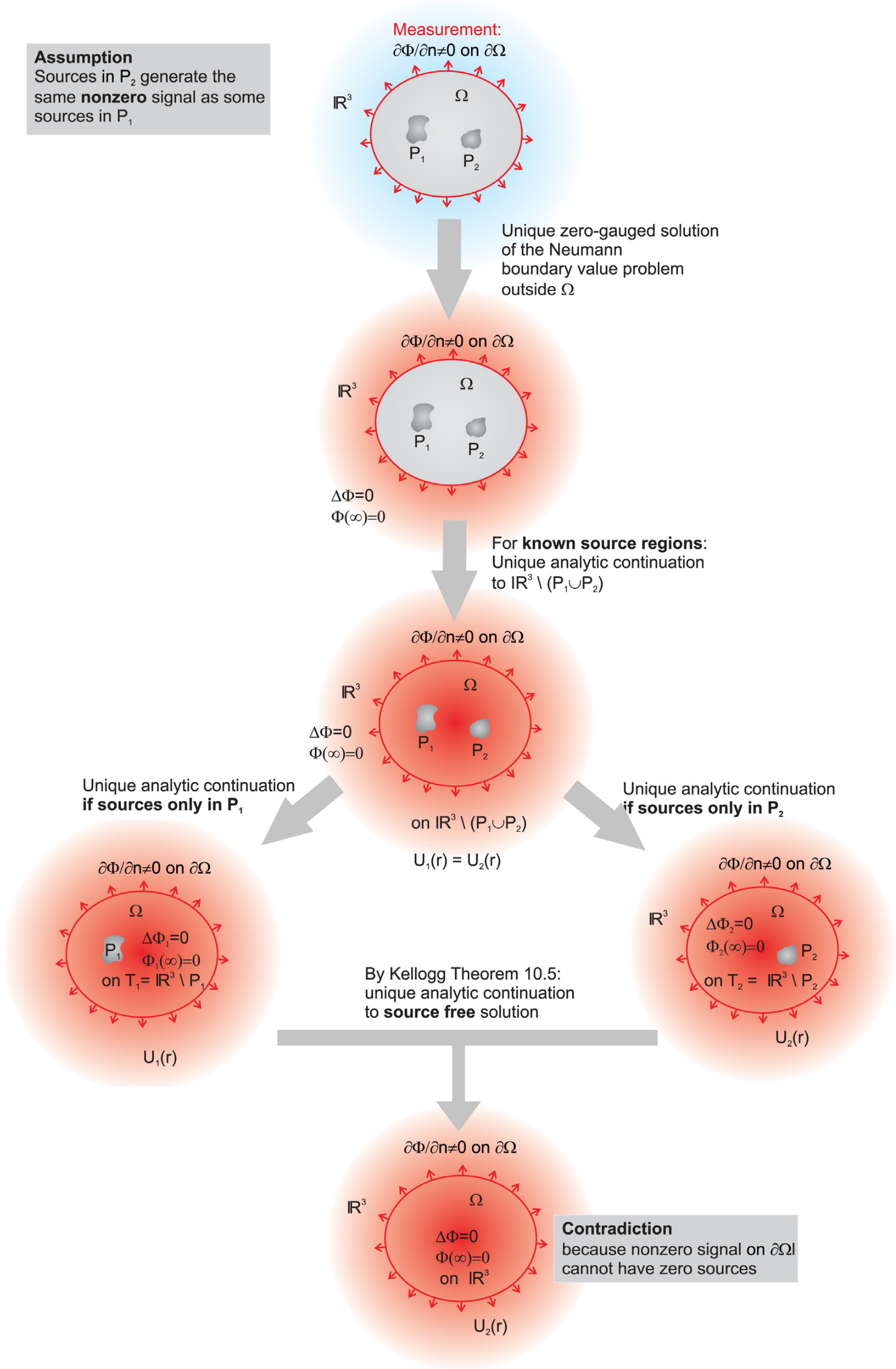

Figure 2. Overview of the proof of the two-region NMA theorem. The measured normal derivatives on the surface $\partial\Omega$ are marked by red arrows. Red shades mark the regions to which the solution has been extended. The assumption that sources in region P_1 generate the same non-zero field on the surface $\partial\Omega$ as sources inside region P_2 leads to a contradiction if T_1 and T_2 are simply connected.

charge distribution inside one of them has a non-zero total charge, then the other must have the opposite total charge to annihilate the field at large distance, but at small distance on the surface $\partial\Omega$ these charges cannot cancel each other. Unfortunately, it appears to be impossible to transform this intuitive picture directly into a mathematical proof if higher multipole orders are taken into account. It will be shown in the following sections by more abstract means that unique-source-assignment and the classical non-uniqueness results are in fact compatible.

Two-region NMA theorem: *Let $\Omega \subset \mathbb{R}^3$ be open and $\partial\Omega$ a smooth manifold and $P_1, P_2 \not\subset \Omega$ be disjoint compact sets, such that $\mathbb{R}^3 \setminus P_1$, $\mathbb{R}^3 \setminus P_2$ and $\mathbb{R}^3 \setminus (P_1 \cup P_2)$ are simply connected, then P_1 and P_2 have the* NMA *property with respect to Ω.*

Proof. The general outline of the proof is sketched in Fig. 2. We derive a contradiction from the assumption that there exists a mutual annihilator

$\rho \in \mathrm{Ann}(P_1 \cup P_2)\backslash(\mathrm{Ann}(P_1) \oplus \mathrm{Ann}(P_2))$.

Because ρ is an annihilator of the union $P_1 \bigcup P_2$, but not a sum of annihilators of the individual particles, there are two non-zero functions $\rho_1, \rho_2 \in L^1(\Omega)$ with supp $\rho_1 \subset P_1$, supp $\rho_2 \subset P_2$, such that

$$\rho = \rho_1 - \rho_2,$$

and the non-zero normal derivatives of their potentials $\frac{\partial \Phi_1}{\partial n}$, $\frac{\partial \Phi_2}{\partial n}$ are identical on $\partial\Omega$. Now recall that the solution of the von Neumann boundary problem for harmonic functions is unique for zero-gauged potentials (Kellogg 1929, theorem 8.4), by which $\Phi_1 = \Phi_2$ on $\mathbb{R}^3\backslash\Omega$, where a potential U is called zero-gauged, if

$$\lim_{||x||\to\infty} U(x) = 0.$$

We now conjure up a bit of mathematical magic in the form of theorem 10.5 in (Kellogg 1929), which essentially encapsulates Gauss theorem of separation of sources. By assumption, the sets $T_1 := \mathbb{R}^3\backslash P_1$ and $T_2 := \mathbb{R}^3\backslash P_2$ are simply connected and open and overlap on the simply connected set $\mathbb{R}^3\backslash(P_1 \cup P_2)$. By analytic continuation on the simply connected open sets T_1 and T_2 (Axler *et al.* 2001, theorem 1.27) there is a unique harmonic function U_1 on T_1 with $U_1 = \Phi_1$ on $\mathbb{R}^3\backslash\Omega$, and a unique U_2 on T_2 with $U_2 = \Phi_2$ on $\mathbb{R}^3\backslash\Omega$. By theorem 10.5 (Kellogg 1929), now there is also a unique harmonic function U on $\mathbb{R}^3$ with $U = U_1$ on T_1 and $U = U_2$ on T_2. This implies that U solves the zero-gauged von Neumann boundary problem $\Delta U = 0$ on $\mathbb{R}^3$ with boundary condition $\frac{\partial U}{\partial n} = \frac{\partial \Phi_1}{\partial n}$ on $\partial\Omega$. Because the unique zero-gauged potential with $\Delta U = 0$ on $\mathbb{R}^3$ is $U = 0$, it follows that $\rho_1 = \rho_2 = 0$, which contradicts the assumption.
□

The above proof makes essential use of theorem 10.5 from Kellogg (1929), which may appear unsatisfactory. In the Appendix this theorem is replicated, and the special case of a two-ball NMA theorem, in which $P_{1,2}$ are simply disjoint balls as in Fig. 1b, is proved by directly applying Gauss theorem of separation of sources. This may help to acquire a more physical understanding of the strength and limitations of the result, and may also lend more credulity to the abstract derivation above. In the next step, the result of the two-region NMA theorem is extended to arbitrary numbers of regions by induction.

Corollary: General NMA theorem: *Let $\Omega \subset \mathbb{R}^3$ be open and $\partial\Omega$ a smooth manifold. For a natural number $N \geq 1$ let $P_1, \ldots, P_N \not\subset \Omega$ be pairwise disjoint compact sets, such that $\mathbb{R}^3\backslash P_k$ and $\mathbb{R}^3\backslash \bigcup_{i=1}^{k} P_i$ are simply connected for all $k = 1, \ldots, N$. Then the P_i have the* NMA *property with respect to Ω.*

Proof. For $N = 1$ there is nothing to prove. Assume that $N > 1$ and that the corollary is true for $N - 1$. Define the sets $P_1' = \bigcup_{i=1}^{N-1} P_i$ and $P_2' = P_N$. The assumptions on the P_k imply that P_1' and P_2' fulfil the conditions to apply the two-region NMA theorem, whereby P_1' and P_2' have the NMA property with respect to Ω which implies

$$\mathrm{Ann}\left(\bigcup_{i=1}^{N} P_i\right) = \mathrm{Ann}\left(\bigcup_{i=1}^{N-1} P_i\right) \oplus \mathrm{Ann}(P_N).$$

Because the corollary is true for $N - 1$ and $P_1, \ldots, P_{N-1}$ fulfil the conditions for its application we have by induction:

$$\mathrm{Ann}\left(\bigcup_{i=1}^{N-1} P_i\right) = \bigoplus_{i=1}^{N-1} \mathrm{Ann}(P_i).$$

Substituting this in the above equation proves the corollary. □

3 UNIQUE SOURCE ASSIGNMENT

The previous two theorems provide all prerequisites to formulate the main result of this paper:

Unique source assignment theorem: *Let $\Omega \subset \mathbb{R}^3$ be open, simply connected, and $\partial\Omega$ a smooth manifold. Assume that $P_1, \ldots, P_N \not\subset \Omega$ are pairwise disjoint compact sets, such that $\mathbb{R}^3\backslash P_k$ and $\mathbb{R}^3\backslash \bigcup_{i=1}^{k} P_i$ are simply connected for all $k = 1, \ldots, N$. If the sources of the zero-gauged potential Φ have compact support on $\bigcup_{k=1}^{N} P_k$, then $\frac{\partial\Phi}{\partial n}$ on $\partial\Omega$ uniquely determines zero-gauged potentials $\Phi_1, \ldots, \Phi_N$, such that Φ_i is harmonic on $\mathbb{R}^3\backslash \bigcup_{k\neq i} P_k$, which implies that it has no sources outside P_i, and*

$$\frac{\partial\Phi}{\partial n} = \sum_{i=1}^{N} \frac{\partial\Phi_i}{\partial n} \text{ on } \partial\Omega.$$

Proof. Because the source of Φ is a charge distribution ρ in $\bigcup_{k=1}^{N} P_k$, there exist zero-gauged harmonic potentials $\Phi_1, \ldots, \Phi_N$ with the required properties, namely those generated by the local charge distributions $\rho_k = \rho|_{P_k}$. □

Uniqueness is now shown by the general NMA theorem. Take any charge distribution ρ' in $\bigcup_{k=1}^{N} P_k$ with zero-gauged potentials $\Psi_1, \ldots, \Psi_N$, such that Ψ_i is harmonic on $\mathbb{R}^3\backslash \bigcup_{k\neq i} P_k$ and

$$\frac{\partial\Phi}{\partial n} = \sum_{i=1}^{N} \frac{\partial\Psi_i}{\partial n} \text{ on } \partial\Omega.$$

Then define $\Gamma_i = \Phi_i - \Psi_i$, such that

$$\Gamma := \sum_{i=1}^{N} \Gamma_i = 0 \text{ on } \mathbb{R}^3\backslash\Omega, \text{ and } \frac{\partial\Gamma}{\partial n} = 0 \text{ on } \partial\Omega.$$

This Γ is the zero-gauged potential from the source distribution $\rho - \rho'$ and a member of $\mathrm{Ann}(\bigcup_{i=1}^{N} P_i)$. By the general NMA theorem for the source regions $\Phi_1, \ldots, \Phi_N$, we have

$$\mathrm{Ann}\left(\bigcup_{i=1}^{N} P_i\right) = \bigoplus_{i=1}^{N} \mathrm{Ann}(P_i),$$

which implies that Γ is the sum of annihilators of the individual source regions P_i, and therefore $\Gamma_i = 0$, or $\Phi_i = \Psi_i$ for $i = 1, \ldots, N$. Thus all zero-gauged Φ_i are uniquely determined by $\frac{\partial\Phi}{\partial n}$ on $\partial\Omega$.

3.1 Unique source assignment is well posed

For the practical application in inversion algorithms it is important to find out whether the above unique decomposition is sufficiently robust with respect to inevitable measurement uncertainties or numerical noise. This kind of robustness is captured by Hadamard's definition of a well-posed inverse problem (Zhdanov 2015). In order to be well posed, the source assignment of the potential-field data needs to (1) have a solution, (2) this solution must be unique and (3) the operator that maps the measurement to the potentials of the individual source regions must be continuous. Because (1) and (2) have been proved above, it remains to show that the solution operator for unique source assignment is continuous.

To simplify defining the inverse-solution operator for one of the regions in the unique-source-assignment theorem, we pick this region and call it P_1, and then call the union of the other regions P_2. The continuity which is of interest here, requires that if a sequence of measurements $m_k,\ k \in \mathbb{N}$ converges to m in $C(\partial\Omega)$, then also the uniquely defined inverse potentials $\Phi_1(m_k)$ converge to $\Phi_1(m)$ on $\mathbb{R}^3\backslash P_1$, or

$$\lim_{k\to\infty} ||m - m_k|| = 0 \Rightarrow \lim_{k\to\infty} ||\Phi_1(m) - \Phi_1(m_k)|| = 0,$$

where the norm on the right-hand side is from $C^2(\mathbb{R}^3\backslash P_1)$. Because Φ_1 is a linear operator, this is equivalent to the case $m = 0$ where it must be proved that

$$\lim_{k\to\infty} ||m_k|| = 0 \Rightarrow \lim_{k\to\infty} ||\Phi_1(m_k)|| = 0.$$

All m_k are measurements on $\partial\Omega$ of fields from zero-gauged potentials $\Psi(m_k)$ generated by sources inside $P_1 \bigcup P_2$. Harnack's theorem (Kellogg 1929, theorem 10.1) now guarantees that these $\Psi(m_k)$ converge on $\mathbb{R}^3\backslash\Omega$ to a zero-gauged harmonic potential $\Psi(0)$. Uniqueness of the von Neumann boundary problem yields $\Psi(0) = 0$. Analytic continuation then implies that the $\Psi(m_k)$ also converge on $\mathbb{R}^3\backslash(P_1 \cup P_2)$ to zero, which in turn guarantees that the $\Psi(m_k)$ converge to zero on $\partial P_1 \bigcup \partial P_2$. By Harnack's theorem now also $\frac{\partial\Psi(m_k)}{\partial n}$ converges to zero on ∂P_1. Because due to unique source assignment $\Phi_1(m_k)$ is the unique zero-gauged potential generated by $\frac{\partial\Psi(m_k)}{\partial n}$ on ∂P_1, it also follows, again by Harnack's theorem, that the $\Phi_1(m_k)$ converge to zero.

The above argument confirms that unique source assignment is a well-posed inverse problem. This guarantees that for each given configuration of source regions with NMA property, there is some level of measurement precision which provides sufficiently dense data and low signal-to-noise ratio, that the inverse problem can be solved in a stable and robust way. As with any inverse problem, one has to confirm that the required level of data quality is reached in practical applications. If this is not the case, the numerical inversion can still be ill-conditioned, which is common in cases where the discretization is too coarse, or the signal-to-noise ratio is low.

4 CONSEQUENCES

The new theorem proved above, provides an astoundingly general condition for when it is theoretically possible to uniquely assign potential-field signals to source regions. To give an intuitive argument why this kind of theorem can exist, consider the simple case when Ω and all P_k are balls. The theorem now guarantees that from the spherical harmonic expansion of the field on $\partial\Omega$ all individual spherical harmonic expansions on the ∂P_k are uniquely determined. Thus the coefficients of one countably infinite basis of an harmonic function space uniquely define N countably infinite coefficient sets on N infinite bases, which is no contradiction in analogy to the Hilbert-hotel paradox (Hilbert 1924/1925).

In rock magnetism, after the pioneering work of Egli & Heller (2000), different magnetic surface scanning techniques are increasingly used to infer magnetization sources and magnetization structure inside rocks (e.g. Uehara & Nakamura 2007; Hankard *et al.* 2009; Usui *et al.* 2012; Lima *et al.* 2013; Glenn *et al.* 2017). Here, the unique-source-assignment theorem enables palaeomagnetic reconstruction from natural particle ensembles (de Groot *et al.* 2018), because it establishes that individual dipole moments from a large number of magnetic particles in a non-magnetic matrix, which are localized by density tomography (micro-CT), can be uniquely recovered from surface magnetic field measurements. In this context, Ω is a half-space in $\mathbb{R}^3$ and the scanning measurement determines the normal component of the magnetic field vector on its surface plane. In de Groot *et al.* (2018), uniqueness of dipole reconstruction was also individually certified by showing that for some specific set of K magnetic particles found by density tomography one can find $3K$ surface measurements such that the a $3K \times 3K$ matrix of the forward calculation is invertible. Based on the uniqueness result proven here, this individual certification becomes unnecessary. The theorem even explains, why false magnetizations assigned to some particles, due to an ill-conditioned inversion matrix, do not influence the correct determination of the other particle magnetizations: the potential fields from the different source regions just do not interfere with each other. The induction proof of the unique source assignment theorem even indicates a divide-and-conquer type strategy for algorithmic implementation of an improved fast inverse reconstruction.

When scanning a rock sample in its natural-remanent magnetization state, and again after applying standard palaeomagnetic stepwise demagnetization procedures, the resulting demagnetization data set can be studied on an individual particle level to identify stable and unaltered remanence carriers. By selecting only optimally preserved and stable remanence carriers from a large collection of measured particles, statistically reliable palaeomagnetic average directions or NRM intensities can be calculated for terrestrial or extraterrestrial rocks that currently cannot be used as recorders of their magnetic history due to unremovable noise.

Unique source assignment can also be significant in other areas of geophysics, for example, for the inversion of gravimetric or aeromagnetic data, when combined with tomographic methods like seismic imaging.

Further potential application are inversion problems in electroencephalography, magnetoencephalography or electrocardiography, where it might enable to uniquely assign externally measured potential-field signals to previously determined brain or heart regions (Baillet *et al.* 2001; Michel *et al.* 2004; Grech *et al.* 2008; Huster *et al.* 2012; Michel & Murray 2012). Empirical inversion techniques that now use numerical and statistical approaches to assess the reliability of their results (Friston *et al.* 2008; Castano-Candamil *et al.* 2015) may profit from unique source assignment to prior known regions.

What remains intrinsically impossible is to assign signals to source regions, which lie inside other source regions, like the nested balls described in Section 2. These cases are excluded because they do not fulfil the condition that for all k, the set $\mathbb{R}^3\backslash P_k$ is simply connected. The fact that this appears to be the main obstruction to unique reconstruction provides a new incentive and direction to study potential-field measurement techniques in combination with *a priori* source localization to recover a maximum of information about the spherical harmonic expansion of the individual source regions.

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APPENDIX

Fundamental mathematical notions

Metric spaces

A *metric space* is any set X for which a 'distance' between two elements can be defined. The distance then is a function

$$d : X \times X \to [0, \infty)$$

with the properties

(1) $d(x, y) = 0 \Leftrightarrow x = y$,
(2) $d(x, y) = d(y, x)$ and
(3) $d(x, z) \leq d(x, y) + d(y, z)$.

Every vector space with a norm $||.||$ has the natural distance function $d(x, y) = ||x - y||$. Thus, all common spaces $\mathbb{R}^n$ or $\mathbb{C}^n$ are metric spaces, but also spaces of m-times continuously differentiable functions $C^m(\Omega)$ with $\Omega \subset \mathbb{R}^n$ are metric spaces with the norm

$$||f - g|| = \max_{|\alpha| \leq m,\, x \in \Omega} |\partial_\alpha f(x) - \partial_\alpha g(x)|.$$

A subset A of a metric space X is *open*, if for each point $x \in A$ there is a $\varepsilon > 0$, such that the ball

$$B(x, \epsilon) := \{y \in X : d(x, y) < \epsilon\}$$

is a subset of A. A subset A of X is *closed*, if its complement $X \backslash A$ is open. Note that $\emptyset$ and X are always open *and* closed in X. For any $A \not\subset X$ one defines the *open core* of A as

$$\mathring{A} := \{x \in A : \exists \epsilon > 0 : B(x, \epsilon) \subset A\},$$

and the *closure* of A in X as

$$\overline{A} := \{x \in X : \forall \epsilon > 0\, \exists y \in A : x \in B(y, \epsilon)\}.$$

The open core can be viewed as the 'inside points' of A, while the closure contains all points in X that have some inside points arbitrarily close to them. Note that the closure of A depends not only on A itself, but also on X. The *boundary* ∂A of A can be defined as those points of the closure of A that are not fully inside, or

$$\partial A := \overline{A} \backslash \mathring{A}.$$

A subset $A \not\subset X$ is *bounded*, if there is an $R > 0$ and $x \in X$, such that $A \not\subset B(x, R)$.

A function f: $X \to Y$ between two metric spaces is *continuous*, if for every open subset $B \not\subset Y$, the set $f^{-1}(B) := \{x \in X: f(x) \in B\}$ is open in X.

Connected, path-connected and simply connected spaces

A metric space X is *connected* if $\emptyset$ and X are its only subsets A that in X at the same time are open and closed, which means $\overline{A} = \mathring{A}$. Note that this definition uses the nice fact that if X has several disconnected pieces, then each of these pieces is also open and closed in X.

A metric space X is *path-connected*, if for any two points $x, y \in X$ there is some curved path fully inside X that connects x and y. Formally, this path is a continuous function

$$p : [0, 1] \to X$$

with $p(0) = x$ and $p(1) = y$. A path-connected metric space X is *simply connected*, if whenever

$$p, q : [0, 1] \to X$$

are two continuous paths with equal start and endpoints $p(0) = q(0)$ and $p(1) = q(1)$, then fully within X, p can be continuously deformed into q while the endpoints remain fixed. Formally, this requests that there is a continuous homotopy map

$$F : [0, 1] \times [0, 1] \to X,$$

such that

$$\forall x \in [0, 1] : F(x, 0) = p(x),\ F(x, 1) = q(x).$$

This condition is also equivalent to the request that all closed loops within X can be continuously contracted to a single point. Intuitively, connected spaces that are not simply connected have 'holes' going through the whole space, like in a torus (doughnut shape) where a loop around the hole cannot be continuously contracted inside the torus. In contrast, if a smaller ball is removed from a larger ball in $\mathbb{R}^3$ the remaining space is still simply connected, because all loops can still be contracted by moving them 'around' the smaller ball.

Here the notion of simply connected regions is important because on them analytic functions can be uniquely continued from any open set to the whole region. If a region X is only path-connected but not simply connected, this cannot be guaranteed because analytic continuation along a non-contractible loop p in the region can lead to different function values at $p(0)$ and $p(1)$, although both points coincide. In disconnected regions, analytic continuation can only be performed within each component.

Other notions

A subset $A \subset \mathbb{R}^3$ is *star-shaped*, if there is a centre point $c \in A$, such that for all $x \in A$ also the line connecting c and x lies in A, that is, $\forall \alpha \in [0, 1] : \alpha c + (1 - \alpha) x \in A$.

If X is a metric space, the *support* of a function $f : X \to \mathbb{R}$ is defined as the closed set

$$\operatorname{supp} f := \overline{\{x \in X : f(x) \neq 0\}}.$$

If $V_1, V_2, \ldots, V_n$ are n linearly independent subvector spaces of V, then their *direct sum* is defined as

$$\bigoplus_{i=1}^{n} V_i := \{\alpha_1 v_1 + \alpha_2 v_2 + \ldots + \alpha_n v_n : v_k \in V_k \text{ and } \alpha_k \in \mathbb{R}\}.$$

Using the notion of the span of a subset of the vector space V, this may also be written as

$$\bigoplus_{i=1}^{n} V_i = \operatorname{span} \bigcup_{i=1}^{n} V_i.$$

Theorems from Kellogg (1929)

For easier reference theorem 10.5 from Kellogg (1929) is here explicitly repeated. In the application of this paper, it guarantees that a harmonic function that can be analytically continued in two different ways onto two different regions, the union of which is $\mathbb{R}^3$, then it also can be analytically continued to $\mathbb{R}^3$.

Kelloggs theorem 10.5: *If T_1 and T_2 are two domains with common points, and if U_1 is harmonic in T_1 and U_2 in T_2, these functions coinciding at the common points of T_1 and T_2, then they define a single function, harmonic in the domain T consisting of all points of T_1 and T_2 (Kellogg 1929).*

The following theorem of Harnack is given as theorem 10.1 in Kellogg (1929). In the application of this paper, all boundaries are compact. The definition of the annihilator was also designed, such that all boundaries of P_k and Ω have finite distance from the sources. This implies that Harnack's theorem guarantees uniform convergence of all derivatives of convergent sequences of harmonic potentials on all boundaries.

Harnack's theorem: *Let R be any closed region of space, and let $U_1, U_2, U_3, \ldots$ be an infinite sequence of functions harmonic in R. If the sequence converges uniformly on the boundary S of R, it converges uniformly throughout R, and its limit U is harmonic in R. Furthermore, in any closed region R', entirely interior to R, the sequence of derivatives*

$$\left[\frac{\partial^{i+j+k}}{\partial x^i\, \partial y^j\, \partial z^k} U_n\right],\ n = 1, 2, 3, \ldots,$$

i, j, k being fixed, converges uniformly to the corresponding derivative of U.

Two-ball NMA theorem

The following is a slightly less general version of the two-region NMA theorem in the main text. Its main advantage is that the proof directly uses the separation-of-sources theorem of Gauss for spherical harmonic expansions, instead of the more abstract theorem 10.5.

Two-ball NMA theorem: *Let $\Omega \subset \mathbb{R}^3$ be open and $\partial\Omega$ a smooth compact manifold and $P_1, P_2 \not\subset \Omega$ be disjoint balls, then P_1 and P_2 have the* NMA *property with respect to Ω.*

Proof. If there exists a mutual annihilator,

$$\rho \in \operatorname{Ann}(P_1 \cup P_2) \backslash (\operatorname{Ann}(P_1) \oplus \operatorname{Ann}(P_2)),$$

then there are two non-zero functions $\rho_1, \rho_2 \in L_1(\Omega)$ with supp $\rho_1 \subset P_1$, supp $\rho_2 \subset P_2$, and $\rho = \rho_1 - \rho_2$, such that the non-zero normal derivatives of their potentials $\frac{\partial \Phi_1}{\partial n}, \frac{\partial \Phi_2}{\partial n}$ are identical on $\partial\Omega$. Because the solution of the Neumann problem for zero-gauged harmonic functions is unique, $\Phi_1 = \Phi_2$ on $\mathbb{R}^3 \backslash \Omega$. Because P_1, P_2 are disjoint, $\mathbb{R}^3 \backslash \overline{P_1 \cup P_2}$ is an open simply connected set and the harmonic functions Φ_1, Φ_2 are defined on $\mathbb{R}^3 \backslash \overline{P_1 \cup P_2}$, and equal on the non-empty open set $\mathbb{R}^3 \backslash \overline{\Omega}$. Because every harmonic function is analytic, this implies $\Phi_1 = \Phi_2$ on $\mathbb{R}^3 \backslash \overline{P_1 \cup P_2}$ (Axler *et al.* 2001, theorem 1.27).

For the potential Φ_1 all sources lie inside P_1 and $\frac{\partial \Phi_1}{\partial n}$ on ∂P_2 is uniquely defined. By Gauss theorem (Gauss 1877; Backus *et al.* 1997), the spherical harmonic expansion of Φ_1 on ∂P_2 is uniquely defined from $\frac{\partial \Phi_1}{\partial n}$ on ∂P_2 and thus only contains terms related to external sources, because supp ρ_1 is outside of ∂P_2. On the other hand, $\frac{\partial \Phi_1}{\partial n} = \frac{\partial \Phi_2}{\partial n}$ on ∂P_2 and the spherical harmonic expansion of Φ_2 on ∂P_2 have only Gauss coefficients from inner sources because supp ρ_2 is inside of $\partial \Omega_2$. Because a non-zero potential cannot at the same time have only inner sources and only outer sources, a mutual annihilator cannot exist. □