

ASTR 288C – Lecture 9

Tuesday, 2 November 2009

Data Analysis III: X-Ray Spectroscopy

XSPEC

XSPEC is a command-driven, interactive, X-ray spectral-fitting program, designed to be completely detector-independent so that it can be used for any spectrometer. XSPEC has been used to analyze data from most space-based X-ray observatories including, *Chandra*, *INTEGRAL*, *Swift*, and *Suzaku*. It is a generalized software package that can be used with any data that is in the correct format. It has become the de facto standard for analyzing X-ray spectra and is being actively supported and upgraded.

The software is fairly easy to use and can be learned in a short amount of time. However, it has the capability to do very sophisticated model fitting.

XSPEC is distributed as part of the HEASOFT software package. It's Web site is <http://swift.gsfc.nasa.gov/docs/xanadu/xspec/index.html>.

The Basics of Spectral Fitting

This section is adapted from the XSPEC Manual, which can be found at <http://swift.gsfc.nasa.gov/docs/xanadu/xspec/manual/manual.html>.

Spectrographs do not measure the true, or intrinsic, spectrum of a source, but instead measure the number of photons that are recorded in individual energy channels in the instrument. A photon entering the spectrograph with an input energy of E can be recorded as having a different energy E' , which can be different from the input energy. The probability of a photon of energy E being recorded as having an energy E' can be determined by calibrating the spectrograph using sources with known spectra. In addition to this shift in energy the efficiency of each channel is not 100%. For any given channel only $N\%$ of the incoming photons will be recorded. Again, this can be calibrated using sources with known spectra.

Therefore, the spectrum that we measure is actually the convolution of the intrinsic spectrum with the response function of the instrument. The response function characterizes how the instrument changes the intrinsic spectrum during the process of recording the spectrum. The recorded number of photons in channel I is $C(I)$. This is related to the intrinsic spectrum, $f(E)$, by:

$$C(I) = \int f(E)R(I, E)dE$$

where $R(I,E)$, is the response function of the instrument. Ideally this equation would be inverted to solve for $f(E)$. However, in practice the recorded spectrum contains noise, and the response function has uncertainties in it, so in general inverting this

equation is unstable and highly sensitive to the noise properties of the data. It is usually not possible to reliably solve this equation.

Instead of solving for the intrinsic spectrum XSPEC uses a technique called forward modeling to estimate the intrinsic spectrum. First a model spectrum is chosen that describes the intrinsic spectrum. For example, if the spectrum is from a thermal spectrum from a hot star then a blackbody model might be used. A blackbody has two free parameters: (1) the temperature of the source and (2) the intensity of the source, or normalization. XSPEC takes initial guesses at the model's parameters then convolves the model with the instrumental response function. Next the convolved model is compared to the data and the model's parameters are adjusted to improve the fit. Once the fit has converged in some statistical sense the parameters of the model are reported to the user. If this procedure works then the model is a good description of the intrinsic spectrum. If it does not work then the user needs to find another model that is a better match to the intrinsic spectrum.

The user needs to have some understanding of the underlying physics of the source that they are interested in in order to pick a reasonable model for their spectrum. Just because a fit converges and returns a reasonable reduced chi-squared value does not mean that the model is an accurate description of the data. For example, gamma-ray bursts do not produce thermal radiation, so fitting a blackbody model to a gamma-ray burst spectrum is not physically realistic, and can lead to nonsense results.

Using XSPEC

Start XSPEC

XSPEC is an interactive software package, so it needs to be run from a command line in a terminal window. To start XSPEC just type `xspec` at a unix prompt. You should end up with something that looks something like this.

```
shogun 19> xspec
```

```
XSPEC version: 12.5.1  
Build Date/Time: Fri Aug 28 16:22:02 2009
```

```
XSPEC12>
```

The `XSPEC12>` is the XSPEC command prompt. This is where you will type commands.

Set Up XSPEC

Once you are running XSPEC you need to tell XSPEC what graphics device you are using. To use the native XWindows graphics support type the command

```
XSPEC12> cpw /xw
```

This will start a PGPLOT server and open a graphics window. There are many set-up options in XSPEC including the ability to set the definition of error bars and choose different statistical techniques for fitting the model to the data. The defaults are usual good unless if you are doing exceptionally complex fitting, or are an expert user.

It is often very useful to plot *X*-ray spectra with energy on the *X* axis instead of wavelength or frequency. XSPEC can be told to do this with the `setplot` command.

```
XSPEC12> setplot energy
```

Read the Data

Once XSPEC is properly initialized for your data set the next step is to read the data. This is done using

```
XSPEC12> data spectrum.pi
```

The data is assumed to be in an OGIP standard format. In general most *X*-ray observatories provide data in a format that can be read by XSPEC. Tool exist to convert most data formats into files that can be used by XSPEC. When the data has been read in XSPEC will print some summary information to the screen.

```
XSPEC12> data PKS0745-19_PC.pi
```

```
***Warning: Detected response matrix energy bin value = 0 (or neg).
```

```
XSPEC will instead use small finite value (response file will not be altered).
```

```
1 spectrum in use
```

```
Spectral Data File: PKS0745-19_PC.pi Spectrum 1
```

```
Net count rate (cts/s) for Spectrum:1 1.343e+00 +/- 5.186e-03 (98.4 % total)
```

```
Assigned to Data Group 1 and Plot Group 1
```

```
Noticed Channels: 1-737
```

```
Telescope: SWIFT Instrument: XRT Channel Type: PI
```

```
Exposure Time: 5.241e+04 sec
```

```
Using Background File PKS0745-19_PCback.pi
```

```
Background Exposure Time: 5.241e+04 sec
```

```
Using Response (RMF) File swxpc0to12s0_20010101v011.rmf for Source 1
```

```
Using Auxiliary Response (ARF) File PKS0745-19_PC.arf
```

Notice that the names of various auxiliary and calibration data files are printed, as well as some information about the instrument that the data was collected with. This information is stored in the input spectral data file. If this information is missing XSPEC will prompt the user for the information that it requires.

Screening the Data

In a perfect world all data would be of the highest quality. In the real world instrumental effects and calibration issues can result in some data being of higher quality than others. Many X-ray data processing pipelines flag bad or uncertain data when the data is processed into files that a user can use. XSPEC recognizes data that is flagged as bad. This data can be ignored using the command

```
XSPEC12> ignore bad
```

```
ignore: 66 channels ignored from source number 1
```

In this case 66 of the 737 channels in the data file have been flagged as having bad data. They will be automatically ignored in the analysis.

Define the Model to be Fit

XSPEC has a large library of predefined models that can be fit to data. It also has the ability for a user to define custom model. In fact, many of the standard XSPEC models were originally written by users and submitted for inclusion in the standard library. An example of a model is a power-law spectrum

$$F(E) = k E^{-\Gamma}$$

where $F(E)$ is the flux in the spectrum at energy E , Γ is the power-law photon index of the spectrum, and k is a normalization constant. This simple model has two parameters, the power-law photon index and the normalization. To use this model in XSPEC use the model command and set the initial guesses at each parameter when prompted for them.

```
XSPEC12> model powerlaw
```

```
Input parameter value, delta, min, bot, top, and max values for ...
```

```
1 0.01 -3 -2 9 10
```

```
1:powerlaw:PhoIndex> 2
```

```
1 0.01 0 0 1e+24 1e+24
```

```
2:powerlaw:norm> 1
```

```
=====
Model powerlaw<1> Source No.: 1 Active/On
Model Model Component Parameter Unit Value
par comp
1 1 powerlaw PhoIndex 2.00000 +/- 0.0
2 1 powerlaw norm 1.00000 +/- 0.0
=====
```

Chi-Squared = 5.396967e+09 using 671 PHA bins.
Reduced chi-squared = 8.067215e+06 for 669 degrees of freedom
Null hypothesis probability = 0.000000e+00
Current data and model not fit yet.

In this case the user is prompted for initial guesses for (1) the photon index and (2) the normalization. The initial guesses should be reasonable and are usually based on pre-existing knowledge of the physics of the source that was observed. If the normalization is not known it can usually be set to one. There is a complete list of models and their parameters in the XSPEC manual.

Models can be combined to create complex multi-component models. For example, the intrinsic spectrum of an accretion disc may be a power law (or something close to a power law), but it could also contain a spectral line. This can be added to the model using an arithmetic syntax. To combine two components, in this case power-law spectrum and a spectral line due to ionized iron (we will assume that the spectral line has a Gaussian shape), just add the two models.

```
XSPEC12> model (powerlaw+gaussian)
```

*There must be **no** spaces in the definition of the model.*

The user is then prompted for the parameters of the two models as before. Additional models can be added. For example, the light from the accretion disc is going to be absorbed by neutral hydrogen in the Galaxy along the line of sight to the source. Since this affects all of the intrinsic spectrum from the source it is combined using multiplication. The model to fit neutral hydrogen absorption is phabs, which stands for photon absorption.

```
XSPEC12> model (powerlaw+gaussian)*phabs
```

Again, XSPEC will prompt the user for the various model parameters.

Input parameter value, delta, min, bot, top, and max values for ...

```
      1  0.01  -3  -2  9  10
1:powerlaw:PhoIndex> 2
      1  0.01  0  0  1e+24  1e+24
2:powerlaw:norm> 1
      6.5  0.05  0  0  1e+06  1e+06
3:gaussian:LineE> 6.7
      0.1  0.05  0  0  10  20
4:gaussian:Sigma> 0.1
      1  0.01  0  0  1e+24  1e+24
5:gaussian:norm> 1
      1  0.001  0  0  100000  1e+06
6:phabs:nH>0.251
```

Model (powerlaw<1> + gaussian<2>)phabs<3> Source No.: 1 Active/On

Model	Model	Component	Parameter	Unit	Value
par	comp				
1	1	powerlaw	PhoIndex		2.00000 +/- 0.0
2	1	powerlaw	norm		1.00000 +/- 0.0
3	2	gaussian	LineE	keV	6.70000 +/- 0.0
4	2	gaussian	Sigma	keV	0.100000 +/- 0.0
5	2	gaussian	norm		1.00000 +/- 0.0
6	3	phabs	nH	10 ²²	0.251000 +/- 0.0

Chi-Squared = 1.080325e+10 using 671 PHA bins.

Reduced chi-squared = 1.624549e+07 for 665 degrees of freedom

Null hypothesis probability = 0.000000e+00

Current data and model not fit yet.

Notice that the chi-squared value for this model is very large before any fitting is done.

The neutral hydrogen absorption along a given line of sight in the Galaxy is often known, so this parameter can be frozen at the known value. Also, the width of a spectral line is often narrower than the instrumental resolution, so the observed width is actually set by the instrument. Therefore, the width of a spectral line can often be fixed to a known value. To fit the width of the spectral line to 0.1 keV and the Galactic neutral hydrogen absorption to $0.251 \times 10^{22} \text{ cm}^{-2}$ use the freeze command.

```
XSPEC12> freeze 4
```

```
XSPEC12> freeze 6
```

Fit the Model

The first step in fitting a model to data is to renormalize the model so that the integrated area under the convolved model is approximately the same as the integrated area under the data. It is important to realize that the model is convolved with the response function of the instrument before any renormalization or fitting is done. To renormalize the model use

```
XSPEC12> renorm
```

Chi-Squared = 63579.69 using 671 PHA bins.

Reduced chi-squared = 95.32187 for 667 degrees of freedom

Null hypothesis probability = 0.000000e+00

Current data and model not fit yet.

Notice that renormalizing has reduced the chi-squared value by a factor of approximately 250.

We are now ready to fit our model. This is done by simply typing fit.

```
XSPEC12> fit
```

XSPEC will print a large amount of information, most of which can be safely ignored unless if you are interested in the statistical details of the fit, or are trying to debug an unsuccessful fit. At the end of the fitting process a table of the best-fit values for each parameter is printed along with a summary of the goodness of fit.

```
=====
Model (powerlaw<1> + gaussian<2>)phabs<3> Source No.: 1  Active/On
Model Model Component Parameter Unit  Value
par comp
 1 1 powerlaw PhoIndex      1.40956    +/- 5.84812E-03
 2 1 powerlaw norm          1.01546E-02 +/- 6.16225E-05
 3 2 gaussian LineE    keV    35.1129    +/- -1.00000
 4 2 gaussian Sigma    keV    0.100000    frozen
 5 2 gaussian norm          4.27217E-04 +/- -1.00000
 6 3 phabs    nH          10^22    0.251000    frozen
=====
```

```
Chi-Squared =      3892.92 using 671 PHA bins.
Reduced chi-squared =      5.83647 for 667 degrees of freedom
Null hypothesis probability = 0.000000e+00
```

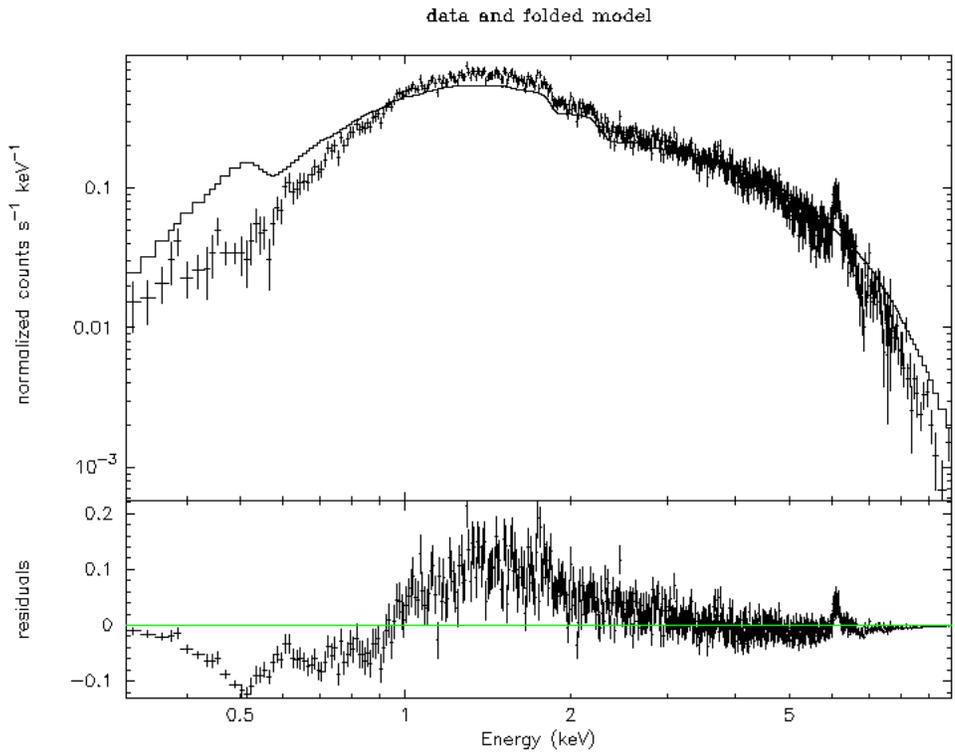
Notice that the parameter that we froze have not been changed. In this case the model that we used appears to be a poor fit. The reduced chi-squared for 667 degrees of freedom is 5.8, which is unacceptably large. This suggests that we either need to add components to the model (such as an additional spectral line) or we need to use a completely different model (such as thermal bremsstrahlung radiation instead of a power law).

Plotting the Results

XSPEC has an extensive plotting capability based on PGPLOT. For most purposes the predefined plotting commands are sufficient. To plot the data along with the convolved model use the plot data command. If you want the Y axis to be on a log scale use the plot ldata command. It is possible to produce multi-part plots. For example, to show the residuals to the fit along with the data and the best-fitting convolved model use

```
XSPEC12> plot ldata residuals
```

This produces a plot that looks something like this.

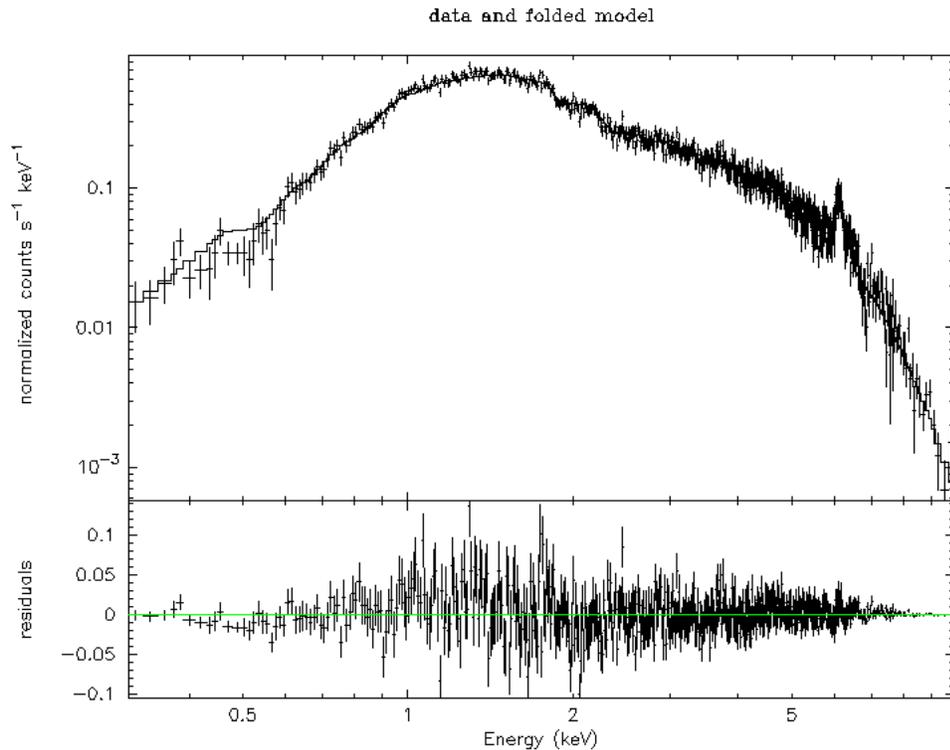


eholland 28-Oct-2008 10:23

This is clearly not a good fit. The model over-predicts the flux at low energies and high energies, and underpredicts the flux between 1 and 2 keV. Further, the spectral line at about 6 keV is not fit.

Refine the Models

By using our knowledge of astrophysics, and of what object we are looking at, we can choose a better model for this spectrum. By choosing the correct set of components we can get a much better fit.



eholland 28-Oct-2008 10:37

Here the convolved model fits the data, including the spectral line, very well. There is, however, a discrepancy at about 0.5 keV. This feature is due to the detector and is not part of the spectrum from the source. Therefore, it is not included in the model.

Finishing Up

To exit XSPEC use the `exit` command.

Getting Help

There is an extensive help facility built into XSPEC. Simply typing `help` at a command prompt will bring up the XSPEC manual. The details of how this is displayed will depend on how your installation of XSPEC is set up. One can also get help on a specific command by typing `help <command>` where `<command>` is the name of a command.

If you are stuck inside an command and can not get back to the command prompt type `/ *` (slash star, with no spaces) and you will be returned to a command prompt.

Lab Work

The purpose of this week's lab exercise is to gain some experience analyzing X-ray spectra. You will find a reasonable multi-component model to fit to an X-ray spectrum of the galaxy cluster PKS 0745–19. This is a large galaxy that has a thermal bremsstrahlung spectrum in X-rays and a heliocentric recession velocity of $30,819 \pm 150 \text{ km s}^{-1}$. *Swift* made extensive observations of this cluster in 2005. We will use an X-ray spectrum that was constructed by Kim Page at the University of Leicester.

To fit this data follow the general procedure that is described in the lecture notes. The fundamental steps, along with some hints, are given below.

Before running XSPEC download the data for this lab from http://lheawww.gsfc.nasa.gov/~sholland/astr288c/autumn_2009/lectures/lecture9/lecture9.tar.gz. Move this file to your working directory, then unzip it and untar it.

- `cd <wherever>`
- `gunzip -v lecture9.tar.gz`
- `tar xvf lecture9.tar`

You should have the following files

- `PKS0745-19_PC.arf`
- `PKS0745-19_PC.pi`
- `PKS0745-19_PCback.pi`
- `swxpc0to12s0_20010101v011.rmf`

You are now ready to run XSPEC and experience the joy of applying science to data.

1. Start XSPEC.
2. Set up XSPEC. You need to initialize the graphics device and set the X axis of your plots to show the energy scale.
3. Read the data. The data file is called “PKS0745-19_PC.pi”. This contains the *Swift*/XRT X-ray spectrum of PKS 0745–19. If you get any warnings about not being able to find files you need to be sure that all four files for this lab are in the same directory, and that you are running XSPEC from that directory.
4. Screen the data.
5. Define the model. PKS0745–19 has a thermal bremsstrahlung spectrum, so a good starting point is to use this as a model. The thermal bremsstrahlung model in XSPEC is called “bremss”. This model has two parameters: (1) the thermal plasma temperature, specified in keV, and (2) the normalization. A reasonable estimate of the plasma temperature in the hot gas in a galaxy cluster is 7 keV.

6. Fit the model.
7. Plot the results. Create a plot with two panels, one showing the data and best-fitting convolved model with a logarithmic Y axis, and the other showing the residuals of the fit. Your plot will look something like the example shown in the notes.

Q1: Is the “bremss” model alone a good fit to the data?

8. Refine the model. If you are not happy with the fit to a thermal bremsstrahlung model then try adding to the model. First, try adding the effects of absorption due to neutral hydrogen in the Galaxy. The Galactic value in the direction of PKS 0745–19 is $N_H = 2.51 \times 10^{21} \text{ cm}^{-2}$. Use the “phabs” model and enter the absorption in units of 10^{22} cm^{-2} . Since we know the value of the Galactic absorption there is no need to fit for this parameter, so freeze it at the input value.

Q2: Does adding Galactic absorption improve the fit? What is the reduced chi-squared value for the new fit?

9. The Galactic absorption does not include the absorption in the galaxy cluster. To fit for this include a third component to account for absorption at the redshift of the galaxy cluster. Use the model “zphabs”. This model is the same as “phabs” but it has redshift as a second parameter. Use NED to find the redshift of PKS 0745–19. When you apply this model remember that absorption due to neutral hydrogen in the cluster affects the model in the same way that absorption in the Galaxy does. Remember to freeze the redshift at its known value.

Q3: Does including the neutral hydrogen absorption in the cluster improve the fit? What is the reduced chi-squared of this fit?

10. There is an emission line at approximately 6 keV that is not fit with our current multi-component model. This is a iron line with a rest-frame energy of 6.07 keV. Model this using a Gaussian spectral line with a fixed width of 0.1 keV. The model name is “zgauss”. You are adding this the the bremsstrahlung model, not using it to modify the bremsstrahlung model, similar to how the spectral line modified the power law model in the notes. Determine the initial guess at the central energy of the spectral line by redshifting the rest-frame energy to a redshift of 0.1028. Remember to freeze the parameters that need to be held at fixed values.

Q4: Record the values and errors for each parameter. Indicate the parameters that are frozen. What is the reduced chi-squared value?

Q5: Save a copy of the plot and submit it with your homework. To send your plot use the following command.

```
XSPEC12> cpd <filename>/ps
```

Where “<filename>” is the name of the file that you want to save your plot to. Use any name you want, but have it end with “.ps” to indicate that it is a PostScript file. To return to plotting to the screen use

```
XSPEC12> cpd /xw
```

Q6: Do you think that you need more model components to properly fit this spectrum? Why or why not? Ignore the detector feature at ≈ 0.5 keV. This is an artefact of the detector, not part of the spectrum of PKS 0745–19.

Q7: Make a second plot of your best fit that is like the first one, only with wavelength on the X axis. Use the XSPEC manual or the “help” command to find out how to do this.

Q8: What is the flux (in $\text{erg cm}^{-2} \text{s}^{-1}$) in your model. Use the “flux” command? What is the energy range that this flux is measured in?

Hand in your answers to the eight questions (including the plots) with your homework assignment.