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Bayesian Hierarchical Analysis for Multi-dimensional Spectra

Yuichi Yokoyama

Japan Synchrotron Radiation Research Institute (JASRI),
1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5198, Japan

In recent years, data-driven science has been attracting remarkable attention. The data-driven techniques such as Bayesian inference enable us to advance the synchrotron radiation X-ray data analysis. To develop innovative analysis methods and incorporate them into beamlines at SPring-8, Synchrotron Radiation Data-driven-science Group was established in January 2023. Our mission is to assist SPring-8 users in maximizing their experimental outcomes. Then, we developed Bayesian analysis methods for synchrotron radiation X-ray measurements, e.g., X-ray photoemission spectroscopy, X-ray absorption spectroscopy, X-ray diffraction, Compton scattering, Mössbauer spectroscopy, small-angle scattering, and so on. Currently, the developments have been completed for 14 beamlines, the majority of the 26 public beamlines at SPring-8.

In this talk, we introduce Bayesian hierarchical analysis for multi-dimensional spectra such as time-series and/or temperature-series spectra. Conventional least-squares fitting has to be the step-by-step analysis as shown in Fig.1. In this analysis, the information available at each step is very limited. The least-squares fitting has initial value dependence and the results are sometimes trapped by local minima. In addition, the least-squares fitting is a point estimation, which means that it is difficult to evaluate the estimation accuracy. Moreover, we have to determine the models such as fitting functions prior to the analysis by human judgement, leading to a human dependent analysis. However, Bayesian hierarchical analysis provides seamless analysis from multi-dimensional spectra as shown in Fig.2, enabling more precise estimation by using posterior probability distributions and quantitative model selection without human judgement. To discuss the effectiveness of Bayesian hierarchical analysis, we present two applications, e.g., the adsorption process of gas molecules on a metal-organic framework observed via time-resolved X-ray diffraction (shown in Fig.3) [1] and the reduction process of a catalyst for automobile exhaust gas observed via temperature-dependent hard X-ray photoemission spectroscopy [2].

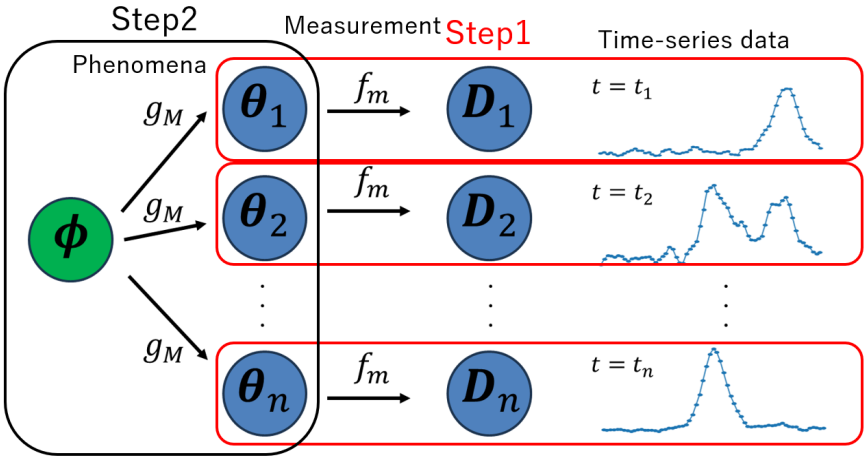

FIGURE 1. Conventional analysis framework for multi-dimensional spectra.

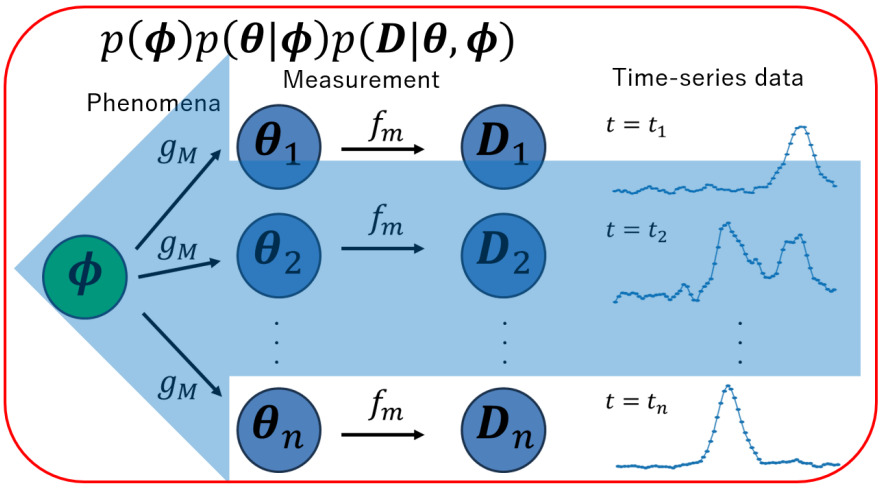

FIGURE 2. Bayesian hierarchical analysis framework for multi-dimensional spectra.

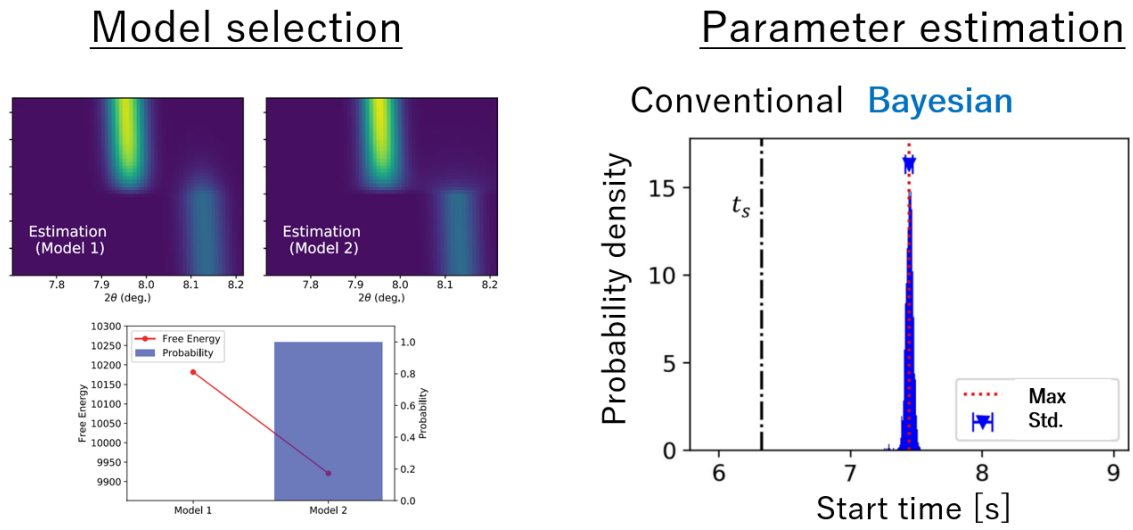

FIGURE 3. Bayesian model selection and parameter estimation based on posterior probability distribution.

REFERENCES

1. Y. Yokoyama et al., Sci. Rep. **13**, 14349 (2023).
2. Y. Yokoyama et al., in preparation.