Simultaneous estimation of melting degree and source composition of MORB: an application of data-driven analysis to Geochemistry

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Geochemical data sets, such as major, trace and isotopic compositions, preserve precious information about various physical and chemical processes. For example, bulk compositions of igneous rocks directly reflect melting of original rocks, magma mixing and rock-fluid interaction in the earth's interior. However, it has been still difficult to extract physical and chemical processes quantitatively due to many unknown factors and insufficient quality of data sets. Recently, many sophisticated data-driven methodologies have been proposed to extract useful information from high-dimensional data sets in information sciences. In this presentation, we will briefly overview data-driven analytical technologies and introduce an application to simultaneous estimation of melting degrees and a mantle source composition from MORB bulk compositions based on Bayesian estimation and Markov chain Monte Carlo (MCMC) optimization.

Keywords: data-driven, Bayesian estimation, sparse modeling, Markov chain Monte Carlo method

Statistical identification of meteorites using X-ray energy spectra measured with handheld-XRF

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Landing explorations of extraterrestrial bodies give us detailed information of their surface materials. Rapid identification of the types of materials is important for planning further in-situ analysis during a remote mission, which includes selecting prime targets to yield optimal science return. Active X-ray fluorescence (XRF) is a candidate for future missions, including being a part of the payload of a surface rover [1] as well as APXS [2], for example, which can perform in-situ measurements of the composition of the surface materials. However, one of the largest problems with XRF measurement is the matrix effect. X-ray excitation intensity is highly influenced by changes in the various matrices (e.g. mineral abundance, crystallinity, and porosity). To remove this effect, fusion bead sample is used for laboratory analyses. Then to calculate quantitative values, abundant numbers of a well-known standard samples are measured to obtain a calibration curve, otherwise the bulk compositions cannot be quantitatively and accurately analyzed. Thus, we are testing whether the meteorite type can be statistically identified without matrix correction using X-ray energy spectra yielded from a hand-held XRF (Olympus Delta). We measured 20 meteorite slab samples stored at the University Museum, University of Tokyo, which include chondrite (carbonaceous and ordinary), achondrite (HED, mesosiderite, and Martian), and primitive achondrite (ureilite). Niihara et al. [3] reported that the compositional values of at least 6 elements (Si, Ti, Al, Fe, Mn, and Ca) could be measured both quantitatively and accurately using a hand-held XRF. Thus, we also perform comparative analysis among the compositional values and the X-ray energy spectra, although the quantitative values include large uncertainty due to the matrix effect; we conduct principal components analysis on both the X-ray energy spectra (10 kV and 40 kV: 40 kV can detect signals from minor to trace heavy elements) and compositional data.
On the PC1 and PC2 space, although the total number of classified types of meteorites is only six, we can distinguish almost every type of meteorite (although mesosiderites are widely distributed) utilizing every data set. Achondrites and primitive meteorites can be easily separated by PC1 for energy spectra or PC2 for compositional data. On PC2, ordinary and carbonaceous chondrites are nearly identical both in 10 kV and 40 kV energy spectra data, while indistinguishable using compositional data. Variations appear to be mainly due to the Fe, Ca, and Si components in the spectral and compositional data sets, consistent with Miyamoto et al.[4], despite the fact that 10 kV and 40 kV spectra have different elemental sensitivities. These three elements are major components of major rock-forming minerals (olivine and pyroxene) and are common in meteorite samples. Based on these result, we suggest X-ray energy spectra could be used to classify meteorites directory without any kind of correction and is useful for primary classification and targeting during future planetary surface explorations.

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Keywords: X-ray energy spectra, Meteorites, PCA

Preliminary results of principal component analysis on visible near-infrared reflectance spectra of meteorites with comparison to the petrological classification

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Classification of asteroids based on spectral observations by ground- and space-based telescope has been studied for decades to obtaining information of constituent materials of asteroids. Tholen [1] first classified asteroids by principal component analysis (PCA) using 8 colors reflectance spectra (wavelength 0.33-1.1 μm) into 13 types. DeMeo et al. [2] also conducted PCA and classified asteroids in more detail (27 types include subtype) by increasing the range of spectra (0.45-2.45 μm; 41 colors). Considering that meteorites are classified into 45 types (at group level) [3], the increase of asteroid class from Tholen [1] to DeMeo et al. [2] is important in order to correspond asteroids with petrological characteristics of known meteorites, which highlights the importance of the wavelength range and resolution of reflectance spectra.
Britt et al. (1992) [4] compared the reflectance spectra of 103 asteroids and 411 meteorites using principal component analysis. They used the Eight Color Asteroid Survey (8 colors), with a range of wavelength of 0.33 to 1.1 μm. They found that HED meteorite (which is believed to originate from asteroid Vesta) correspond well with V-type asteroids, however, the other major meteorite types do not have clear resemblance with any asteroid types. Because they used reflectance spectra shorter than 1.1 μm, they could not utilize the strong absorption band of pyroxene locating near 2 μm where another major mineral olivine does not have absorption. Our motivation of this study is to conduct principal components analysis using reflectance spectra of meteorites with wider wavelength region from 0.45 to 2.45 μm to compare with conventional petrological classification.
We compiled 709 reflectance spectra of meteorites within the wavelength range from 0.45 to 2.45 μm with high wavelength resolution (41 colors) from the database of RELAB facility at Brown University [6] and conducted principal component analyses. We find that a carbonaceous chondrite and an aubrite have the highest and the lowest PC1, respectively, with aubrites being widely distributed in terms of PC1. The 0.9 μm absorption band of olivine and pyroxene is the primary factor to contribute to PC1 dispersion. PC2 are contributed with 0.9 μm and 2 μm absorption band. On the PC1 space, ordinary chondrites, ureilite meteorites and carbonaceous chondrites (which are all primitive meteorites) locate close to each other, while ureilite meteorites scatter between ordinary and carbonaceous chondrites, suggesting that PC1 may represent the primitiveness of meteorites. In addition, based on PC2, we could be able to distinguish primordial of meteorites (which have information of early solar system) and differentiated meteorites that have experienced large scale melting/differentiation (HED meteorites and Mars) on PC2.
Although the primary minerals of meteorites are olivine and pyroxene, each meteorites has significant diversity such as mineral composition, grain shape and chemical composition, which should affect reflectance and the center of absorption band. Especially only pyroxene minerals have 2 μm absorption, thus the abundance of pyroxene could significantly contribute to the dispersion of PC2. Our spectral analyses using wider wavelength region of meteorites reflectance spectra suggest that based on PC1 and PC2, we may be able to distinguish meteorites at least Class level defined by conventional petrological classification [3].
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Keywords: Principal Component Analysis, meteorite, visible near-infrared reflectance spectra, asteroid, spectra

Statistically independent components controlling enrichment of rare-earth elements in deep-sea sediments

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Rare-earth elements and yttrium (REY) are critical materials that are indispensable in high-tech devices and green technology applications including electric vehicles, smart phones, LED bulbs, wind power generation, and so on. Recently, deep-sea sediments highly enriched in REY, known as REY-rich mud, have been discovered in the Pacific and the Indian oceans (Kato et al., 2011; Yasukawa et al., 2014, 2015). Because of their huge potential economic value as a new resource for REY, it is becoming an important issue to understand the origin of REY-rich mud.
Elucidating the controlling factors of REY-enrichment in deep-sea sediments is key in finding areas of high resource potential worthy of detailed exploration and for revealing latent relationships between the Earth's system and marine mineral resources. Here we construct a hemisphere-scale compositional dataset of ~4,000 bulk sediment samples from more than 100 sites in the Pacific and the Indian oceans, and we apply Independent Component Analysis originally established in the fields of neuroscience and information science in 1990s, to the huge, multi-elemental data matrix. As a result, we successfully extract the statistically independent geochemical signatures including components controlling the REY-enrichment in deep-sea sediments. The features of the REY-controlling components, including hydrothermal, hydrogenous, and biogenic calcium phosphate components, indicate that an underlying key factor of significant REY-enrichment is a sufficiently low sedimentation rate that enables the mud to accumulate REY from the overlying seawater.
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Keywords: deep-sea sediment, REY-rich mud, Independent Component Analysis

CONSTITUTIVE DYNAMICAL SYSTEMS OF SOLID EARTH MECHANICS FROM DATA DRIVEN SCIENCE

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CONSTITUTIVE DYNAMICAL SYSTEMS OF SOLID EARTH MECHANICS FROM DATA DRIVEN SCIENCE
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Explosive massive data flow of seismic activities in the solid earth and related to the volcanic activities takes a new insight of dynamic processes involving complicated basic mechanisms and various inhomogeneities of present systems by means of reconstruction of the attractors in the high dimensional phase space. Recent data science studies of global geochemical data of ridge basalts clarified the global chemical inhomogeneity of the whole mantle hemisphere, indicating the long term mantle hydration by plate subduction by Iwamori (1). Besides, Toriumi (2) studied the seismic activities of the plate boundary zones using the cross correlation method to apply the dimension reduction of the local mechanical states of the crust and mantle. Further, Kuwatani et al. (3) applied the Markov random field model for fluid phase regional patterns in the uppermost mantle from tomographic data.
Reconstruction of the attractors of the dynamical systems of plate boundary mechanics is possibly obtained by means of dimension reduction method using deep learning processing of time series data of seismicity and eruption related seismicity. In this paper, the author intends to discuss the possibilities of big data analyses for constitutive dynamical system in the solid earth process in the case of mechanical evolution of the plate boundary and the volcanic process.
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Keywords: reconstructive dynamical system, solid earth processes, dimension reduction

Relationship between albedo and reflectance spectra of asteroids: implication to asteroids' thermal processes

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Large amounts of visible and near-infrared reflectance spectra data of asteroids have been obtained by ground- and space-based telescopic observations. Using the reflectance spectra, asteroids have been classified into several types based on principal component analysis [1]. Different types of meteorite samples, however, can yield similar reflectance spectra such as black ordinary chondrites and carbonaceous chondrites [2]. Thus the degeneracy of reflectance spectra may suggest that there is an application limit of the classification scheme based solely on reflectance spectra. Albedo data also have been accumulated, however, their relationship with reflectance spectra are not fully understood [3]. Our objective is to combine albedo with reflectance spectra in an attempt of improving asteroid classification.
We compiled visible/infrared reflectance spectra within the region of 0.45 to 2.45 μm based on published databases. Most of the spectra are from IRTF Near-IR Spectroscopy of Asteroids [3]. All the spectra were sampled with cubic spline fits at a wavelength interval of 0.05 μm, resulting in 41 data points. We defined the spectral type index *R*, which is the difference between correlation coefficients with average S and C-type spectra. Positive *R* values more closely approximate C-type spectra, while negative *R* values S-type. We also compiled geometric albedo data mostly from Supplemental IRAS Minor Planet Survey [4].
The albedo-spectra map indicates that there is a general trend in the distribution of asteroid types. V-type, C-type and S-type asteroids are distinctly separated from each other on the albedo-spectra map. The variance of each cluster appears to increase in the order of V-type, S-type and C-type. It appears that geometric albedo plays a significant role in the resulting spectral signature. There are many possible factors which could influence albedo, such as (1) mineral and/or elemental composition, (2) fragmented particle size, (3) space weathering and (4) crystal size. We consider, however, crystal size to be the primary factor in the resultant albedo-spectra map because: (1) based on the analyses of meteorites, there is no significant difference between ordinary and carbonaceous chondrites in terms of carbon content or modal composition, (2) smaller particles tend to yield higher albedo, though not enough to explain the significant albedo difference observed among asteroids, and (3) spectral darkening due to space weathering requires reduced Fe (noting that there is no clear evidence that C-type asteroids, which are significantly darker than S-type or V-type asteroids, have higher Fe abundances). With the above consideration, we discuss the crystal size in the context of thermal processes of asteroids to help explain albedo-spectra map.
Smaller crystals generally result in darker reflectance. V-type asteroids are believed to have experienced differentiation and magmatism, as evidenced by the analyses of HED meteorites. Thus the crystals would become coarser due to a slow cooling rate, resulting in brighter and more pyroxene-rich surface spectra. On the other hand, S- and C-types would be undifferentiated chondrite asteroids, believed to correspond to ordinary and carbonaceous chondrites, respectively. Those meteorites preserve chondrules generally having finer crystals due to rapid cooling in the presolar nebula [5]. This would result in dark featureless surface spectra of C-types. S-type asteroids have experienced moderate thermal metamorphism after their accretion, causing recrystallization which results in larger crystals and in more evident pyroxene signals than C-type.

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Keywords: asteroids, reflectance spectra, albedo, meteorites, crystal size

Data driven construction of thermodynamic model of hydrous melt using machine learning technique

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H_2O in silicate melt drastically changes the phase relation of magma. Phase relations and physico-chemical properties of hydrous magma have been determined based on various experiments. However, each experiment was carried out under independent P-T condition and melt composition. To model the phase relation of hydrous magmas in continuous P–T–composition space of a natural melting zone, numerical model must be developed.
In order to conduct a numerical modeling, we need to develop a consistent set of a thermodynamic equation and its parameter values. Generally, thermodynamic equation is constructed based on a priori information such as theoretical predictions or observations using natural samples. However, little is known about the microstructure and physico-chemical properties of hydrous melt. It means that modeling of hydrous melt lacks a pripri information. In this situation, we have to construct both the non-linear model equation and parameter values based on small size of experimental data set. In addition, silicate melt exhibits a multi-component system. The degree of freedom in terms of composition, pressure and temperature ranges are large. In this case, previous methods used in earth science field such as analytical or empirical methods are not effective for the modeling.
In order to obtain the optimal thermodynamic parameter values based on experimental results obtained within discrete and limited P-T-compositional conditions, we use cross-validation technique. In the cross-validation, we divide the dataset (experimental results) into two groups. We optimize parameter values to make the best fit of the first group (the training data). The external validity (generalization ability) of the parameter set is obtained using the second group (the test data).
For the selection of the model equation, we test all possible combinations of coefficients of the thermodynamic equation. For the each combination of coefficients, we use leave-one-out cross-validation, in which the one experimental result is used for the test data, and the rest is used for the training data. All the possible ways to divide the original data are tested, and the average residual is regarded as the validity of the model equation. The combination of coefficients to minimize average residue is regarded as the model equation and the optimized parameter is regarded as the optimal thermodynamic parameter set.
We develop a thermodynamic model to calculate phase equilibrium between hydrous melt and olivine as a model system. We use experimentally determined melt composition, H_2O concentration, pressure, temperature and olivine composition during the melting of hydrous and anhydrous mantle peridotite (e.g., Hirose and Kushiro, 1993; Hirose and Kawamoto, 1995) as a dataset. Specific heat of melt and non-ideality model for the olivine solid solution are taken from previous studies. We assume the regular solution for the basic equation of the non-ideality of melt, in which non-ideal free energy is described as linear functions of concentrations of end-member components. Especially for the H_2O, polynomial of degree 2 is considered because a strong non-linear relationship between H_2O concentration and phase relation has been reported.
The optimal model uses the first-degree term against all end-member components. However, the second-degree term of the H_2O component is not selected for the optimal model equation. Forward calculations conducted using the optimized model equation and parameter set reproduce the experimentally determined genetic conditions of hydrous magmas. The method presented in this study, data driven method for construction of the thermodynamic model can be applicable to various systems

such as modeling of rock forming minerals and multi-phase systems.

Keywords: Machine learning, Thermodynamics, Hydrous melt, Phase equilibrium

Forward modeling of microboudinaged columnar grains: simplified microboudin palaeo-piezometer

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Proportion of microboudinaged columnar grains embedded within metamorphic rocks is the key gauge to evaluate the differential stress during plastic deformation. We present the forward modeling for microboudinaged grains, and propose the simplified microboudin palaeo-piezometer.
The modeling consists of the weakest-link theory and shear-lag model. The weakest-link theory for the fracturing of fibre minerals are derived the probability density function of fracture strength as a function of aspect ratio and strength (Masuda et al., 1989). We obtain the fracture strength of each columnar grain from generating sample numbers at random from above probability density function by the inverse transform method. Shear-lag model (Zhao and Ji 1997) is the stress-transfer model for stress distribution along a fibre connecting the far-field differential stress with the tensile stress. If the tensile stress is higher than the fracture strength on a certain grain, we regard this grain becoming the microboudinaged grain. We also assume that the distribution of fracturing points in each grains conform to the Beta distribution. We collected the shape data of the columnar grains from tourmaline grains embedded with in the metachert from East Pilbara Terrane. We measured the width, length, and fracturing point of the microboudinaged grains of 1432 tourmaline grains with their long axes ±15° to the mean orientation. Base on the tourmaline grain shape data, we calculate the variation of the proportion of microboudinage grains with respect to the far-field differential stress from 0 to 20 MPa.
Our calculation shows that the increasing of proportion of the microboudinaged grains coincides with the increasing of the far-field differential stress. At 20 MPa, 70% of grains were microboudinaged. The proportion of microboudinaged grains with respect to aspect ratio, which is fundamental data in the microboudin stress analysis, shows significantly similar distribution pattern in natural microboudinaged tourmaline grains. Thus, our modeling surely reproduced the microboudinage of columnar mineral grains. We focus the results on the proportion of the microboudinaged grains with respect to far-field differential stress, and construct the simplified microboudin palaeo-piezometer to estimate the far-field differential stress from the proportion of the microboudinaged grains. We demonstrate the stress analysis to tourmaline grains embedded within metachert using the simplified microboudin palaeo-piezometer, and compare with usual microboudin palaeo-piezometer.

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Keywords: Microboudin structure, Palaeo-piezometer, Numerical modeling

Selection of observation points in kriging based on non-convex programming

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Kriging (Matheron, 1963) is a method of interpolation for a stochastic field in the spatial domain. The procedure of kriging is as follows: the first step is to estimate the semivariogram, which determines the spatial covariation of stochastic field and the second step is to solve a linear equation with respect to observations and the semivariogram so that the predictions are the best linear unbiased predictors. Kriging is widely used in various fields such as solar radiation forecasting (Alsamamra et al., 2009), radon concentration prediction (Zhu et al., 1996), and circuit variability analysis (Yelten et al., 2012).
Since the ordinary kriging uses all observation data, it requires prohibitive computational cost when immediate estimates at many points are needed in the case of, for example, an urgent evaluation of earthquake hazards. For reduction of the computation cost, Yang et al., (2014) proposed to implement least absolute shrinkage and selection operator (lasso) on kriging. However, a convex regularization term is not efficient enough to select observation points because it does not match the constraint that the predictions are unbiased. Therefore we propose to carry out kriging based on non-convex programming.
The non-convex programming problems here have the hyperplane constraint, and the objective function is the sum of a quadratic form and a non-convex penalty term such as 1) L1-L2 regularization term proposed by Lou et al., (2015) and 2) L1-largest-K regularization term proposed by Gotoh et al., (2015). These problems belong to DC programming, in which objective functions can be represented as the difference of two convex functions. Approximate solutions of such problems can be obtained by DC algorithm proposed by Tao (1986), which is now a general approach to DC programming.
A numerical experiment shows that the L1-L2 regularization term and L1-largest-K regularization term work well for selection of observation points in kriging although lasso does not work efficiently.

Keywords: Kriging, DC Programming, Selection of observation points

Preliminary spatial modeling of ore grades over a deposit by a combination of geostatistics and physical law

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This study is aimed to develop a method for highly precise spatial modeling of metal contents in a metal deposit. For this, a combination of geostatistics and a physical law is examined. Matsumine and Fukazawa mines, typical large kuroko deposits in the Hokuroku district, Akita Pref., northern Japan, are selected for a case study of the combination. Kuroko is a Japanese term for massive, compact black-ore mainly composed of sphalerite, galena, and pyrite. Kuroko deposits were originated from felsic to intermediate submarine volcanic activity (e.g. Yamada and Yoshida, 2013). The metal contents of Cu, Zn, and Pb (chief metals of kuroko) in the drilling cores were used for the spatial analyses.
After semivariogram analysis to clarify the spatial correlation structure of the metal data, kriging and sequential Gaussian simulation were used to produce a 3D spatial model of ore grade. Assuming that the transport of ore solutions and the deposition of metals are approximated by an advective-diffusion spread phenomenon, theoretical solution of an advective-diffusion equation was applied to the ore grade data by solving unknown parameters such as advective velocity and diffusion coefficient. Then, ore grades over the study area were assigned from the physical model. Finally, geostatistical and physical models were combined by a kriging technique so that the calculated ore grades by these models were coincident with the sample grade data. The combined model shows roughly main paths of ore solutions, which may contributes to interpret the deposit formation process. Our next step is a multi-scale spatial modeling by extracting and characterizing distributions of sulfide minerals in kuroko ore samples.
Acknowledgments: The authors wish to express their gratitude to Dowa Metals & Mining Co., Ltd. and Hanaoka Eco-System Co., Ltd. for providing the precious drilling investigation materials and cooperating to organize them.
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Keywords: Kuroko, kriging, advection-diffusion equation, copper grade, ore-solution path

Approximate Bayesian Computation of surface-area model selection in water-rock interactions

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Water-rock interaction is one of the key ingredients in understanding the dynamic processes of surface and subsurface environments of the Earth. It has been, however, frequently remarked that there exist several orders of discrepancy in kinetic rates between laboratory and fields, which is attributed to a large uncertainty in estimates of the surface areas in the various geological situations.
In order resolve the problem, it is highly desired to establish an analytical method which provides an accurate estimation of the kinetic rate constant from reaction solvent data obtained by laboratory and also fields. In particular, it is of significant for the considered method to have an ability to identify a model of the surface areas.
In this study, we firstly applied Approximate Bayesian computation (ABC) method to select model of surface areas of minerals and evaluate the reaction rate constant from the solution chemistry data. ABC has recently attract attention in the field of machine learning as an efficient inference technique for some problems in which a likelihood function is difficult to evaluate. Here, we discuss one of the simplest chemical reaction systems which is realized in laboratory experiments. Chemical equations are given by a set of ordinary differential equations for each chemical constituent concentrations. For a given set of reaction rate constants and an initial condition, time evolution of the concentrations is obtained relatively easily in numerical simulations, while to evaluate the likelihood function under an observation noise is a non-trivial task. This is the situation that ABC should work effectively. We propose a framework to evaluate the reaction rate constants from partially observed data for the case where time evolution of an intermediate product is only observable from experimental measurements. Actual numerical calculations are based on a population-type Monte Carlo method which is one of various technique in the ABC scheme. It is found that the proposed method successfully evaluates the rate constants for a synthesis data of the intermediate product. In addition, we show some results of the model selection of the surface areas on the basis of ABC.

Keywords: water-rock interactions, Approximate Bayesian Computation, surface-area model

