Composite Spectral Energy Distribution and Bayesian Machine Learning for Spectral Data

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Keywords

galaxies: evolution, methods: data analysis, methods: Bayesian non-parametric

Abstract

Composite SEDs and Bayesian non-parametric clustering. Photometry and medium bands: surveys Spectral Energy Distributions: fitting template, FAST, EAZY Composite SEDs: evolution from grouping methods Bayesian non-parametric on functional data: 1. Dirichlet Processes for clustering 2. Gaussian Processes on Spectral data 3. Clustering on functional data

Contents

1. INTRODUCTION

improvement of Photometry data on redshift rage 3-4.

2. GALAXY EVOLUTION IN TERMS OF COMPOSITE SPECTRAL ENERGY DISTRIBUTIONS (SEDs)

2.1. Medium-Band Photometry

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2.2. Composite Spectral Energy Distributions (SEDs)

3. BAYESIAN MACHINE LEARNING FOR CLUSTERING AND MODELING SPECTRAL DATA

Bayesian machine learning is a branch of machine learning which aims to solve machine learning problems in a Bayesian perspective. Instead of optimizing the parameters of interest from data using an empirical loss function (e.g., a least-squared function), Bayesian methods build generative models to randomly sample data from parameters and try to maximize the likelihood between observed data and hidden parameters (Barber 2012).

The difference between Bayesian statistics and Bayesian "machine learning" is that Bayesian "machine learning" is trying to approximate *non-linear* functions (Bishop & Tipping 2003). After the publish of Rasmussen & Williams (2005), learning unknown complicated functions from observed data using *Gaussian processes* (GP) became popular.

GP: :
Gaussian Processes

$\sim$ Normal: :
Sampling from a Gaussian (normal) distribution

Bayesian ML: :
Bayesian Machine Learning

K: :
Covariance function (matrix)

μ: :
Mean function

3.1. Modeling Spectral Data using Gaussian Processes (gp)

A *Gaussian process* is a bunch of random variables, and any finite subset of these random variables is a joint Gaussian distribution (Rasmussen & Williams 2005). GP could be a powerful tool to model any kind of functional data (continuous data) in a non-parametric way. By non-parametric, it actually means we use infinite many parameters to describe our function (Gelman et al. 2014). GP could be treated as a random function (or a stochastic process) which draws samples from the n-dimensional distribution,

$$\mu(x_1), ..., \mu(x_n) \sim Normal((m(x_1), ..., m(x_n)), K(x_1, ..., x_n)). \quad (1.)$$

The construction of a GP could be considered as finding the mean function ($m(\vec{x})$) and a suitable covariance function ($K(\vec{x}, \vec{x}')$). In normal cases, a zero mean is usually used as a prior for GP regressions. For $K(\vec{x}, \vec{x}')$, pre-defined covariance functions (e.g., squared potential function $\exp(\frac{-r^2}{2\ell^2})$) are often been implemented. However, the usage of GP in modeling functional data will also be restricted by the intrinsic properties of the covariance functions. Learning a suitable covariance function is the most crucial part of machine learning in GP.

Finding a suitable choice of covariance often reflects our interpretations of the characteristics of our data (Rasmussen & Williams 2005). For example, the usage of the squared potential function $\exp(\frac{-r^2}{2\ell^2})$ implies the assumption that we believe each point on the function would have less impact to each other if they are far away on the functional space. Therefore, we need a special kind of covariance function to suit our purpose of modeling spctral data.

Garnett et al. (2017) took a machine learning approach to learn the covariance function, with a wavelength range from Ly_∞ to Lyα, from training data (quasar spectra). The optimization choice was to firstly decompose covariance matrix with (Garnett, Ho & Schneider 2015),

$$\mathbf{K} = \mathbf{M}\mathbf{M}^T, \tag{2.}$$

and then use the first 10 principle components of the flux of quasar spectra, $\mathbf{Y}$, to constitute the matrix $\mathbf{M}$. The optimization was done by maximizing the log likelihood, $\mathcal{L}$, of the data by given $\mathbf{M}$ and absorption noise ω,

$$\mathcal{L}(\mathbf{M}, \omega) = \log p(\mathbf{Y} \mid \lambda, \mu, \mathbf{M}, \mathbf{N}, \omega, z_{\mathrm{qso}}, Model). \tag{3.}$$

The goal of optimizing above function is to find optimal covariance matrix, $\mathbf{M}$, and absorption parameter, ω, with some given conditions. Those conditions are: a given mean vector μ, the noise on the spectra $\mathbf{N}$, the redshift of the QSO, and with a given model. In a perspective of generative modeling, optimizing the data likelihood implies we are trying to find a covariance matrix to better generate our spectral data.

The covariance matrix built in Garnett et al. (2017) with a wavelength range from Ly_∞ to Lyα is in Fig 1. The scale in Fig1 represents the strength of correlations between pairs of rest-frame wavelengths on the QSO spectra. The features of Lyman series are distinct. The off-diagonal term demonstrates the correlations of pairs of corresponding emission lines.

The mean function of GP modeling in Garnett et al. (2017) can be simply obtained by stacking the training spectra,

$$\mu_j = \mathrm{median}(y_{ij}), \tag{4.}$$

where y_{ij} are the fluxes for spectrum. Fig 2 shows the mean function with a range from Ly_∞ to Lyα. The features emission line of Lyman series are also visible in the figure.

Generally, the GP model for spectral data could be described as

$$p(\mathbf{y} \mid \lambda, \mathbf{v}, \omega, z, Model) = Normal(\mathbf{y}; \mu, \mathbf{K} + \mathbf{\Omega} + \mathbf{V}), \tag{5.}$$

where $\mathbf{y}$ is the observed flux of the spectrum, λ is the spectroscopic grids we chose to bin the flux, $\mathbf{v}$ is the instrumental noise given by the observed data (it is SDSS QSO catalogue (Pâris, I. et al. 2012) in Garnett et al. (2017)), z is the redshift dependence of the GP model,

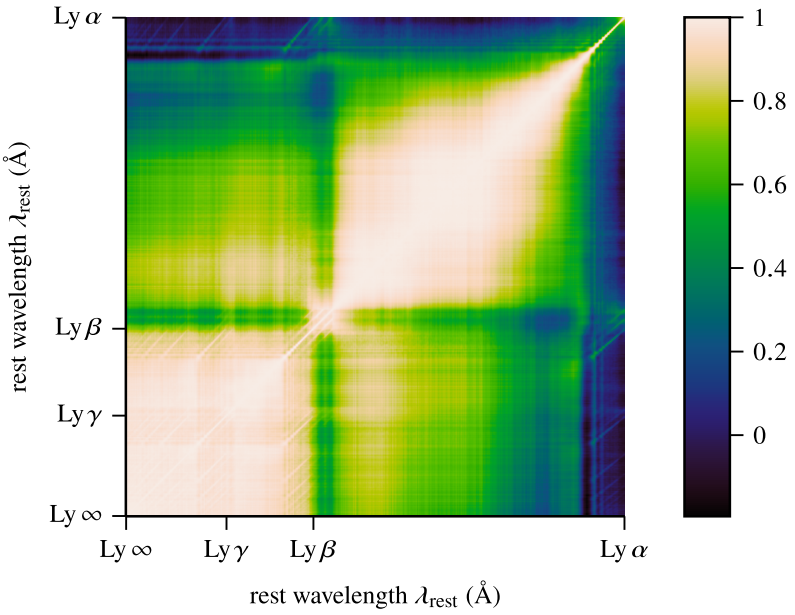

Figure 1

Covariance function for quasar spectra in Garnett et al. (2017)

and ω is the absorption redshift dependence (it was used to model Lyα forest in Garnett et al. (2017)).

The beauty of generative modeling the spectrum using GP framework is that we are able to fully control the modeling of instrumental noise and redshift dependence uncertainties. In addition, the whole framework is transparent and flexible, which implies it is interpretable and future improvements are achievable.

SUMMARY POINTS

1. *Gaussian Processes.* A flexible Bayesian non-parametric framework which allows us to model any kind of function.
2. Learned covariance matrix **K**. To model spectral data, we can optimize the covari-

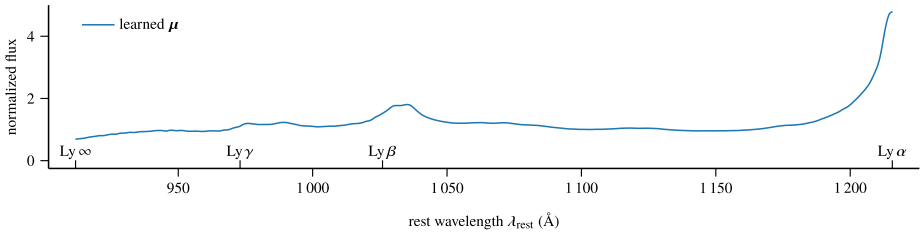

Figure 2

Mean function for quasar spectra in Garnett et al. (2017)

ance matrix using training data to acquire customized covariance function of any given range of wavelengths.

3.2. Dirichlet Processes

The *Dirichlet process* (Teh et al. 2006) is a Bayesian non-parametric method to model infinite mixture models and also could be used for clustering. We haven't seen any application of *Dirichlet processes* (DP) in spctral data clustering. A recent astronomical application of DP is building a mixture model for binary neutron stars in gravitational-wave data (Del Pozzo et al. 2018). Since we expect the application of DP in the clustering of spectral data is achievable in future, we decided to roughly review the basic concept of DP here.

The DP is a stochastic process which is often used to model mixture models. Each random sample in DP is itself a distribution, which means we can treat random samples of a DP as cluster centers of a mixture model. Similar to GP, a finite subset of a DP could be described by Dirichlet distributions.

To model the data v using the Dirichlet mixture model, the clustering memberships could be described by the following conditional probability (Barber 2012),

$$p(v^{1:N} \mid \theta) = \sum_{z^{1:N}} p(v^{1:N} \mid z^{1:N}, \theta) p(z^{1:N}), \tag{6.}$$

where $p(z^{1:N})$ gives the priors over each cluster and θ describe the parameters of the cluster model. The choice of priors over clusters ($p(z^{1:N})$) is crucial

3.2.1. Chinese Restaurant Process. The clustering property of DP is hard to understand simply via mathematical forms above. However, there's an intuitive metaphor described in Teh et al. (2006) to mimic the process of drawing samples from DP using a real-life example: *Chinese Restaurant process* (CRP).

The name of CRP was developed in 1980's. CRP is a process to describe the distribution over partitions.

Now, imagine this: there are infinite number of round tables in a Chinese restaurant, and there are also infinite number of seats in each round table. Each customer will come

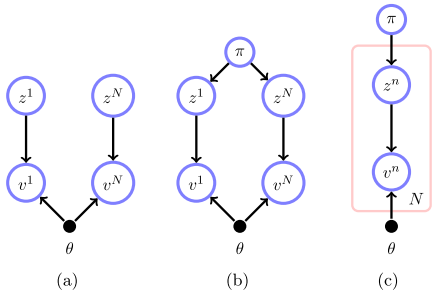

Figure 20.12: **(a)**: A generic mixture model for data $v^{1:N}$. Each z^n indicates the cluster of each datapoint. θ is a set of parameters and $z^n = k$ selects parameter θ^k for datapoint v^n. **(b)**: For a potentially large number of clusters one way to control complexity is to constrain the joint indicator distribution. **(c)**: Plate notation of (b).

Figure 3

The probabilistic graphical model of DP in plate notation in Barber (2012). The symbols here: z is the indicator and $p(z^n)$ implies the prior over n^{th} cluster; v is data; θ is used to describe the parameters on the cluster model (the shared model) while z could be treated as the hidden variable used to described component models (the individual models); π here is the parameter of a Dirichlet distribution, which is used to describe distributions.

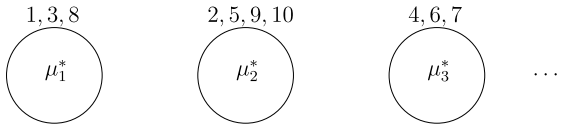

Figure 4

An illustration of CRP in Blei (2007).

to the restaurant one by one (just like sampling). Let's assume the first customer choose the first table. Which table would be next person choose?

SUMMARY POINTS

1. Summary point 1. These should be full sentences.

FUTURE ISSUES

1. Future issue 1. These should be full sentences.

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