[Poster Titles]
(Additional information on authors, affiliations and abstracts follows)

1. Predicting Drosophila behavior from a small number of neuron types
2. Topological data analysis of across-sniff habituation in olfactory cortex
3. Towards accurate spatial modeling of hydrothermal-originated metal grade by a combination of geostatistics and physical law
4. Sparse estimation of neural circuits for internal rewards
5. Analysis of x-ray fluorescence holography data using sparse modeling on Mn-doped Bi2Te3 topological insulator
6. Analysis of x-ray fluorescence holography data using sparse modeling on the traditional Fe65Ni35 Invar alloy
7. Statistical properties of interaction parameter estimates in direct coupling analysis
8. Statistical Mechanics Analysis of Compressed Sensing for Hamiltonian Estimation of the Ising Spin Glass
9. Time-series reconstruction using compressed sensing with ADMM in 2D magnetic resonance spectroscopic imaging
10. Solid-state NMR signal assignment by covariance NMR combined with Monte Carlo integration
11. Statistical mechanical analysis of sparse linear regression as a variable selection problem
12. Geodetic data inversion for spatial distribution of slow slip events using sparse modelling
13. Simultaneous Screening for Positive-Unlabeled Sparse Support Vector Machines
14. Geochemical-petrological evolution under the paleo subduction zone identified by machine-learning techniques
15. Bayesian inference of an effective interaction between atomic defects on the surface of SrVO3
16. Principal component analysis with electronic wavefunctions for exploration of organic polymer device materials
17. (Cancelled)
18. Many-variable variational Monte Carlo method with sparse modeling
19. Direct imaging of supermassive black hole by sparse modeling
20. Variational Bayes method for matrix factorization to two sparse factorized matrices
21. Approximate analysis of matrix factorization/completion problem by variational Bayes method with sparse prior

22. Comparison between asteroids and meteorites through multivariate analysis of visible to near-infrared reflectance spectra
23. Low-rank matrix completion by simulated annealing
24. Analytical continuation of quantum Monte Carlo data using sparse modeling
25. Regression model for stabilization energy of various anion ordering in perovskite oxynitrides
26. TimeTubes: Visual Fusion for Detailed and Precise Analysis of Time-Varying Multi-Dimensional Datasets
27. Model selection on chemical kinetics in water-rock interaction using exchange Monte Carlo method
28. Bayesian spectroscopy of x-ray photoelectron spectra in graphenes having atomic thicknesses on SiC substrates
29. Bayesian spectroscopy for spectral and normal mode analyses in solid-state materials
30. Seismic wavefield imaging of long-period ground motion in the Tokyo metropolitan area, Japan
31. Bayesian common parameter model in systems biology
32. Bayesian inference for chemical kinetics of catalytic reaction using temporal analysis of products
33. Bayesian spectroscopy of excitonic photoluminescence spectra in Cu_2O thin crystals
34. Break the Limit of Live Imaging Technology using sparse modeling.
35. Deta-driven analysis of first-principles simulation of chemical reaction
36. Extracting Neuronal Nonlinear Dynamics Based on Sparse Modeling
37. Bayesian inversion analysis of nonlinear spatiotemporal dynamics of heterogeneous reactions in rock-water interactions
38. Application of compressed sensing for efficient measurement of scanning tunneling microscopy and spectroscopy
39. Bandit Algorithms for Fast Diagnosis by Interactive Measurement

[Posters]

1. Predicting Drosophila behavior from a small number of neuron types

Takuya Hiroshima[A], Laurent Badel[B], Hokto Kazama[B], and Keiji Miura[A]

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Although various hypotheses on population coding such as a grandmother cell hypothesis have been proposed, it remains unclear how many neurons are essential to trigger fly behaviors. Here we tried to predict fly aversive responses to abundant odors from the recorded neural activity of olfactory glomeruli by using algebra-based sparse estimation of input-output relationships. We found that at least 6 cells are necessary to explain the behaviors, suggesting that a grandmother cell hypothesis is insufficient under broad olfactory contexts.

2. Topological data analysis of across-sniff habituation in olfactory cortex

Yuki Usui, Ayaka Onishi, and Keiji Miura

Kwansei Gakuin University

Although it is well known that animals habituate to odors across sniffs, its neural basis is still unclear. While many neurons we recorded from the olfactory cortex (anterior piriform cortex) decreased firing rates for the continued odor stimulation, some increased firing rates. Therefore, it is necessary to characterize the responses dynamically as a whole to understand the habituation in the olfactory cortex. The principal component analysis revealed that the neural responses at the first and second sniffs after the odor delivery looked different. In fact, the topological data analysis revealed that the orbit of the neural responses for the two sniffs did not necessarily repeat the same loop twice. These findings suggest that the olfactory cortex could underlie the odor habituation across sniffs.

3. Towards accurate spatial modeling of hydrothermal-originated metal grade by a combination of geostatistics and physical law

Lei Lu[A], Katsuaki Koike[A], Koki Kashiwaya[A], Mohamad N. Heriawan[B], and Ryoichi Yamada[C]

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This study is aimed to develop a method that combines geostatistics and a physical law for highly precise spatial modeling of metal contents in hydrothermal-originated ore deposits . Semivariogram clarified spatial correlation structure of the metal data and then kriging estimations and conditional simulation were used to generate three-dimensional distribution of ore grade. Transports of ore fluid and depositional process of metals were assumed to be approximated by a physical process with partial differential equation. Numerical solution of advection-diffusion equation was applied to metal grade from borehole sampling data. Suitable values of the advective velocity and diffusion coefficient were determined at each location according to the geostatistical estimation and simulation. The Spatial modeling by a joint use of Physical law & Geostatistics (SPG) method was verified by two types of ore deposits, kuroko (volcanogenic massive sulfide) type in Japan and porphyry copper type in Sulawesi Islands, Indonesia. Matsumine and Fukazawa mines, typical kuroko deposits in the Hokuroku district, Akita Pref., northern Japan, were selected to verify SPG As the result. High metal content zones are well clarified and characterized, and a fluid flow pattern that formed the zones is expressed as a colloidal texture which could suggest temperature and pressure changes in the shallow subvolcanic activities.

4. Sparse estimation of neural circuits for internal rewards

Shintaro Nakamura[A], Ju Tian[B], Naoshige Uchida[B], Mitsuko Watabe-Uchida[B], and Keiji Miura[A]

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Dopamine neurons, representing an internal joy, are known to promote the learning in which animals select future actions based on past reward experience. Although the activities of dopamine neurons themselves should be determined by the projections from the other types of neurons, the functional connections within the reward system are still unclear. In this study, we construct a sparse regression model that can reproduce electric activities of dopamine neurons from the others.

5. Analysis of x-ray fluorescence holography data using sparse modeling on Mn-doped Bi2Te3 topological insulator

Shinya Hosokawa[A], Jens R. Stellhorn[A], Tomohiro Matsushita[B], Naohisa Happo[C], Koji Kimura[D], Koichi Hayashi[D], Mamoru Kitaura[E], and Minoru Sasaki[E]

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Mn K-alpha x-ray fluorescence holography (XFH) measurements were performed on a Bi2Te3Mn0.1 topological insulator single crystal at 300 and 100 K to search for the Mn impurity sites in this functional crystal. Possible impurity sites are twofold, i.e., an interlayer site with an octahedral symmetry and a substitutional site of Bi and/or Te in the layer. Local structural information was obtained by detailed analyses using a L1-regularized linear regression for the experimental data, such as the ratio of the Mn impurity sites, the Mn-Te interatomic distances, the lattice distortions, and the positional fluctuations around the impurity Mn atoms. A distinct temperature dependence is seen in the positional fluctuations of the impurity Mn atoms. These findings for the impurity sites cannot be obtained by diffraction or XAFS experiment in the usual way, but only using a combination of the XFH and XAFS measurements

6. Analysis of x-ray fluorescence holography data using sparse modeling on the traditional Fe65Ni35 Invar alloy

Yuki Ideguchi[A], Jens R. Stellhorn[A], Shinya Hosokawa[A], Tomohiro Matsushita[B], Naohisa Happo[C], Kunio Yubuta[D], Koji Kimura[E], and Koichi Hayashi[E]

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Fe and Ni Kα x-ray fluorescence holography (XFH) measurements were carried out on a single crystal Fe₆₅Ni₃₅ Invar alloy at 100 and 300 K to investigate the temperature dependence of the three-dimensional local structures around the Fe and Ni atoms, respectively. Local structural information was obtained by detailed analyses using a L1-regularized linear regression for the experimental data. At 100 K, the local atomic arrangements around both the elements show fcc structures. At 300 K, however, only the image around Fe shows a bcc-like neighboring arrangement. In addition, the atomic image around Fe exhibits a fcc structure by choosing the incident x-ray energy at the high-spin (HS) shoulder in the XANES spectrum, i.e., the atomic arrangements around the HS atoms are fcc-like. From these XFH data, we propose a model that by increasing temperature that an Fe atom enters around an Fe atom with the low-spin (LS) state at the central position of the fcc lattice and is stabilized there.

7. Statistical properties of interaction parameter estimates in direct coupling analysis

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We consider the statistical properties of interaction parameter estimates obtained by the direct coupling analysis (DCA) approach to learning interactions from large data sets, which help to filter out the insignificant elements from learning results. Two inference methods are considered: the L2 regularized naive mean-eld inference procedure (regularized least squares, RLS), and the pseudo-likelihood maximization (plmDCA). Numerical simulations indicate that background distribution can be characterized by a few system parameters with finite scaling properties. This property holds for both RLS and plmDCA and may be exploitable for inferring the distribution of extremely large interactions from simulations for smaller system sizes.

8. Statistical Mechanics Analysis of Compressed Sensing for Hamiltonian Estimation of the Ising Spin Glass

Chako Takahashi[A], Masayuki Ohzeki[A], Shuntaro Okada[B], Masayoshi Terabe[B], Shinichiro Taguchi[B], and Kazuyuki Tanaka[A]

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Recently, several powerful machines dedicated to solver of the optimization problems such as D-wave machine with quantum mechanics have appeared. To input problems on the machines, a method to estimate coupling constants from several pairs of energy and spin configurations is needed. In this presentation, we propose such a method by use of compressed sensing. Compressed sensing is a technique for reconstructing an unknown sparse vector from low dimensional data. This technique has spread to many fields because of its simple principle, straightforward implementation, and extensive availability for various applications. We consider compressed sensing for the above case in fully-connected Ising model, and analytically evaluate the estimation performance of the coupling constants. Then we employ the replica method, which was used in the performance analysis of the compressed sensing in the ordinary problem setting as in [Kabashima et al., 2009]. We show that our result coincides with the results in [Donoho & Tanner, 2005] and [Kabashima et al., 2009]. Finally, we compare our analytical result with numerical result using the alternating direction method of multipliers.

9. Time-series reconstruction using compressed sensing with ADMM in 2D magnetic resonance spectroscopic imaging

Utako Yamamoto[A], Hirohiko Imai[A], Kei Sano[A], Masayuki Ohzeki[B], Tetsuya Matsuda[A], and Toshiyuki Tanaka[A]

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In order to reduce the imaging time, we employ the compressed sensing, which can make the image of dynamics of the substances in vivo even from the under-sampling observation data of 2D 1H-13C heteronuclear multiple quantum coherence (HMQC) magnetic resonance spectroscopic imaging (MRSI).

For MR measurement, an animal 7T MR device (Bruker BioSpin) and a 1H-13C nuclear transmission / reception volume coil were used. Using a sequence incorporating 2D 1H-13C HMQC, signals were collected with a sampling pattern based on the Sobol sequence which is a set of quasi-random numbers. Metabolic processes of about 7 hours after 13C -labeled glucose was intraperitoneally administered to tumor-bearing mouse were measured. For reconstruction by compression sensing, alternating direction method of multipliers (ADMM) was used. Time series changes of the spatial distribution of each substance were reconstructed using the base spectrum of three substances (glucose, lactic acid, and fat).

Under the current imaging condition, in the case of the conventional full sampling, the imaging time is about 4.5 hours. On the other hand, our approach allowed us to reconstruct 2D spatial distribution of metabolites with a time resolution of 8.5 minutes from the data collected in about 7 hours.

10. Solid-state NMR signal assignment by covariance NMR combined with Monte Carlo integration

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Solid-state NMR can exhibit tremendous power for structural and dynamical analyses of large and/or insoluble proteins. However, the analyses are often prevented due to difficulty of peak picking in chemical shift assignment. Covariance NMR approach that can integrate several spectra into the high dimensional space using covariance calculation between spectra, can reduce the difficulty of peak picking because signals are dispersed in a high dimensional space. The most concerned problem was the covariance map calculation in a high dimensional space requires high computational cost. To tackle this problem, we applied Monte Carlo integration to obtaining the covariance map. The approach was verified using 3D-CANCO, NCACO and NCOCA solid-state NMR spectra of GB1 microcrystal. We could construct the 6D covariance map within a few minutes using a laptop computer. Thereby, we successfully assigned the backbone chemical shifts of GB1 derived from the approximated 6D covariance map without human intervention. Thus, our Monte Carlo integration based covariance NMR approach is helpful for backbone chemical shift assignments.

11. Statistical mechanical analysis of sparse linear regression as a variable selection problem

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The information theoretic performance of compressed sensing or related variable-selection problems is analytically evaluated when a design matrix is given by an overcomplete random matrix. The replica method is employed to derive the result. The analysis is conducted through evaluation of the entropy, an exponential rate of the number of combinations of variables giving a specific value of error to given data which is assumed to be generated from a linear process using the design matrix. This reveals the achievable limit of the fit error to the data when solving a representative L0 problem, as well as the presence of unfavorable phase transitions preventing local search algorithms from reaching the minimum-error configuration. The associated phase diagrams are shown. A noteworthy outcome of the phase diagrams is, however, that there exists a wide parameter region where any phase transition is absent from the high temperature to the lowest temperature at which the minimum-error configuration or the ground state is reached. This implies that certain local search algorithms possibly find the ground state with moderate computational costs in that region. A numerical simulation based on simulated annealing is conducted, which well supports this theoretical prediction.

12. Geodetic data inversion for spatial distribution of slow slip events using sparse modelling

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We estimated spatial distribution of the long-term slow slip events (L-SSEs) beneath the Bungo channel in southwest Japan. The total slip distributions of these L-SSEs estimated by geodetic data have been smoothed to some extent due to prior constraints on inversion analyses. In this study, by using fused regularization, a type of sparse modelling suitable for detecting discontinuous changes in the model parameters, we found that the largest slip abruptly becomes zero at the down-dip limit of the seismogenic zone, and is immediately reduced to half at the up-dip limit of the deep low-frequency tremors, and becomes zero near its down-dip limit. Such correspondences imply that some thresholds exist in the generation processes for both tremors and SSEs. It suggests that geodetic data inversion with sparse modelling can detect such abrupt changes in the slip distribution.

13. Simultaneous Screening for Positive-Unlabeled Sparse Support Vector Machines

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Sparse support vector machine (Sparse SVM) is a standard method for classification problem. However, when the number of samples and features are very large, it requires large computational cost. Therefore, finding efficient algorithms for sparse SVM is an important problem. In many real real-world applications, given data are not completely labeled. In particular, we often have a few positive labeled data and many unlabeled data. Learning from such dataset is referred to as positive-unlabeled learning (PU-learning). In this study, we propose an efficient algorithm for the PU-learning version sparse SVM problem (PU pparse SVM). We introduce a new convex loss function for PU sparse SVM problem. Then we adopt the simultaneous screening method for sparse SVM to our loss function. We evaluate the proposed method in real-world dataset.

14. Geochemical-petrological evolution under the paleo subduction zone identified by machine-learning techniques

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Geochemical-petrological evolutions of the subducting rocks are identified by means of multivariate statistical analyses applied for the metamorphic rocks formed under ca. 15-60 km of the paleo subduction zone. Chemical composition of metamorphic rocks is commonly represented by more than 10 components such as SiO2, TiO2, and others. To detect the characteristics of a series of rock compositions, this contribution performed k-means cluster analysis (KCA) combined with the whitening of the dataset (Iwamori et al., 2017) and non-negative matrix factorization (NMF) to the dataset of metapelites of the Sanbagawa metamorphic belt in central Shikoku, collected by Goto et al. (1996) and Kiminami & Ishihama (2003) which comprise 235 samples with 14 elements. Both multivariate analyses indicate an evolutional change of chemical composition during the progressive metamorphism. In the higher metamorphic grade part, a decrease in SiO2 and Na2O and compensating increase in other components are recognized. To be noted, the endmember decomposition using NMF revealed that the change of rock composition is approximated to a stoichiometric increase of garnet-like component. This metamorphic evolution can be best explained by the precipitation of garnet and leaching of other components during progressive dehydration.

15. Bayesian inference of an effective interaction between atomic defects on the surface of SrVO3

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We invented the new methodology to extract atomic positions from STM topography data [arXiv:1703.08643]. We thus applied our method to real experimental data of an oxide metal, SrVO_3. On the surface of the material, the oxygen atoms take a cubic lattice arrangement, and there are atomic defects that correspond to lower electron density spots in a topography image. According to our further analysis, it is found that these atomic defects are randomly distributed in space beyond four lattice constants, meanwhile it exhibits an exclusive distribution within the distance. In order to understand the spatial distribution, we infer an effective interaction between the atomic defects by using a lattice gas model through the Bayesian statistics. In our poster, we show our inference framework by using MCMC and our recent results.

16. Principal component analysis with electronic wavefunctions for exploration of organic polymer device materials

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Principal component analysis (PCA) was carried out so as to analyze large-scale electronic state calculation data for exploration of organic polymer device materials [1]. The method is given by the dimensional reduction of electronic wavefunctions, since the original data size is huge. The reduction is realized, when the participation ratio of wavefunctions, a measure of quantum localization, is chosen as the descriptor. The proposed method was used as an extension of our previous research in organic polymer devices materials [2]. The computation was carried out for electronic states for 40,000 samples of disordered organic polymers with 1,200 atoms by our large-scale electronic state calculation code ELSES on the K computer. As results, the polymer samples are classified into four groups correctly and the physical meaning of the principal components is clarified. The present method is general and forms a rigorous foundation of the data-driven material science. References: [1] H. Imachi et al., in ASIAN19, National Chiao Tung Univ., Taiwan, 31. Oct.- 2. Nov. (2016); H. Imachi, D. Thesis, Tottori U., Mar. 2017; Manuscript in preparation. [2] T. Hoshi, et al., Proc. ScalA16 in SC16, pp.33-40, (2016).

17. (Cancelled)

18. Many-variable variational Monte Carlo method with sparse modeling

Yuichi Motoyama, Takahiro Misawa, and Kazuyoshi Yoshimi
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The variational Monte Carlo (VMC) method is one of the most powerful solver for strongly correlated quantum system. In VMC, we search for the ground state of the Hamiltonian by minimizing the energy of a parametrized wave function. In order to obtain the real ground state, the Hilbert space spanned by the parametrized wave functions should include it. It is non-trivial unfortunately how we can construct a good parameter space. Many-variable VMC (mVMC) method overcomes this obstacle simply by increasing the number of variables. This causes another problem, that is, an increase of numerical cost, but this has been resolved by advance in hardware and optimization method referred as stochastic reconfiguration. Now mVMC can treat many of condensed matter physics problems, for example a spin liquid phases in quantum spin model. However, there remain some models that mVMC method has not yet been able to deal with because of a slow optimization. In this study, we combine the sparse modeling framework with the mVMC method to prepare a better initial parameter than random one and to speed up optimization steps.

19. Direct imaging of supermassive black hole by sparse modeling

Mahito Sasada[A], Fumie Tazaki[A], Kazuki Kuramochi[A,B], Kazuhiro Hada[A], Mareki Honma[A], Kazunori Akiyama[A,C], Shiro Ikeda[D], Mariko Kimura[E], Taichi Kato[E], Daisaku Nogami[E], Makoto Uemura[F], Taise Abe[F], and Yurika Yamada[F]

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Black hole is one of the most interesting topics in the universe. Direct imaging of the black hole is the primary purpose of the project of Event Horizon Telescope (EHT), which is an international collaboration on a very long baseline interferometer (VLBI) observation. A current specification of the EHT observation will achieve a spatial resolution of 25 microarcsec. The angular size of black hole is, however, considered from 35 to 50 microarcsec in the case of Sgr A*. We develop a new imaging tool to obtain a higher-resolution image of black hole with a sparse modeling (SpM) algorithm. An image with the SpM imaging technique has achieved over three times higher resolution than a conventional method of a VLBI analysis from the same data set. A polarimetric image is also generated with over three times higher resolution. We apply the SpM to not only the simulation but also an actual data. We try to apply the SpM to other astronomical topics. In this presentation, we will report results of application of SpM to the VLBI imaging and other astronomical studies.

20. Variational Bayes method for matrix factorization to two sparse factorized matrices

Tomoki Tamai and Koujin Takeda
Ibaraki University

Matrix factorization is the problem of finding two low-rank matrices from their product. This idea is used in many areas such as collaborative filtering, sentiment analysis and drug interaction analysis. For this problem we use variational Bayes method. In the past study of Bayesian analysis, multivariate Gaussian prior is used for both factorized matrices for convenience of analysis. In our study, we assume that the observed matrix is the product of two sparse matrices, and the prior of each matrix element is exponential distribution. This describes the case of nonnegative matrix factorization, which is significant in the application to many practical problems. Under these assumptions, we will report the result of our analysis and matrix factorization experiment.

21. Approximate analysis of matrix factorization/completion problem by variational Bayes method with sparse prior

Ryota Kawasumi and Koujin Takeda
Ibaraki University

We study matrix factorization, which is the problem of finding low-rank factorized matrices from their product. This can be applied to various problems like collaborative filtering, which is used for quick and precise analysis of customer preference. We also study matrix completion, where some elements in matrix product are unobserved and we need to fill such elements by the idea of matrix factorization. Here we mainly deal with the matrix factorization with noise, where the observed matrix is expressed by the product of dense and sparse matrices with additional noise. For the analysis we use variational Bayes method, where Gaussian prior for dense matrix and Laplace prior for sparse matrix are assumed. With this method and under several approximations, we obtain an analytical expression of matrix factorization solution for a given observed matrix. Using our analytical result, we conduct numerical experiment of matrix factorization for the product of dense and sparse matrices with additional noise, and compared the result with another analytical work, where Gaussian priors are assumed for both factorized matrices. We also report Bayesian formulation of matrix completion, and the result of numerical experiment.

22. Comparison between asteroids and meteorites through multivariate analysis of visible to near-infrared reflectance spectra

Peng K Hong, Takafumi Niihara, and Hideaki Miyamoto
The University of Tokyo

Asteroids and meteorites have been considered as remnants of the early evolution of the solar system. Although meteorites are considered to originate from asteroids, their spectral relationship, remains poorly constrained except for a few cases. The major obstacle to compare asteroids with meteorites is that the classification schemes for the two are fundamentally different, because the two databases have significantly different data coverage, precision and resolution. In order to connect asteroids with meteorites, we develop large databases for the application of multivariate analysis. Our reflectance spectra database ranges from 0.4 to 4 μm, including 3 μm region, where one can observe absorptions due to hydrated silicates. We performed principal component analyses and found that using spectra from 0.4 to 2.5 μm, accuracy of separation among ordinary chondrites, carbonaceous chondrites, HED meteorites is significantly improved compared with the case using spectra from 0.4 to 1.0 μm. We also found that the accuracy of separation is not significantly improved when using meteorite spectra from 0.4 to 4 μm. These results suggest that unlike previous expectation, 3 μm band may not be useful for classification of some meteorites, because 3 μm band is widely observed among chondrites and achondrites.

23. Low-rank matrix completion by simulated annealing

Joji Mikami, Yuya Seki, Masayuki Ohzeki, and Kazuyuki Tanaka
GSIS

The method to solve L0-norm sparse approximation by using simulated annealing has been proposed. We apply a similar method to find the low-rank matrix by selecting the relevant components. In our method, we randomly select a singular value and decide whether or not to delete it by using an energy function following the Monte-Carlo manner. This is a kind of the simulated annealing to find the optimal selection of the singular values. When the temperature is high, singular values are randomly deleted. As temperature decreases, it is often to decide to decrease the value of the energy function. When the temperature becomes near 0, the planted solution can be found. We investigated its performance in the noiseless and noisy cases by numerical experiments. Also, we compared its performance by using quantum annealing.

24. Analytical continuation of quantum Monte Carlo data using sparse modeling

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In quantum Monte Carlo simulation, dynamic physical quantities such as single particle and magnetic excitation spectrum can be obtained by analytical continuation of imaginary-time data. However, analytical continuation is the ill-conditioned inverse problem and thus sensitive to noise and statistical errors. To solve this problem, analysis using the maximum entropy method or statistical method, etc., has been proposed, but a definitive method has not yet been established. In this presentation, we propose a method of analytical continuation using sparse modeling [1]. In this method, analytical continuation becomes robust against noise since relevant basis unaffected by the noise is automatically selected. We also show that these compression basis gives the model-independent compact representation of imaginary-time data [2]. In addition, we will introduce the open source software "SpM" implementing the new method of analytical continuation [3]. [1] J. Otsuki, M. Ohzeki, H. Shinaoka, and K. Yoshimi, Phys. Rev. E 95 (2017), 061302(R). [2] H. Shinaoka, J. Otsuki, M. Ohzeki, and K. Yoshimi, Phys. Rev. B 96 (2017), 035147. [3] https://github.com/j-otsuki/SpM"

25. Regression model for stabilization energy of various anion ordering in perovskite oxynitrides

Masanori Kaneko[A,B], Mikiya Fujii[A,B], and Koichi Yamashita[A,B]

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Recently, Perovskite ABX3 has been studied for various applications due to its various interesting properties, e.g., as a water splitting photocatalyst and solar cell. ABO3-xNx (0<x<1) has better activity than ABO3 and ABO2N in some cases. When first-principles calculations are performed to study ABO3-xNx (0<x<1), it is necessary to consider anion-ordering and tilting. There are a huge number of combinations of the structure configuration. Thus, performing a quantum chemical calculation for each combination. However, we cannot calculate all-structures because of the high computational cost of quantum chemical calculations. The most expensive calculation in the quantum chemical calculation is structure optimization. Therefore, we have developed a model that can predict a stabilization energy by structure optimization from the unoptimized structure with good accuracy using ridge regression. Using this model, we can omit the structure optimization and predict the stabilization energy by the structure optimization from only the unoptimized structure. Finally, using this method, it is possible to predict the most stable anion-ordering without optimizing the structure.

26. TimeTubes: Visual Fusion for Detailed and Precise Analysis of Time-Varying Multi-Dimensional Datasets

Naoko Sawada[A], Masanori Nakayama[A], Hsiang-Yun Wu[A,B], Makoto Uemura[C], and Issei Fujishiro[A]

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TimeTubes is a visualization tool for observed datasets of blazars. It allows astronomers to geometrically analyze the dynamic behavior of and relationship among multiple time-varying variables in the datasets. This poster mainly focuses on a novel functionality of TimeTubes—visual data fusion, which is intended to visually fuse multiple datasets from different observatories for the same blazar. To analyze the behavior of blazars, temporally denser observation is required, because blazars fluctuate drastically in a wide time range, which can be from a few minutes to several years. However, there are many intrinsically unobservable periods in a dataset, due to daylight, bad weather, and so on, which may cause astronomers to miss important events of the blazar. Thus, by increasing the amount of observed data to visualize, visual data fusion can meet astronomers' need of a more detailed and precise analysis. Additionally, comparison of multiple datasets for the same blazar, taking into account observation conditions and precision, can contribute to the reduction of unreliability caused by errors in datasets. Our interface effectively supports a more precise analysis, which can be achieved by visually fusing multiple datasets by allowing for their global gaps.

27. Model selection on chemical kinetics in water-rock interaction using exchange Monte Carlo method

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Earth is a water planet, and water-rock interaction plays essential roles on various geological phenomena in surface and crustal environments. Chemical reactions among rock and water are essentially complex heterogeneous reactions, where reactive surface of mineral is important, and often are associated with mass transport, and the observable data (i.e. solution chemistries and dissolved or precipitated minerals) are noisy and sparse. Accordingly, estimates of kinetic parameters for the water-rock interaction is quite difficult inversion problem. In this study, we conducted a long-term (over 6 months) experiments under hydrothermal conditions for development of reaction zones at the boundaries between mantle (olivine, Mg_2SiO_4) and crustal rocks (quartz, SiO_2). This reaction system produces talc ($Mg_3Si_4O_{10}(OH)_2$), serpentine ($Mg_3Si_2O_5(OH)_4$), and brucite ($Mg(OH)_2$) with increasing the distance from the olivine-quartz boundary, which spatial variations in the abundance of product and reactant minerals and pores can be modeled by one-dimensional equation of coupled seven reactions and diffusion processes. We estimated eight kinetic parameters (the reaction rate constant and diffusion coefficient) by using the exchange Monte Carlo method (Hukushima and Nemoto, 1996). We also carried out the cross validation for selecting the most appreciate models of reactive surface areas of minerals.

28. Bayesian spectroscopy of x-ray photoelectron spectra in graphenes having atomic thicknesses on SiC substrates

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We have analyzed x-ray photoelectron spectra(XPS) in graphenes having atomic thicknesses on a SiC substrate by Bayesian spectroscopy. To elucidate binding energies and their chemical shifts of bonding states in materials, we have to decompose the XPS to spectral components for the respective species in such materials. In graphene samples formed on SiC substrates, it is considered that two kinds of buffer layers exist between graphenes and the SiC substrate. In this report, we performed the Bayesian spectroscopy to decompose a C-1s XPS to spectral components in such layers. We employed four kinds of symmetric Doniach-Ŝunjić spectral functions for peak structures of graphenes, two buffer layers and the SiC, where we assume that each spectral function has spectral widths of a common homogeneous broadening and a common inhomogeneous broadening. In addition, a Shirley spectral function was also considered to reproduce the background component in the XPS. Through sufficient samplings by a replica exchange Monte Carlo method, we succeeded for getting posterior probability distributions of all spectral parameters for the graphene monolayer, two kinds of buffer layers and the substrate. In addition, we can reproduce a measured XPS by using the mean values of their distributions.

29. Bayesian spectroscopy for spectral and normal mode analyses in solid-state materials

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We analyze excitonic absorption spectra and coherent phonon (CP) signals in solid-state materials by the Bayesian spectroscopy. In absorption spectra due to electronic elementary excitations, since multiple excitonic absorption peaks appear being overlapped with other background optical transitions, their spectral decomposition is difficult. However, with the Bayesian spectroscopy, the band gap and the excitonic binding energies can be estimated accurately by introducing physical laws concerning to the excitonic transitions. On the other hand, the Bayesian spectroscopy for the CP signals can also estimate the frequency and vibrating initial phase of the normal mode with high accuracies. Although the conventional Fourier transform spectrum has a broad spectral width on accounting of damping behaviors of the CP signals, the Bayesian spectroscopy with a physical model of a damped oscillation improves the estimation accuracy of the normal mode frequency in two orders of magnitude compared to the Fourier transform method. We also present the results of virtual measurement analyses to discuss the abilities of the Bayesian spectroscopy in the both cases of the absorption spectra and the CP signals.

30. Seismic wavefield imaging of long-period ground motion in the Tokyo metropolitan area, Japan

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Long-period ground motions due to large earthquakes can cause devastating disasters, especially in urbanized areas located on sedimentary basins. To assess and mitigate such damage, it is essential to rapidly evaluate seismic hazards for infrastructures, which can be simulated by seismic response analyses that use waveforms at the base of each infrastructure as an input ground motion. The present study reconstructs the seismic wavefield in the Tokyo metropolitan area located on the Kanto sedimentary basin, Japan, from seismograms of the Metropolitan Seismic Observation network. The obtained wavefield fully explains the observed waveforms in the frequency band of 0.10–0.20 Hz. This is attributed to the seismic wavefield imaging technique, which implements the replica exchange Monte Carlo method to simultaneously estimate model parameters related to the subsurface structure and source information. Further investigation shows that the reconstructed seismic wavefield lower than 0.30 Hz is of high quality in terms of variance reduction, and that the velocity response spectra show good agreement with observations up to 0.90 Hz in terms of the combined goodness of fit. Inputting the reconstructed wavefield into seismic response analyses, we can rapidly assess the overall damage to infrastructures immediately after a large earthquake.

31. Bayesian common parameter model in systems biology

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Kyushu University

In systems biology, ordinary differential equation (ODE) models are conventionally employed to describe biological or life phenomena in the level of molecular biology. Although the parameters of ODE models are estimated from experimental data sets, generally, the parameter estimation is not easy because the parameter estimation problem is equivalent to nonlinear regression and the sample size of data set is not enough large. To elucidate the mechanism of disease, the comparison between healthy and disease subject of ODE model is demanded. Given that, the mechanism of disease is described by the different values of parameters of between disease and healthy ODE model rather than the model structure, we can consider that the disease ODE model has common parameters with the healthy ODE model, because the biochemical pathways necessary for survival need to be kept normal. We developed the parameter estimation method from Bayesian approach to detect the different values of parameters between two models, which have same model structure. The developed methods is based on hierarchical Bayes model and the posterior probability distribution is computed by replica exchange Monte Carlo method.

32. Bayesian inference for chemical kinetics of catalytic reaction using temporal analysis of products

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We develop a Bayesian inference framework to estimate chemical kinetics of catalytic reactions from temporal analysis of products (TAP) data. In TAP experiments, reactant gas is injected from a pulse valve into a reactor with catalyst sample and exit gas flow is measured with sub millisecond time resolution. By analyzing TAP data, we study chemical kinetics of the reaction between the catalytic surface and reactant gas. It is important to estimate effective diffusivity and reaction rate constant of a reaction-diffusion equation system which models the behavior of reactant gas. The purpose of this study is to solve these problems by approximate Bayesian computation which is a combination between Bayesian inference and numerical simulations. This time, we took account of the property of experimental apparatus in a reaction-diffusion equation model and examined the validity of the model by applying it to argon data. In this presentation, we report the results of estimating parameters such as effective diffusivity with the method of least squares.

33. Bayesian spectroscopy of excitonic photoluminescence spectra in Cu_2O thin crystals

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We analyze polarization dependences of photoluminescence (PL) spectra in Cu_2O thin crystals sandwiched by paired MgO plates with Bayesian inference. In such thin crystals, the degeneracy of the yellow exciton states in Cu_2O will be lifted by stress effects induced by a small lattice mismatch between the Cu_2O and MgO. Consequently, the PL spectra exhibit obvious/remarkable As the result, the thin crystal provides complicated PL spectra, which include multiple resonance PL peaks of the split exciton states, their phonon side-band PL and another PL band. To study the stress effects and energy structure of the split exciton states, we have to decompose such complicated PL spectra into the respective spectral components and we introduced a physical model with Gaussian and Maxwell-Boltzmann spectral functions, which explain the PL profiles of the resonance PL and the phonon side-band PL, respectively. In synthesized spectra composed by these spectral components, we can completely reproduce the complicated spectra and can satisfactory get the probability distributions of spectral parameters in such functions. In addition, a measured PL spectrum was also successfully decomposed to the resonance PL peaks and other spectral components.

34. Break the Limit of Live Imaging Technology using sparse modeling.

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Live imaging is a novel method which is received the most attention in the field of life science and medicine. However, detailed observation of biological events in the live imaging for a long time often suffers from the fluorescence diminishment. Also as the imaging duration increases, the imaging area decreases. And so the information that can be obtained per unit time is reduced. What is needed for live imaging in the future is how to use photon budget on optimal conditions and increase the information obtained per unit time. But these problems are currently hampered by the performance limit of the microscope. To solve the crucial problem in the live imaging, we developed a new technique for obtaining the detailed cell morphological data, by using the compressed sensing, which can elucidate the most relevant part from a small amount of data, and by the reduction of the laser irradiation mass for decrease in the damage to fluorescence protein. By using this technology, we succeeded in reducing imaging duration by half, and reduced fluorescent damage becomes possible in live imaging.

35. Deta-driven analysis of first-principles simulation of chemical reaction

Yasunobu Ando

CD-FMat, AIST

In this poster, we present the data-driven analysis of first-principles simulation for chemical reactions. First principles simulation based on the density functional theory is common tool for the research on the chemical reactions. By using it, we can calculate the activation energy of reactions and identify the transition states on reaction coordinates. Once we simulate them, we obtain several data sets corresponding to the reactions. For example, reaction pathway, electronic structure along reaction pathway, and activation barriers. It is truly difficult to analyze these whole data sets because these are high dimensional. To achieve deep understanding of the chemical reactions from the simulation data sets, data-driven analytical procedure based on machine learning is indispensable. From this perspective, we attempt to develop new method to create low-dimensional reaction coordinate form high dimensional ones, and to catch up the differences of density of states along reaction coordinates to find important energy range of electrons and atoms in the system. These method is based on the simple machine learning way; principle component analysis, and k-means clustering. We would like to present that such simple methods give us simple viewpoints to understand what is happening in the chemical reactions in the simulation.

36. Extracting Neuronal Nonlinear Dynamics Based on Sparse Modeling

Shinya Otsuka and Toshiaki Omori
Kobe University

We propose a sparse modeling approach for extracting nonlinear dynamics in single neurons from observable data. Using our proposed sparse modeling approach, we show that latent neuronal dynamics can be extracted from a number of candidate nonlinear dynamics.

37. Bayesian inversion analysis of nonlinear spatiotemporal dynamics of heterogeneous reactions in rock-water interactions

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We propose a Bayesian statistical framework for extracting nonlinear spatiotemporal dynamics of surface heterogeneous reactions from sparse and noisy observable data. Surface heterogeneous reactions are chemical reactions with conjugation of multiple phases, and they have the intrinsic nonlinearity of their dynamics caused by the effect of surface-area between different phases. Using our proposed method, we show that the rate constants of dissolution and precipitation reactions, which are typical examples of surface heterogeneous reactions, and the diffusion constants, as well as the spatiotemporal changes of solid reactants and products, were successfully estimated only from the observable temporal changes in the concentration of the dissolved intermediate product.

38. Application of compressed sensing for efficient measurement of scanning tunneling microscopy and spectroscopy

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The interference of electrons is one of the manifestations of their particle-wave duality in quantum mechanics. When electrons are scattered by local disordered structures, the reflected electronic wave interferes with the injected one to form a spatial modulation of surface charge density, called a quasi-particle interference (QPI) pattern. QPI patterns is observable with scanning tunneling microscope (STM), and the Fourier transform of the patterns taken at various energies enables us to obtain the energy dispersion of the quasiparticles closely related to the band structure of the system. But on the other hand, this experiment requires quite a long measurement time, which sometimes even becomes a week, making it difficult to work on. Here, we apply data analysis methods based on statistical theory, called compressed sensing (CS), to the QPI measurements. These techniques allow efficient detection of an original signal that is mostly composed of zero-value data points. We have numerically examined the effectiveness of random down sampling and the performance of a sparsity-inducing algorithm based on QPI data taken on a noble metal surface, demonstrating the possible significant reduction of the measurement time.

39. Bandit Algorithms for Fast Diagnosis by Interactive Measurement

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Hokkaido University

For some disease diagnosis, existence of bad cells can be effectively checked by some measurement like Raman-spectra measurement. In such measurement, interactive measurement that minimizes the number of points to measure seems important technology to achieve fast diagnosis. We regard this problem as a kind of multi-armed bandit problem, in which the player judges the existence of an arm whose expected reward is more than a given threshold by drawing as small number of arms as possible. We first consider a simpler problem called an arm discrimination problem whose solver algorithm must discriminate whether a given slot machine has an expected reward at least a given threshold or not by drawing as small number of arms as possible. We give an algorithm for this problem and show an upper bound of the sample complexity (the number of arm draws). We construct a successive elimination algorithm and a successive checking algorithm that make use of the algorithm for the arm discrimination problem as a subroutine, and also show the sample complexity upper bounds of those algorithms.