BayesVP: a Bayesian Voigt profile fitting package

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ABSTRACT

We introduce a Bayesian approach for modeling Voigt profiles in absorption spectroscopy and its implementation in the python package, BayesVP, publicly available at https://github.com/cameronliang/BayesVP. The code fits the absorption line profiles within specified wavelength ranges and generates posterior distributions for the column density, Doppler parameter, and redshifts of the corresponding absorbers. The code uses publicly available efficient parallel sampling packages to sample posterior and thus can be run on parallel platforms. BayesVP supports simultaneous fitting for multiple absorption components in high-dimensional parameter space. We provide other useful utilities in the package, such as explicit specification of priors of model parameters, continuum model, Bayesian model comparison criteria, and posterior sampling convergence check.

Key words: methods:data analysis – quasars:absorption lines

1 INTRODUCTION

Absorption line spectroscopy is undoubtedly one of the most important tools for probing the physical properties of absorbing gas in a variety of astrophysical environments. Spectral analyses are ubiquitous in astrophysics and have a long and rich history in studies of stars, galaxies, gas, cosmology and more.

One of the basic tasks in such analyses is identification and characterization of spectral absorption lines. The most common way to do the latter is to fit the Voigt profile (VP) to the absorption profile and then use its parameters to extract basic properties of the absorbing gas, such as column density, Doppler parameter, and central velocity/redshift.

A number of codes for modeling absorption lines with the Voigt profile are available publicly. For example, VPFIT is a popular $\chi^2$-based code commonly used in the community over many years (Carswell et al. 1991). autoVP is another $\chi^2$ grid-search based code, an automated Voigt profile fitting procedure that chooses the number of absorption components, designed for Ly$\alpha$ forest statistics (Davé et al. 1997).

While these codes have provided immense values to the community, there are fundamental limitations in methods based on $\chi^2$ grid-search in the Voigt profile fitting. For example, such methods cannot constrain model parameters of non-detections in a statistically rigorous manner. The methods make very specific assumptions about the likelihood and the nature of the flux errors. In addition, it is challenging to capture the degeneracy between column density and Doppler parameter when absorption lines are saturated.

Therefore, uncertainties of the best-fit parameters can be under- or overestimate estimated in a coarse grid of the parameter space. Furthermore, the grid search becomes prohibitively computationally expensive or impossible when fitting multiple absorption components because the number of parameters and thus the number of dimensions of parameter space is large. Thus, one cannot reliably and rigorously find the best fit model for physical properties of the gas using the optimal number of absorption components. This can affect our physical interpretation of the kinematics of the gas (i.e., number of velocity components and the total dispersion) and the column density distribution function (for example, see Appendix in Gurvich et al. 2017).

Motivated by these problems, we developed a Bayesian approach to the Voigt profile fitting combined with efficient algorithms for sampling posterior distribution of parameter values. We introduce an implementation of such method in the python package BayesVP, which simultaneously addresses these issues and provides additional benefits. These include explicit control of the priors of parameters and providing constraints in a form of posterior distributions, which allows uniform treatment of detections and non-detections. Using efficient parallel sampling methods, BayesVP can fully explore high-dimensional parameter space efficiently, providing more accurate parameters uncertainties and their degeneracies. This allows us to reliably find the best number of absorption components and to include an additional continuum model. One can also explicitly compare models using Bayesian model comparison criteria. In section 2, we describe the Bayesian approach to absorption line fitting and our specific implementation of this approach in the BayesVP package. We include a short tutorial on the basic usage of the package in the Appendix.
2 THE PACKAGE: BAYESVP

2.1 Posterior Distribution and Sampling

In the Bayesian approach we constrain the posterior distribution, \( \pi(\vec{\theta}) \), of model parameters vector of column density, Doppler broadening factor, and redshift, \( \vec{\theta} = \{ N, b, z \} \), given the vector of spectral fluxes and their uncertainties, \( \vec{F} \). The joint posterior distribution is simply proportional to the product of likelihood \( \mathcal{L}(\vec{F}|\vec{\theta}) \) and the prior pdf of the parameters:

\[
p(\vec{\theta}\,|\,\vec{F}) \propto \mathcal{L}(\vec{\theta}\,|\,\vec{F})p(\vec{\theta}),
\]

where the total likelihood \( \mathcal{L} \) is the product of all likelihoods of the individual pixels within a spectral segment of interests:

\[
\mathcal{L}(\vec{\theta}\,|\,\vec{F}) = \prod_i \ell_i(\vec{\theta}\,|\,F_i).
\]

Using methods, such as Markov Chain Monte Carlo (MCMC), that allow sampling of unnormalized distributions, we can sample the unnormalized posterior:

\[
\pi(\vec{\theta}\,|\,\vec{F}) = \mathcal{L}(\vec{\theta}\,|\,\vec{F})p(\vec{\theta}),
\]

The individual likelihood \( \ell_i \) of a given pixel \( i \) at \( F_i \) depends on the noise model. The specific noise characteristic depends on properties of telescopes and their instruments. In the limit of a large number of photons, we usually assume that the properties of telescopes and their instruments. In the limit of a large number of photons, we usually assume that

\[
\ell_i(\vec{\theta}\,|\,F_i) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp \left[ -\frac{(F_i(\vec{\theta}) - F_i)^2}{2\sigma_i^2} \right]
\]

where \( \sigma_i \) is the uncertainty of the flux \( F_i \) at pixel \( i \). However, the noise model can be modified and a different likelihood can be used for low photon counts (e.g., Poisson distribution). Although currently BayesVP implements only Gaussian likelihood, this can be easily changed to a different likelihood by supplying a different input log-likelihood function to the posterior class in Likelihood.py. In BayesVP, we also provide an easy way to specify prior priors based on knowledge of the specific problem in mind.

We sample the posterior distribution defined by eq.\(^3\) using an efficient sampling method. This is particularly useful in the Voigt profile fitting because it is common to fit multiple absorption components simultaneously. The number of parameters can thus grow quickly, since each absorption component adds three parameters (e.g., \( N, b, z \)). In addition, many sampling methods can be easily parallelized, which allows efficient sampling of the high-dimensional parameter space. Due to blending between components and the relationship between Doppler parameters and column densities in the saturated regime, Voigt profile parameters can be highly correlated. The simplest Metropolis-Hasting MCMC algorithm that samples the parameter space with isotropic steps is thus not optimal. We thus use two MCMC sampling algorithms designed to efficiently sample narrow distributions of highly correlated parameters and in high dimensional spaces. In particular, BayesVP is set up to use the affine-invariant ensemble sampling algorithm of (Goodman & Weare 2010) implemented in the emcee python package (Foreman-Mackey et al. 2013)\(^4\) and an additional powerful kernel-density-estimate based MCMC sampler kombine\(^5\).

2.2 Voigt Profile Model

The Voigt profile is parameterized by the absorber column density \( N \), Doppler parameter \( b \), and redshift \( z \). The normalized flux at frequency \( \nu \) (or wavelength \( \lambda \)) is simply:

\[
F(\nu|N, b, z) = \exp[-\tau(\nu)]
\]

where the optical depth \( \tau \) at frequency \( \nu \) of a system with \( (N, b, z) \) is:

\[
\tau(\nu|N, b, z) = N\sigma_0 f_{\text{osc}} \Phi(\nu|b, z)
\]

and \( \Phi(\nu) \) is the convolution of a Gaussian profile (due to the Doppler broadening) and a Lorentzian profile (due to pressure broadening). For computation speed, we compute the Voigt profile function \( \Phi(\nu) \) via the real part of the Faddeeva function \( w(x+iy) \) routine in the SciPy package\(^7\):

\[
\Phi(\nu|b, z) = \Re\{w(x+iy)\}/\sqrt{\pi\nu D}
\]

where \( x = \Delta\nu/\Delta\nu_D \) and \( y = \Gamma/(4\pi\Delta\nu_D) \). Also, \( \Delta\nu = \nu - \nu_0(1+z)^{-1}, \Delta\nu_D = b\nu/c \). In addition, \( \sigma_0 = \sqrt{\frac{\pi e}{m_e c^2}} \) is the cross section.

Collectively, the set of atomic constants \( \{ e, m_e, f_{\text{osc}}, \nu_0, \Gamma \} \) are the charge and mass of the electron, oscillator strength, rest-frame frequency and damping coefficient of an atomic transition. We include atomic parameters from the UV to optical wavelength regimes compiled from Morton (2003). Any additional transitions can be easily added in the supplementary data file included in BayesVP.

2.3 Continuum model

We implement a polynomial continuum model in addition to the Voigt profile model fitting. The addition of the continuum model moves some of the error budget from systematic uncertainties to statistical uncertainties. The continuum is parametrized as a polynomial in BayesVP:

\[
C(\lambda|a_i) = \sum_i a_i (\lambda - \bar{\lambda})^i + \bar{F}
\]

\[
F_{\text{model}}(\lambda) = C(\lambda|a_i) \times F_{\text{Voigt}}(\lambda|N, b, z)
\]

where \( \{a_i\} \) are the continuum parameters. Although BayesVP can fit a high order polynomial, in our experience for typical wavelength ranges used in absorption line fits, linear or quadratic polynomial are sufficient to model continuum accurately. Thus, we recommend fitting up to a quadratic polynomial (i.e., three continuum parameters). In any case, the degree of the polynomial should be considerably smaller than the number of spectrum pixels dominated by continuum.

Note that we have pivoted the polynomial fit from the observed wavelength \( \lambda \) to \( (\lambda - \bar{\lambda}) \), where \( \bar{\lambda} \) and \( \bar{F} \) are the median wavelength and flux of the input data. In Figure\(^3\) we show a test that includes a continuum model in a synthetic absorption line, where BayesVP successfully captures the correct input parameters.

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1. https://github.com/dfm/emcee
2. https://github.com/bfarr/kombine
3. https://docs.scipy.org/doc/scipy/reference/generated/scipy.special.wofz.html
4. http://ab-initio.mit.edu/wiki/index.php/Faddeeva_Package
2.4 Convergence Criteria

When sampling a posterior, it is important to demonstrate the convergence of sample chains in order to trust the resulting posterior and statistics derived from it. BayesVP package provides functionality for convergence tests using the Gelman-Rubin indicator. The basic idea is that the chains should reach a state where the parameter distributions are stationary. To do so, the GR indicator compares the variances of parameters within and across independently sampled chains. We adopt the definition used in Gelman & Rubin (1992):

$$R = \frac{V}{W} = \frac{N_w + 1 \sigma_w^2}{N_w W} - \frac{N_s - 1}{N_w N_s}$$  \hspace{1cm} (10)

where $W$ and $V$ are the “within-chain” variance and “between-chain” variance. And $\sigma_w^2$ is the estimator for the true variance of a parameter. In addition, $N_w$ and $N_s$ are the number of independent chains (or “walkers”) and the number of steps (length of the individual chains), respectively. A perfect convergence would correspond to the “within-chain” and “between-chain” variances matching each other ($R = 1$). Figure 2 shows an example the GR indicator as a function of the steps for the parameters in the continuum model fit shown in Figure 1.

2.5 Model Comparison

Observed absorption lines are frequently blended. The best number of absorption components for the observed profiles is not always clear. The column densities and Doppler parameters are strongly affected by the number of components that we choose to fit the data. Our physical interpretation of the absorbers may also change depending on the number of velocity components. One of
the main advantages of a Bayesian approach is the ability to select the best fit model based on some objective criteria when it is not clear how many components one should choose. In BayesVP, we implement some measures for choosing the best fit models: the Bayesian information criterion ($BIC$) for a given model $M$ (Ivezić et al. 2014):

$$BIC = -2 \ln(L^0(M)) + 2k + k \ln N$$  \hspace{1cm} (11)

where, $L^0(M)$ denotes the maximum value of the likelihood of model $M$, and $k$ is the number of model parameters and $N$ is the number of points in the MCMC chains. The objective for the best-fit model is to minimize $BIC$.

In general, odds ratio is also useful for comparison of two models $M_1$ and $M_2$:

$$O_{21} = \frac{L(M_2)}{L(M_1)}$$  \hspace{1cm} (12)

For this measure, model 2 is preferred if $O_{21} \gg 1$. However, it is computationally expensive to compute $L(M)$ because it involves integrating the posterior distribution over all $k$ model parameters, $L(M) = \int \pi(\theta) d\theta$. Instead, we calculate $L(M)$ using the local density estimate of the points sampled by MCMC chains $\tilde{\rho}(\theta)$ and the posterior $\pi(\theta)$, i.e. $L(M) = N\tilde{\pi}(\tilde{\theta})/\tilde{\rho}(\tilde{\theta})$ (see section 5 in Ivezić et al. 2014 for more details.)

The basic idea for these criteria (e.g., $BIC$) is that the models with a larger number of parameters are penalized and have to compensate with the larger values of $L(M)$ or $L^0(M)$. As an example, in Figure 3 we show results of a two-component Voigt fit for a blended absorption profile (with two input absorption components) and the corresponding posterior distributions of the model parameters. Clearly, the two-component fit describes the observed flux quite well. The choice of a two-component fit is also supported by the comparison criteria shown in Figure 4.

2.6 Uniform treatment for upper limits, lower limits and detections

Absorption line fits for weak lines in noisy spectra often result in unconstrained parameters. In the $\chi^2$ based analyses, these are usually treated as upper or lower limits. For example, in observational analyses of the absorption profiles of the circumbinary medium, lines of sights of large impact parameters usually result only in upper limits (e.g., Liang & Chen 2014). The inclusion of such limits when fitting a model of the column density profile or comparing to simulation results (e.g., Liang et al. 2016) is challenging and requires strong assumptions about their posterior form.

Thus, there has been a substantial effort in trying to model the probability of the column density of upper-limit systems in order to maximize their utility, such as constraining the gas properties (e.g., density and metallicity; Crighton et al. 2015; Fumagalli et al. 2016; Stern et al. 2016). On the other hand, when the absorption lines are saturated, it is difficult to constrain the column density precisely due to its degeneracy with the Doppler parameter. In this case, lower limits are often quoted in the literature. An improvement over the lower limits is bracketed ranges using the absence of damping wings (e.g., Johnson et al. 2015). In both of these cases, when the original data is available, this probability distribution can be directly measured as a marginalized posterior. In this case, no assumptions about the shape of the probability distribution are needed. We refer readers to Figure 6 in our companion paper (Liang et al. 2017) to see the diversity of the posterior distributions for the cases that would usually be identified as upper or lower limits and compared to the posterior distributions of “detections.”

3 SUMMARY

We present a python package BayesVP, which implements a Bayesian approach for modeling absorption lines with the Voigt profile. The package can be used to simultaneously fit multiple absorption components to constrain column density, Doppler parameter, and redshifts of the absorbing gas. The parameter constraints are derived in the form of marginalized posterior distributions, which allows for uniform treatment of the non-detections (i.e., upper limits) and detections in subsequent analyses, model fits, and comparisons of observations with simulations. The BayesVP package is set up to use the affine-invariant MCMC method implemented in the MCMC emcee package and the kernel-density-estimate-based ensemble sampler KOMBINE to efficiently sample the posterior distributions of highly correlated parameters. It also provides other useful utilities, such as convolution with instrumental line spread function (LSF), explicit control of parameter priors, Bayesian model comparison criteria, and sampling convergence check. The BayesVP package is designed to have a simple user interface with a single configuration file that users can explicitly define the line spread function, the number of walkers, MCMC steps, and parallel threads. BayesVP is publicly available at https://github.com/cameronliang/BayesVP. In the Appendix below we present an example showing how to use the package to fit absorption lines.

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APPENDIX

We describe the basic usage of the package in this section. $BayesVP$ is meant to run with a configuration file in the background, as it can take a few minutes for MCMC sampling, depending on the chosen number of walkers, steps, and parallel processes. This section illustrates the basic interactive use of the code and setting up a configuration file.

For this example, we will explicitly change the path to the location of the package for importing $BayesVP$.

```python
In [1]:
import sys
sys.path.append('/Users/cameronliang/BayesVP')
```

We can now import $BayesVP$. Let us also import an object, $WriteConfig$, that interactively asks the user a few questions to create a config file.

```python
In [2]: import BayesVP, WriteConfig
```

Let us assume that the spectrum in question is located in the following directory:

```python
In [3]: spectrum_path = '/Users/cameronliang/BVP_tutorial/spectrum'
```

The file name of the example spectrum is OVI.spec, with three of columns of data: wave, flux, error. We can use the $WriteConfig$ routine to set up the config file like so:

```python
In [4]: config = WriteConfig.interactive_QnA()
```

Path to spectrum:
/Users/cameronliang/BVP_tutorial/spectrum/

Spectrum filename: OVI.spec
filename for output chain: o6
atom: O
state: VI
Maximum number of components to try: 1
Starting wavelength(Å): 1030
Ending wavelength(Å): 1033

Enter the priors:
logN [cm$^{-2}$] = [10.000, 18.000]
b: [min, max] = [0.000, 100.000]
redshift: [min, max] = [-0.00100, 0.00100]

Written config file: /Users/cameronliang/BVP_tutorial/spectrum/bvp_configs/config_OVI.dat

The config file is automatically written within a subdirectory where the spectrum is located. We can now run the MCMC fit shown below. Note that $BayesVP$ can be run by supplying the full path to the config file as a command line argument. $BayesVP$ will print to screen the relevant information from the config file. In this example, we are fitting an OVI transition with rest wavelength of 1031.926 Å.

```python
In [5]: config_fname = spectrum_path + '/bvp_configs/config_OVI.dat'
In [6]: BayesVP.bvp_mcmc(config_fname)
```

The data products will be written in a subdirectory

```
Written chain: /Users/cameronliang/BVP_tutorial/spectrum/bvp_chains_0.000000/o6.npy
```

We complete the fitting process after the step above since the output chain (a binary file ends with .npy) contains all the information that we need. We would like to plot the results and write the best fit spectrum into a file. There are tools in the package that can help us do so:

```python
In [7]: import PlotModel as pm
from Config import DefineParams
```

We first extract all of the relevant information using the $DefineParams$ function:

```python
In [8]: config_params = DefineParams(config_fname)
```

Config file: /Users/cameronliang/BVP_tutorial/spectrum/bvp_configs/config_OVI.dat

```python
In [9]: output = pm.ProcessModel(config_params)
In [10]: redshift = 0.0; dv = 300;
output.plot_model_comparison(redshift,dv)
output.write_model_summary()
output.write_model_spectrum()
output.plot_gr_indicator()
output.corner_plot()
```

The data products will be written in a subdirectory
processed_products_0.000000, where the redshift of the system is appended to the subdirectory name. The final posterior and the best fit data are shown in Figure 5 and Figure 6.

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