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Numerical strategies for magnetic mineral unmixing

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ABSTRACT

Iron-bearing minerals are sensitive to a wide spectrum of natural processes and thus carry important environmental information. In environmental magnetism, various techniques are used to identify and quantify magnetic mineral assemblages in natural materials, with the aim of drawing inferences concerning past environments and environmental change. Natural materials typically contain a number of magnetic mineral subpopulations with different origins that can reflect multiple environmental processes. Thus, it is essential that the information carried by such mixed magnetic mineral assemblages can be quantified in terms of environmentally meaningful component parts. Magnetic unmixing techniques are designed to perform this quantification and can, thus, act as a cornerstone for interpreting complex environmental magnetic data. In this review, numerical strategies for unmixing magnetic mineral assemblages are discussed and are illustrated with examples. Emphasis is placed on the extent of available *a priori* knowledge concerning a magnetic mineral mixture and the ways that such information can be incorporated into a meaningful unmixing model.

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1. Introduction

Naturally occurring assemblages of fine magnetic particles in rocks and sediments carry environmental information spanning a wide spectrum of temporal and spatial scales. At the shortest time scales, magnetic particles can record wildfire burning of landscapes (Gedye et al., 2006; Blake et al., 2006). Magnetic particles in sediments and soils can record anthropogenic pollution in a local catchment over periods of years and decades (Shankar et al., 1994; Hanesch and Scholger, 2002; Blundell et al., 2009). Spanning centuries and millennia, magnetic particles have recorded anthropogenic processes and provide an essential archeological tool (Oldfield et al., 1985; Dalan and Banerjee, 1998; Church et al., 2007). Moving beyond the last ten thousand years, the waxing and waning of the ices ages is recorded by sedimentary magnetic particles on continents (Heller and Liu, 1986; Maher and Thompson, 1992; Guo et al., 2002; Ding et al., 2005) and in the oceans (Bloemendal and deMenocal, 1989; Larrasoaña et al., 2003; Roberts et al., 2011b), which can help to understand Earth's climate system. Magnetic particles in ancient sediments provide key insights into environmental change driven by major catastrophic events (Ellwood et al., 2003; Chang et al., 2012; Font and Abrajevitch, 2014), and periods of time characterized by extreme global warming (Kopp et al., 2007; Larrasoaña et al., 2012).

A given geological material may have been influenced by a variety of natural processes originating from the atmosphere, biosphere, hydrosphere, and cryosphere, which in concert produce a mixed magnetic mineral assemblage that carries convolved information concerning a number of environmental mechanisms (Evans and Heller, 2003). Environmental magnetism aims to identify and quantify such natural processes based on the composition of magnetic mineral assemblages. Thus, separation of bulk rock magnetic signals into meaningful parts is an essential task. This has led rock and environmental magnetists to develop and adapt experimental and data processing techniques to "unmix" complex magnetic mineral assemblages into environmentally informative parts. A wide variety of tools is now available with which to decompose mixed signals to obtain information pertinent to environmental investigations.

The primary route to unmixing magnetic assemblages is via a sequence of well-designed experiments, with each step targeting a different part of the system. In mixed magnetic particle assemblages the results of such experiments can be ambiguous and detailed analysis frameworks have been developed in conjunction with visualization tools to facilitate interpretation. The ideas underlying these techniques have been reviewed recently with a range of illustrative examples (Liu et al., 2012). This paper focuses on techniques designed to unmix rock and environmental magnetic data numerically, which enables estimation of both the composition and abundance of environmentally relevant components. Numerical unmixing is a challenging, often ill-posed, problem that necessarily relies on a statistical foundation, while being required to respect known magnetic phenomena. Over the past thirty years numerical unmixing analysis of rock magnetic data has taken a variety of forms, but has focused on a single goal; to mathematically partition experimental data in such a manner that the individual subpopulations that contribute to a mixed assemblage can be identified, characterized, and quantified.

In this paper, ideas underlying different families of numerical unmixing techniques will be discussed with illustrative examples. In Section 2, a general overview is provided of the key concepts that underpin magnetic unmixing. Different forms of numerical unmixing models, the assumptions involved, and the level of *a priori* knowledge they require are discussed in subsequent sections.

2. Magnetic mineral mixtures

The complexity of natural systems means that most materials of geological and environmental interest will contain a variety of magnetic minerals with different grain sizes and concentrations. The aim of magnetic unmixing is to identify these magnetic mineral "subpopulations" or "components" on the basis of their rock magnetic properties and, where possible, to characterize them in detail and quantify their abundance. In its simplest form the combined behavior of a collection of components can be represented by the linear mixing model:

$$X = \sum_{j=1}^{c} A_j S_j, \tag{1}$$

where X is a bulk sample property resulting from the combined behavior of c components. Specifically, A_j is the abundance of the j^{th} mixture component and S_j is the corresponding property for that component. When dealing with experimental data sets, it is necessary to extend the linear mixing model to include an error term (e) to account for differences between the model and the data:

$$X = \sum_{j=1}^{c} A_j S_j + e, \tag{2}$$

which may arise from measurement noise, shortcomings of the model, etc. In Eq. (2), X represents a single property, for example, the saturation magnetization, but the model can be extended easily to represent collections of parameters or spectral data composed of a sequence of measurements (e.g., hysteresis loops or remanence acquisition curves), with $\boldsymbol{X}$ becoming a vector:

$$X_i = \sum_{j=1}^{c} A_j S_{ij} + e_i, \tag{3}$$

where i represents the i^{th} parameter in the sequence. In order to make Eqs. (2) and (3) physically meaningful it is typically necessary to apply constraints to $\boldsymbol{A}$ and $\boldsymbol{S}$. For example, subpopulation abundances in a mixture should be non-negative and in the case of relative abundances will sum to a constant (normally 1):

$$\begin{array}{ll} \text{Non-negativity} & A_j \geq 0, \quad j = 1, \ldots, c \\ \text{Sum-to-one} & \sum_{j=1}^{c} A_j = 1. \end{array} \tag{4}$$

Appropriate constraints on $\boldsymbol{S}$ should ensure that known magnetic phenomena are respected. This can be as simple as ensuring that parameters of interest lie within physically realistic intervals (for example, saturation magnetization, M_s, must be non-negative) or as complex as imposing shape constraints on the form of hysteresis loops (Jackson and Solheid, 2010; Heslop and Roberts, 2012a).

Depending on the unmixing problem at hand, an investigator may constrain estimates of either $\boldsymbol{A}$ or $\boldsymbol{S}$, or potentially $\boldsymbol{A}$ and $\boldsymbol{S}$ together. Although the structure of a linear mixing model is conceptually simple, any numerical approach to solving Eqs. (2) and (3) will depend on the specific problem and any simplifying assumptions made. In the case of mixed magnetic mineral assemblages, special consideration must be given to how the abundances of the mixture subpopulations can be represented and the appropriateness of a linear model.

2.1. Defining subpopulation abundances

A key aim of magnetic unmixing is to estimate the abundances of the subpopulations that make up a mixed magnetic mineral assemblage. There is, however, a level of ambiguity associated with the abundance term in the linear mixing model (Eqs. (2) and (3)) that is specific to magnetic mineral mixtures. To give an experimental example, the S-ratio (Stober and Thompson, 1977; Bloemendal et al., 1992) is an estimate of the relative abundance of high coercivity (e.g., hematite and goethite) and low coercivity (e.g., magnetite) minerals in a bulk