A uniqueness theorem in potential theory with implications for tomography-assisted inversion

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Inversion of potential field data is a central technique of remote sensing in physics, geophysics [Zhdanov, 2015], neuroscience [Baillet et al., 2001, Michel et al., 2004, Grech et al., 2008, Michel and Murray, 2012, Huster et al., 2012] and medical imaging [France and Johnson, 2016]. In spite of intense research, uniqueness theorems for potential-field inversion are scarce[Zhdanov, 2015]. Applied studies successfully improve potential-field inversion results by including constraints from independent measurements, but so far no mathematical theorem guarantees that source localization improves the inversion in terms of uniqueness of the achieved assignment. Empirical inversion techniques therefore use numerical and statistical approaches to assess the reliability of their results [Friston et al., 2008, Castano-Candamil et al., 2015]. Especially when inverting magnetic field surface measurements, even seemingly advanced mathematical approaches require substantial additional assumptions about the source magnetization to achieve a useful reconstruction [Baratchart et al., 2013]. Here, standard potential field theory is used to prove a uniqueness theorem which

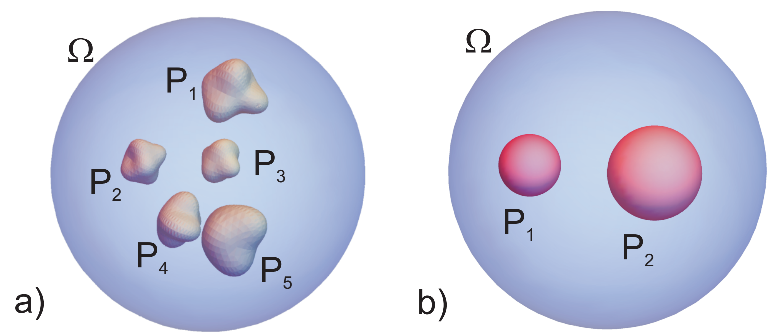

Figure 1: Geometric situation a) in the general case, and b) for the simplified model.

completely characterizes the mathematical background of source-localized inversion. It guarantees for an astonishingly large class of source localizations that it is possible by potential field measurements on a surface to differentiate between signals from different source regions. Non-uniqueness of potential field inversion only prevents that the source distribution within the individual regions can be uniquely recovered.

That a completely unique reconstruction of a charge distribution inside a sphere is impossible by potential field measurements on or outside this sphere is long known. For every charge distribution inside each sphere can be replaced by an equivalent surface charge distribution creating the same outside potential [Kellogg, 1929]. To still infer localized information in spite of this non-uniqueness, we previously suggested to constrain the source regions inside Ω by additional tomographic information [de Groot et al., 2018]. Thus a new type of inversion problem occurs, namely to assign parts of the total measured signal to charge distributions inside the tomographically outlined regions $P_1, \ldots, P_N$. Is it now still possible that some charge distribution, for example inside particles P_1, P_2, P_4, P_5 of Fig. 1a, creates exactly the same measurement signal as a charge distribution in P_3? Below it is shown that for topologically separated regions $P_1, \ldots, P_N$ this is not the case. Accordingly, a potential field measurement at the surface of Ω can be uniquely decomposed into signals from these individual source regions. By that, the inevitable non-uniqueness of potential-field inversion is completely constrained to the uncertainty of the internal source distribution of the individual regions.

Let $\Omega \subset \mathbf{R}^3$ be open and $\partial\Omega$ a nonempty, smooth compact manifold. For a set G with $\overline{G} \subset \Omega$ the (Neumann) annihilator of G in $\partial\Omega$ is defined as

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

N pairwise disjoint compact sets $P_1, \ldots, P_N$ with $P_i \subset \Omega$ have the *no-mutual-annihilator* (NMA) property if

$$\mathrm{Ann}\Big(\bigcup_{i=1}^{N} P_i\Big) \;=\; \bigcup_{i=1}^{N} \mathrm{Ann}(P_i).$$

The NMA property implies, that it is impossible to have a charge distribution ρ within the region $\bigcup_{i=1}^{N} P_i$ which generates a zero signal on the boundary, but 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 which do not have the NMA property are two nested spherical shells. A well-known annihilator in this case are constant charge distributions of opposite sign whose integrals over the shells cancel[Zhdanov, 2015]. Setting the charge distribution in one of the shells to zero clearly leads to a non-zero field on $\partial\Omega$. It is also known that the annihilator sets $\mathrm{Ann}(G)$ for $\overline{G} \subset \Omega$ are large. For star-shaped G, any charge distribution $\rho \in L^1(G)$ for which there exists a harmonic function $h \in C^2(\Omega) : \Delta\, h = 0$ with

$$\int_G h(r)\, \rho(r)\, dV \;=\; 0$$

generates no field on $\partial\Omega$, such that $\rho \in \mathrm{Ann}(G)$ [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 result so far that if a gravity field is generated by a star-shaped body of constant density $\rho(r) = \rho_0$, the gravity inverse problem has a unique solution [Novikov, 1938]. It therefore may appear incredible that a far-reaching uniqueness result, as claimed above, is mathematically possible. We will now show that it is. To make the proof easier to follow, it is first shown under relatively weak topological conditions that two disjoint regions have the NMA property. By induction this can then be easily generalized to a finite number of N regions. From that the main theorem on unique source assignment follows by the linearity of the boundary problem. So the main mathematical content is embodied in the following two-region NMA theorem, that can be regarded as a generalization of Gauss theorem about separating the internal and external components of the geomagnetic field [Gauss, 1877, Backus et al., 1997], and 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].

Two-region NMA theorem. *Let $\Omega \subset \mathbf{R}^3$ be open and $\partial\Omega$ a smooth compact manifold and $P_1, P_2 \subset \Omega$ be disjoint compact sets, such that $\mathbb{R}^3 \backslash P_1$, $\mathbb{R}^3 \backslash P_2$, and $\mathbb{R}^3 \backslash (P_1 \cup P_2)$ are simply connected then P_1 and P_2 have the* No-Mutual-Annihilator *property with respect to Ω.*

Proof. We derive a contradiction from the assumption that there exists a mutual annihilator

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

By definition, then there are two nonzero functions $\rho_1, \rho_2 \in L_1(\Omega)$ with $\operatorname{supp} \rho_1 \subset P_1$, $\operatorname{supp} \rho_2 \subset P_2$, 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 Neumann problem for harmonic functions is unique for zero-gauged potentials [Kellogg, 1929, Theorem 8.4], by which $\Phi_1 = \Phi_2$ on $\mathbf{R}^3 \backslash \Omega$, 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 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 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 [Kellogg, 1929, Theorem 10.5], there now also is 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 the zero-gauged Neumann 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. □

Because the above proof is quite mathematical in nature, in the supplementary information the special case of a two-ball NMA theorem, in which $P_{1,2}$ are disjoint balls, is proved by directly applying Gauss theorem of separation of sources. This may help to acquire a physical understanding of the strength and limitations of the result, and may also lend more credulity to the 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 $\Omega \subset \mathbf{R}^3$ be open and $\partial\Omega$ a smooth compact manifold. For a natural number $N \geq 1$ let $P_1, \ldots, P_N \subset \Omega$ 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* No-Mutual-Annihilator *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 fulfill the conditions to apply the two-region NMA theorem, whereby P'_1 and P'_2 have the *No-Mutual-Annihilator* property with respect to Ω which implies

$$\mathrm{Ann}(\bigcup_{i=1}^{N} P_i) \;=\; \mathrm{Ann}(\bigcup_{i=1}^{N-1} P_i) \cup \mathrm{Ann}(P_N).$$

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

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

Substituting this in the above equation proves the corollary. □

We have now all prerequisites to formulate the main result of this article:

Unique source assignment theorem. *Let $\Omega \subset \mathbf{R}^3$ be open, simply connected, and $\partial\Omega$ a smooth compact manifold. Assume that $P_1, \ldots, P_N \subset \Omega$ 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 Γ with

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

is the zero-gauged potential from the source distribution $\rho - \rho'$, which thereby is a member of

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

The equality is due to the general NMA theorem and its right hand side implies that $\Gamma_i = 0$, or $\Phi_i = \Psi_i$ for $i = 1, \ldots, N$. Thus the zero-gauged Φ_i are uniquely determined by $\frac{\partial \Phi}{\partial n}$ on $\partial\Omega$. $\square$

When denoting by $H_0(\mathbb{R}^3 \backslash P)$ the space of harmonic, zero-gauged functions outside a compact region P, the linear operator for solving the inverse problem

$$A : H_0(\mathbb{R}^3 \backslash (P_1 \cup P_2)) \to H_0(\mathbb{R}^3 \backslash P_1), \quad \Phi \mapsto \; \Phi_1$$

has the nullspace $H_0(\mathbb{R}^3 \backslash P_2)$ which is closed in $H_0(\mathbb{R}^3 \backslash (P_1 \cup P_2))$, whereby A is continuous (Rudin, theorem 1.18). Accordingly the source assignment problem a) has a solution, b) this solution is unique, and c) the operator that maps the measurement to the solution is continuous, which by definition[Zhdanov, 2015] implies that the inversion even is a well-posed problem.

This new theorem provides a clear and astoundingly general condition for when it is theoretically possible to uniquely assign potential field signals to source regions. To give a 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].

Unique source assignment is significant in geophysics for gravimetric, or aeromagnetic interpretation, when combined with tomographic methods like seismic imaging. It also lies the foundation for reading three-dimensional magnetic storage media. For our own rock-magnetic research this leads to a breakthrough for paleomagnetic reconstruction from natural particle ensembles [de Groot et al., 2018], because it confirms that individual dipole moments from a large number of magnetic particles that are localized by density tomography (micro-CT) can be uniquely recovered from surface magnetic field measurements. When scanning a sample in its natural-remanent magnetization state, and again after standard stepwise demagnetization procedures, the resultant data set can be individually studied to select stable and unaltered remanence carriers. By selecting only optimally preserved and stable remanence carriers from a large collection of measured particles, reliable statistical average directions or intensities can be calculated from terrestrial or extraterrestrial rocks which currently have to be discarded as recorders of their magnetic history.

Further significant applications of NMA theorems are EEG, MEG, or ECG inversion for example to uniquely assign EEG signals to previously determined brain regions. What essentially remains impossible by this method is to assign signals to source regions which lie inside other source regions. In this sense the new theorem 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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Supplementary information

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]*

Two-ball NMA theorem. *Let $\Omega \subset \mathbf{R}^3$ be open and $\partial\Omega$ a smooth compact manifold and $P_1, P_2 \subset \Omega$ be disjoint balls, then P_1 and P_2 have the* No-Mutual-Annihilator *property with respect to Ω.*

Proof. If there exists a mutual annihilator

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

then there are two nonzero functions $\rho_1, \rho_2 \in L_1(\Omega)$ with $\operatorname{supp} \rho_1 \subset P_1$, $\operatorname{supp} \rho_2 \subset P_2$, 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 $\mathbf{R}^3 \backslash \Omega$. 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 $\mathbb{R}^3 \backslash \overline{\Omega_1 \cup \Omega_2}$, and equal on the nonempty 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 $\operatorname{supp} \rho_1$ 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 has only Gauss coefficients from inner sources, because $\operatorname{supp} \rho_2$ 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. □