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O-20

Bayesian Estimation for Spectral Deconvolution

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In this review, we introduce the framework of Bayesian estimation in spectral deconvolution. In Bayesian estimation, we can trace the causal relationships by Bayes' theorem to extract the underlying structure behind the spectral data. By applying Bayesian estimation to spectral deconvolution, we can estimate the number of peaks in the spectral data based on the framework of model selection. Furthermore, by using an algorithm called exchange Monte Carlo method, it is possible to solve the problem that is trapped in the local optimum solution.

Spectral deconvolution is the data analysis method for regressing the spectral data obtained by spectroscopy such as into the sum of basis function such as Gaussian function or Lorentzian function. The peak position obtained by spectral deconvolution depends on the composition and chemical state of the material, and the half width at half maximum depends on the lifetime of the electron.

One of the general approaches for spectral deconvolution is to search the model parameter set θ minimizes the mean squared error function $E(\theta)$ between the spectral data $D = \{x_i, y_i\}_{i=1}^{n}$ and model function $f(x, \theta)$ as follows;

$$E(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i;\theta))^2 , \qquad (1)$$

This method has two problems. One is the problem for trapping local minima. The other is to objectively choose the optimal number of peaks.

In this review, we introduce the Bayesian estimation for spectral deconvolution, which is proposed by Nagata et. al., to overcome these two problems[1,2]. Bayesian estimation enables us extract the latent structure behind the obtained data by tracing the causal relationships using Bayes' theorem. Figure 1 shows the schematic figure of Bayesian estimation for spectral deconvolution. In this case, the number K of peaks is probabilistically obtained by the probability $p(K)$ firstly. Then, the peak parameter set θ is given by the conditional probability distribution $p(\theta|K)$. After given

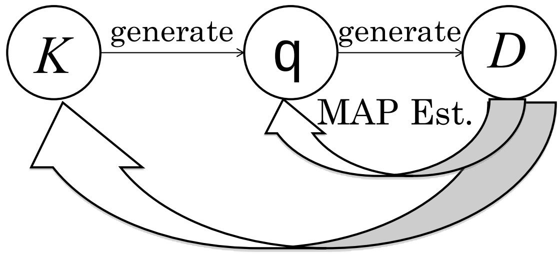

Fig. 1 Schematic figure of Bayesian estimation for spectral deconvolution.

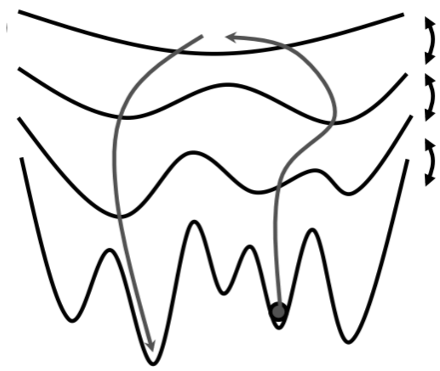

Fig. 2 Exchange Monte Carlo method.

the number K of peaks and the parameter set θ, the spectral data D is given by the conditional probability distribution $p(D|\theta,K)$. This is an example of causal relationship for spectral deconvolution. Bayesian estimation is the probabilistic inference based of Bayes' theorem. By using Bayesian estimation, we can obtain not only the statistically optimized peak parameter but also the number K of peaks by the Bayesian model

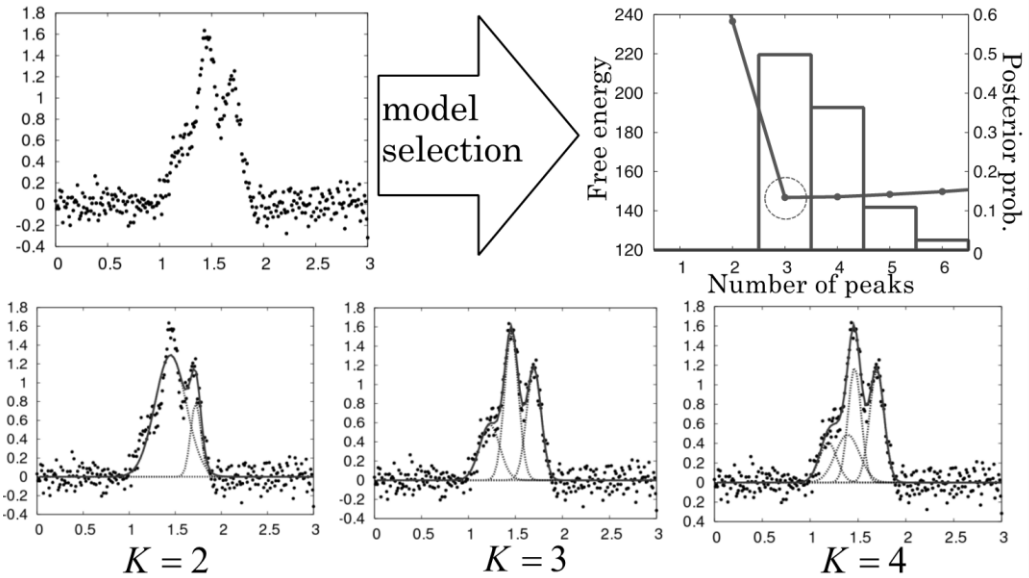

Fig. 3 Result of Bayesian estimation for spectral deconvolution. Upper left figure shows synthetic spectral data generated by computer simulation. Upper right figure shows the result of model selection. Lower figures show the fitting result for K=2, K=3 and K=4.

selection. Specifically, we can obtain the statistically optimal number K of peaks by minimizing the following function called Bayesian free energy;

$$F(K) = -\log \int \exp(-nE(\theta))\, p(\theta|K) d\theta \quad (2)$$

In order to calculate the Bayesian free energy, it requires the multiple integral for the model parameter set θ, which is difficult for analytical calculation. Then, we use replica exchange Monte Carlo (REMC) method[3] to tackle this problem. The REMC method is an algorithm of Markov chain Monte Carlo (MCMC) method, and prepare for the replica system for the optimization problem formed by the Bayesian estimation. The procedure of REMC method is constructed by two processes. One is the fundamental update such as Metropolis algorithm. The other is the exchange process between the neighboring replicas, which has the effect for annealing process. By the exchange process, we can escape the local minima trap, which is shown in Fig.2. Moreover, we can efficiently simulates the numerical calculation for multiple integral for the Bayesian free energy.

Figure 3 shows the example of applying the Bayesian estimation for spectral deconvolution. The upper left figure in Fig.3 shows the obtained synthetic spectral data, which is computationally generated from three Gaussian functions added with Gaussian noise. More specifically, we first set the three Gaussian functions and make the composite function by the sum of these functions. After that, we added this composite function with Gaussian noise with mean 0 and standard deviation 0.1. For this synthetic data, the result of Bayesian model selection is shown in upper right figure in Fig.3. In this figure, the bar indicates the probability distribution of the number K of peaks given by the spectral data. From this result, we can see that the optimal number K of peaks is K=3, which maximize the probability $p(K|Y)$ of K given the data set Y. In this way, we can estimate not only model parameter set θ but also the number K of peaks by using Bayesian estimation.

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