Inference of phase properties from sorting experiments and MLA data

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1 Introduction

Geometallurgy is a discipline on the intersection of geology, mineralogy, mineral processing and metallurgy, which aim is the adoption of mineral processing and metallurgy to the ore properties. From crushing to optical sorting, flotation, magnetic separation and so on, the behaviour of every mineral grain within the several processing steps is of interest. With this knowledge it is possible to model the output of each step and, given a certain input feed, predict the grade and recovery of the desired value mineral in the concentrate. Of course this result depends on the chosen process parameters.

Each of these processing steps is based on a certain property or property set of the particle, e.g. its hardness, density, size, etc. Knowing these values for the considered sample the perfect parameter setup could be chosen in order to get the desired grade and recovery. But this information is hard to infer. The aim of this paper is to provide a method to estimate such properties from the results of sorting experiments.

This contribution deals with magnetic separation. In order to characterize the performance of an isodynamic separator (McAndrew (1957)) its separation function is needed. Here the magnetic susceptibility defines the behaviour of the particle. The higher the susceptibility of a particle the less magnetic field strength is needed to separate this particle from the rest. The field strength is controlled by amperage at an isodynamic separator.

Unfortunately, quite often only the magnetic susceptibility of a bulk sample is measured in an experiment due to several reasons, e.g. if the composition consists of too many distinct components and the contained mineral particles consist of several mineral phases. Instead, during separation the sample is split into several classes. The susceptibility can then only be measured for such a class. It is given by

$$\overline{\chi_j} = \sum_{i=1}^{n} \frac{m_i}{m_j} \chi_i$$

($\overline{\chi_j}$: susceptibility of class j, χ_i: susceptibility of the i-th mineral phase, m_j: mass of class j, m_i: mass of the i-th mineral phase; McAndrew (1957)). If we had enough classes, at least as many as mineral phases, we would be able to calculate the mineral susceptibilities directly. But usually the number m of classes is much smaller than the number of mineral phases n.

2 Mathematical model

Given a sample mixture S consisting of a large number of distinct mineral phases i, we want to characterise a certain property p_i (e.g. the magnetic susceptibility) for each single phase $i = 1, \ldots, n$. S consists of several polymineralic particles. S is split into m classes in an sorting experiment and the average property $\overline{p_j}$ measured for each occurring class $j = 1, \ldots, m$. Knowing the mineral composition of each class, i.e. the portion $x_{j,i}$ of phase i in class j, the

following system of equations has to solved:

$$\begin{array}{ccccccccc} x_{1,1}p_1 & + & x_{1,2}p_2 & + & \dots & + & x_{1,n}p_n & = & \overline{p_1} \\ x_{2,1}p_1 & + & x_{2,2}p_2 & + & \dots & + & x_{2,n}p_n & = & \overline{p_2} \\ \vdots & & & & \ddots & & & & \vdots \\ x_{m,1}p_1 & + & x_{m,2}p_2 & + & \dots & + & x_{m,n}p_n & = & \overline{p_m} \end{array}$$

As mentioned before we usually have $n \gg m$. Furthermore the exact composition of every class is not known. We rather have e.g. MLA measurements of the class composition, i.e. 2D cuts of three-dimensional particles (Barbery (1991); Jones (1974)). We assume that these cuts are random, implying that the observed two-dimensional composition is representative for the original three-dimensional volume one. An MLA, Mineral Liberation Analyser, is a scanning electron microscope with automated software for high resolution images of rock specimen and sample compounds from mineral processing, which provides quantitative mineralogical microstructural information. (Fandrich (2007))

Since property p can only be retrieved with some error in measurement, we would like to apply a linear model to solve this problem. But as mentioned before, usually $n \gg m$. On the other hand, using data from machines like MLA, we do not only have information concerning modal mineralogy for the whole measured sample, but each particle in it. Therefore we chose to create subsamples out of every class. In each class we arbitrarily choose n_r particles for such a subsample. This procedure is repeated n_s times. Then we have a new equation for each subsample k of class j

$$x^k_{j,1}p_1 + x^k_{j,2}p_2 + \cdots + x^k_{j,n}p_n = \overline{p_j}$$

The mean of property p is $\overline{p_j}$ for each particle being chosen for class j during the sorting experiment. Therefore $\overline{p_j}$ is likewise the mean for each subsample we created. So the equation is reasonable and we now have enough of them to solve this problem using a linear model.

3 Simulation results

In order to confirm our approach we use the following simulation setting: we simulate 10^5 particles, consisting of up to 16 different phases. To each phase i the property p_i is assigned with the following values

phase	1	2	3	4	5	6	7	8
p	-25	-0.1	0.1	0.5	3	3.2	12	24
phase	9	10	11	12	13	14	15	16
p	24.5	25.5	27.8	33	55	79.5	100	110

Additionally we simulate a random cut through these particles to incorporate the 2D-3D problem mentioned before.

We consider two different sorting experiments: One experiment sorts the sample correctly. For the second the sorting is distorted with standard normal error, i.e. each particle is classified according to its susceptibility $p+\varepsilon$ with a random noise $\varepsilon \sim N(0,1)$ Both sortings result in five distinct classes

group	1	2	3	4	5
threshold values	< 10	$10 \dots 20$	$20 \dots 40$	$40 \dots 60$	≥ 60

Furthermore we consider another sorting splitting the sample into two groups, where the mean value for p over all p_i is used as threshold.

The simulations run 200 times each, the results are shown in Figure 1. The red dots indicate the correct values for the property.

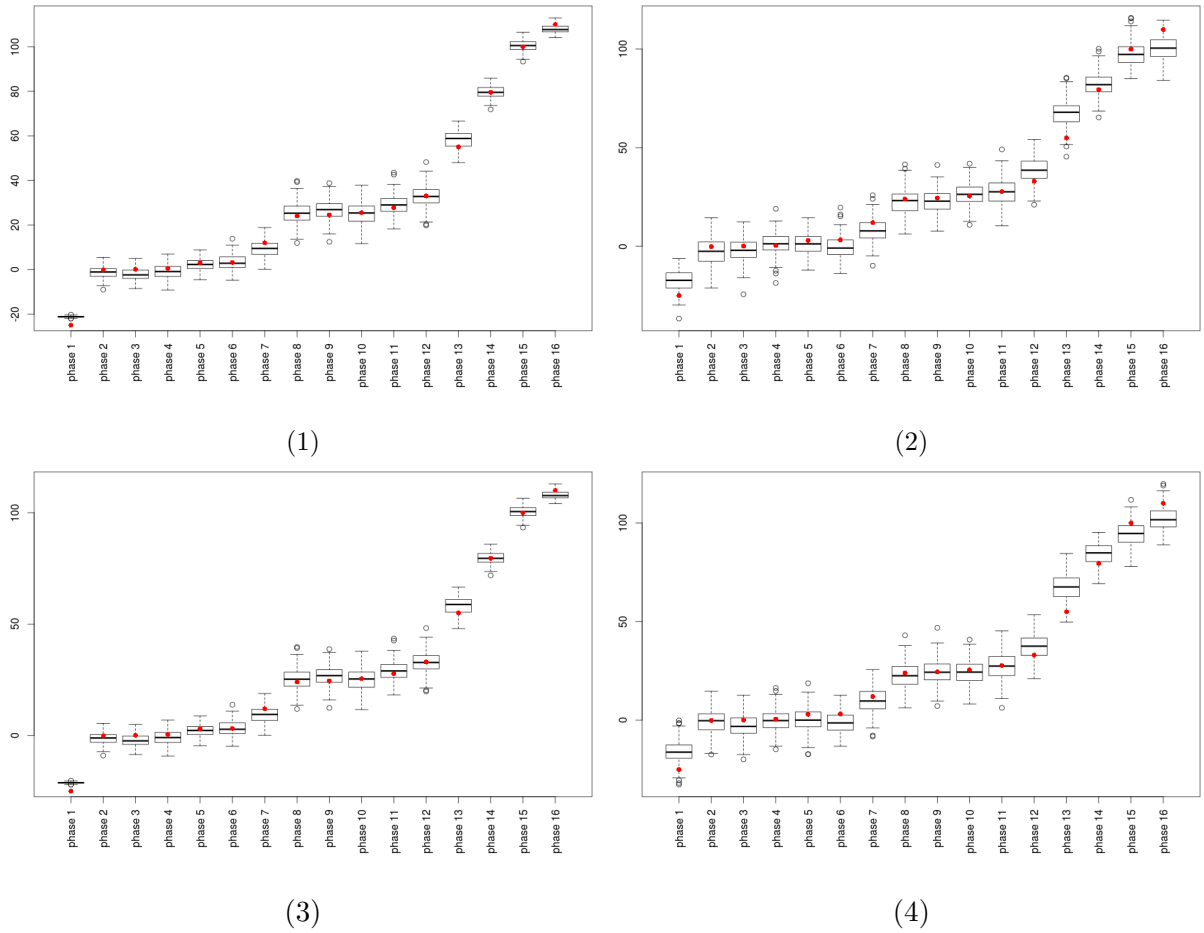

Figure 1: Predicted magnetic susceptibility (y-axis) for the simulated experiments as boxplots for the different phases considered. Red dots show the true value of theses susceptibilities. (1) five classes with no decision error, (2) two classes with no decision error, (3) five classes with decision error, (4) two classes with decision error

4 Assessing the reliability of estimates

In order to get a rating for the calculated values, we solve the linear model using singular value decomposition (Knüsel (2008)). Here we are looking for a decomposition of

$$X = \begin{pmatrix} x_{1,1}^1 & \dots & x_{1,n}^1 \\ \vdots & \ddots & \vdots \\ x_{m,1}^{n_s} & \dots & x_{m,n}^{n_s} \end{pmatrix} = U \cdot D \cdot V^T,$$

where $D = \mathrm{diag}(s_1, \dots, s_k)$ is a diagonal matrix matrix consisting of the singular values. U and V are orthogonal matrices. Since

$$X \cdot p = \overline{p}, \quad p = \begin{pmatrix} p_1 \\ \vdots \\ p_n \end{pmatrix}, \ \overline{p} = \begin{pmatrix} \overline{p_1^1} \\ \vdots \\ \overline{p_m^{n_s}} \end{pmatrix}$$

we have

$$\begin{aligned} UDV^T p &= \overline{p} \\ p &= VD^{-1}U^T\overline{p} \end{aligned}$$

A slightly different approach leads to a maximum entropy solution (Csiszar (1991)), which allows us to judge the calculated solution. Instead of X we are looking for a singular value decomposition of X^TX. Then

$$X^TXp = X^T\overline{p}.$$

In this case the two orthogonal matrices are the same, so

$$\tilde{V}D^2\tilde{V}^Tp = X^T\overline{p}$$

Each singular value deemed "too small" is now set to zero (depending on user's choice). Let us denote the arising matrix by $\tilde{D} = \text{diag}(s_1^2, s_2^2, \ldots, s_r^2, 0, \ldots, 0)$. This leads to the orthogonal matrix $\tilde{V} = [V|V_0]$. The columns of V form a basis of the part of the solution space being determinable, the columns of V_0 form a basis of the orthogonal complement, i.e. of the indeterminable subspace. Hence we use singular values close to zero as evidence for the associated vectors being in this orthogonal complement. Now

$$p = \tilde{V}\tilde{D}^-\tilde{V}^TX^T\overline{p},$$

where $\tilde{D}^-$ is a generalised inverse of $\tilde{D}$ with

$$\tilde{D}^- = \text{diag}(1/s_1^2, 1/s_2^2, \ldots, 1/s_r^2, 0, \ldots, 0).$$

Remember that the $s_{r+1}^2, \ldots, s_k^2$ were corrected to zero.

This decomposition in a determinable and an indeterminable subspace allows us to assess how determinable each individual phase susceptibility is. The i-th row vector of the matrix $\tilde{V}$ identifies phase i. The projection of this vector on the indeterminable subspace (i.e. the norm of the i-th row vector of matrix V_0) is the quantity sought. This is 1 if the i-th variable is completely indeterminable, and it is 0 if it be can perfectly determined. To simplify this interpretation, we assign up to three $*$ to every p_i. Hereby $***$ means, that this value is very reliable. Then this vector is orthogonal to the indeterminable subspace and the variable can be perfectly determined from the data available. If there is no $*$ assigned,then this value strongly depends on the orthogonal subspace, i.e. do not rely on it.

5 Application to real data

The following example uses real data from a rare earth mineral deposit. We wanted to calculate the magnetic susceptibility of each of the 31 mineral phases, but the sorting only split the sample into eight classes. We repeated the approach given before 200 times for the data. Figure 2 shows the corresponding boxplots. The following table shows the reliability of the calculated values.

phase	1	2	3	4	5	6	7	8	9	10	
reliance	**	**	**	*		**	*	*		**	
phase	11	12	13	14	15	16	17	18	19	20	
reliance	*	*	**	*	**	*	*			*	
phase	21	22	23	24	25	26	27	28	29	30	31
reliance	**	**	**	*	**	*	**	**		**	**

Compared to the little number of magnetic susceptibilities of the observed mineral phases found in the literature (Hunt (1995); Bleil (1982); Carmichael (1990); Rosenblum (1999)), which is one reason, why we wanted to compute them, at least the values marked with $**$ seem quite reasonable. But some of them, especially the values labelled with no $*$ and the ones with a large variance within the 200 calculations, appear to be unrealistic.

The given approach is applicable to other phase properties, too. But then this property has as well to be additive, e.g. density, in order to end up in a system of linear equations as shown above.

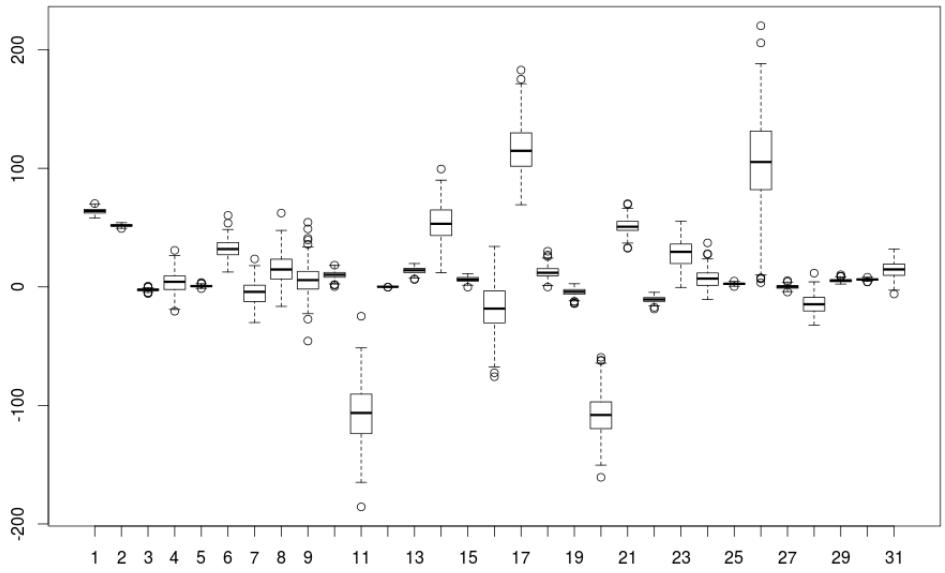

Figure 2: Boxplots for the calculated magnetic susceptibilities for each mineral phase considered in a sample of a rare earth deposit

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