# **PyXspec Documentation**

Release 2.0

# CONTENTS

1	Build and Install	3
2	Tutorials	7
3	PyXspec Class Reference	27
4	Notes	63
5	Authors	67
In	Index	

PyXspec is an object oriented Python interface to the XSPEC spectral-fitting program. It provides an alternative to Tcl, the sole scripting language for standard Xspec usage. With PyXspec loaded, a user can run Xspec with Python language scripts or interactively at a Python shell prompt.

Note: The source code distribution of XSPEC is required for using PyXspec

CONTENTS 1

2 CONTENTS

**CHAPTER** 

ONE

## **BUILD AND INSTALL**

# 1.1 Build and Install PyXspec

# 1.1.1 Requirements

Since we do not distribute Python with the HEASOFT packages, you'll need to have it already installed on your system (which it is with most Linux and Mac OSX distributions). PyXspec is compatible with Python versions **2.6**, **2.7**, and (beginning with PyXspec 2.0) Python **3.x**. The **python** executable must be in your path, and with the library and header files located in the standard directories relative to the executable (see the **Troubleshooting** section for more info).

# 1.1.2 Building/Installing

PyXspec is fully integrated into the general HEASOFT build procedure, as described at http://heasarc.gsfc.nasa.gov/lheasoft/install.html . So it will be **built and installed automatically** with the rest of XSPEC/HEASOFT, requiring no additional effort from the user.

By default, the HEASOFT configure/build process will first search for **python2** versions on your system, and only if it finds none will it then search for **python3**. You can override this behavior by setting your PYTHON environment variable to the full path to your **python3** executable *before* running the HEASOFT configure. You can also switch between **python2** and 3 *after* your original build. Please see *Changing between Python 2 and 3* for details.

Once HEASOFT is finished building and installing, you should find PyXspec's code files and lib\_pyXspec.so library in the directory \$HEADAS/lib/python/xspec.

When you run the HEASOFT initialization script (\$HEADAS/headas-init.csh or .sh), it will add \$HEADAS/lib/python to your PYTHONPATH environment. This allows Python find the PyXspec module so that you may load it into your session from anywhere, using the *import xspec* statement.

# 1.1.3 Changing between Python 2 and 3

If you wish to change the Python version from which PyXspec was built during the original HEASOFT configure/build, you can do so by manually editing the file:  $heasoft-<ver>/Xspec/BUILD_DIR/hmakerc$ . This file contains definitions for the 2 variables: PYTHON\_INC and PYTHON\_LIB, which set the compiler paths for the Python header file inclusion and dynamic library linkage, and these must be changed to point to your new Python location.

For example, to point to an Anaconda Python3 distribution on your system, your new settings might look something like:

```
PYTHON_INC="-I/path/to/your/anaconda_py3/anaconda-4.0.0-x86_64/include/python3.5m"
PYTHON_LIB="-L/path/to/your/anaconda_py3/anaconda-4.0.0-x86_64/lib -lpython3.5m"
```

**Note:** You can determine the Python path information with the *python-config* (or *python3-config*) utility. Call it with the *-cflags* option for the include path information, and with *-ldflags* for the library path information.

After making these edits, simply rebuild PyXspec by doing:

```
cd /path/to/heasoft-<ver>/Xspec/src/XSUser/Python/xspec
hmake clean
hmake
hmake install
```

# 1.1.4 Running on Mac OS X

These issues apply only to Mac OS X users. Linux users may skip this section.

## Using the default XCode Python

You may use the default Xcode Python (normally /usr/bin/python) if your HEASOFT distribution was built using the **Xcode gcc and g++ compilers**, with only the Fortran compiler coming from a 3rd party such as Fink or MacPorts. But if you built HEASOFT with ALL of your compilers coming from Fink or MacPorts, you cannot use the Xcode Python.

## Using the MacPorts or Fink Python

This applies only to users who have built HEASOFT using Fink or MacPorts for **ALL 3 of their compilers** (gcc, g++, gfortran). Note that you can avoid all of this if you build HEASOFT using Mac's own Xcode gcc and g++, and only use Fink or MacPorts for gfortran.

You are going to have to get the corresponding Fink or MacPorts distribution of Python for both building and running PyXspec. The standard Xcode Python (*in /usr/bin*) will conflict with libraries pulled in by the Fink and MacPorts gcc.

To rebuild PyXspec using the Fink or MacPorts Python, please follow the same instructions as in *Changing between Python 2 and 3* for modifying the PYTHON\_INC and PYTHON\_LIB settings in the file *heasoft-<ver>/Xspec/BUILD\_DIR/hmakerc*. In this case they should point to the location of the Python header files and dynamic library of your Fink or MacPorts Python distribution. Then clean and rebuild PyXspec as described in the previous section.

# 1.1.5 Troubleshooting

If the HEASOFT configuration stage fails when it's processing PyXspec, it will just issue a warning and continue. Its failure should not affect the rest of the XSPEC and HEASOFT build. Standard XSPEC will still be fully functional, but its Python interface won't be available.

The most likely cause of a PyXspec build failure is that the HEASOFT configuration script can't find a **python** executable and/or its accompanying library and header files. You should first check that the command "which python" can find an executable on your path (python is generally a symbolic link to a version-specific executable).

If you don't explicitly set the PYTHON environment variable, the configuration script first looks for **python2** versions followed by **python3**. Once it's found an executable, it looks for the files *Python.h* and

*libpython[m.n].so* (or .dylib) with the help of the *python-config* (or *python3-config*) utility. The configuration fails if it is unable to find either file.

If you are manually trying to reset the PYTHON\_INC and PYTHON\_LIB variables (in *heasoft-* <*ver>/Xspec/BUILD\_DIR/hmakerc*) to point to these files in a different Python distribution (for instance if switching between Python 2 and 3, or to a 3rd-party Python distribution installed on your system), we recommend using the *python[3]-config* utility to help you determine the correct path information.

#### **Other Errors**

If you are running on **Mac OS X** and get a Python "ImportError" message containing such statements as **no suitable image found** and **mach-o, but wrong architecture**, it's likely you are trying to run a 32-bit mode Python while your default HEASoft build is now 64-bit.

If you are running on a **Mac** and have built your HEASOFT installation with **all 3 compilers** (**gcc**, **g++**, **gfortran**) coming from **Fink** or **MacPorts**, AND you get a runtime error that begins with something like:

then it likely means there's a conflict between your default Python distribution and the compiler libraries used to build PyXspec. Please see the **Using the MacPorts or Fink Python** section above for switching away from the default Xcode Python distribution.

**CHAPTER** 

**TWO** 

# **TUTORIALS**

# 2.1 Quick Tutorial

This assumes the user already has a basic familiarity with both XSPEC and Python. Everything in PyXspec is accessible by importing the package **xspec** into your Python script.

PyXspec can be utilized in a Python script or from the command line of the plain interactive Python interpreter. PyXspec does not implement its own command handler, so it is NOT intended to be run as the Python equivalent of a traditional interactive XSPEC session (which is really an *enhanced* interactive Tcl interpreter). In other words you launch an interactive PyXspec session with:

```
LINUX> python
>>> import xspec
>>>
```

#### rather than:

```
LINUX> xspec
XSPEC12>
```

Note that in all the tutorial examples the **xspec** package name qualifier is left off. You must either include the **xspec** qualifier:

```
s = xspec.Spectrum("file1.pha")
```

or use a variation of the Python import or from . . . import commands:

```
from xspec import *
s = Spectrum("file1.pha")
```

# 2.1.1 Jumping In: The *Really* Quick Tutorial

A simple Xspec load-fit-plot Python script may look something like this:

```
#!/usr/bin/python
from xspec import *

Spectrum("file1.pha")
Model("wabs*pow")
Fit.perform()
Plot.device = "/xs"
Plot("data")
```

Keeping this template in mind, we'll proceed to fill in the details...

## 2.1.2 Terminology

This description uses the standard Python object-oriented terminology, distinguishing between **classes** and *objects*. **Class** is used when referring to the *type* or definition of an *object*. An *object* refers to a specific instance of a **class** and is normally assigned to a variable. For example a user may load 3 data files by creating 3 spectral data objects *s1*, *s2*, and *s3*, which are all instances of the class *Spectrum*.

The functions and stored data members that make up the definition of a **class** are referred to as **methods** and **attributes** respectively.

The term **Standard XSPEC** refers to the traditional ways of using XSPEC, either with a Tcl script or an interactive XSPEC session.

# 2.1.3 Getting Help

Documentation for PyXspec classes can be found in the *Classes* section of this manual. You can also access the same information from the Python shell command line using Python's built-in help(<class-name>) function.

# 2.1.4 The 6 Global Objects

An XSPEC session fundamentally consists of loading data, fitting that data to a model, and plotting the results. To manage these operations, PyXspec offers the user 6 global objects: *AllChains*, *AllData*, *AllModels*, *Fit*, *Plot*, and *Xset*. Note that these are NOT the names of classes. They are instantiated *objects* of the **class** types shown below.

**Note:** Operations involving these 6 global ojbects should ALWAYS be performed through the object names and NEVER their class names. Their class names should never appear in your code.

Object Name	Class	Role	
AllChains	ChainManager	Monte Carlo Markov Chain container	
AllData	DataManager	Container for all loaded data sets (objects of class <i>Spectrum</i> )	
AllModels	ModelManager	Container for all <i>Model</i> objects	
Fit	FitManager	Manager class for setting properties and running a fit	
Plot	PlotManager	Manager class for performing XSPEC plots	
Xset	XspecSettings	Storage class for XSPEC settings	

PyXspec instantiates these objects immediately upon the importing of the **xspec** package. You cannot create any other objects of these class types, as they each allow only 1 instance of their type. (They are **singletons** in the language of design patterns.)

# 2.1.5 Loading And Removing Data

Spectral data files can be loaded in several ways. You can create an object of the *Spectrum* class by passing it the data file name:

```
s1 = Spectrum("file1.pha")
```

which also adds the new object s1 to the AllData container. Or you can simply add the new file directly to the container without retrieving a Spectrum object:

```
AllData += "file1.pha"
```

Later you can always obtain a *Spectrum* object reference to any of the loaded spectra by passing *AllData* an integer:

```
s2 = AllData(2) # s2 is a reference to the 2nd loaded spectrum
```

For more complicated data loading, you have access to the same functionality in Standard XSPEC's **data** command. Simply pass a string to the *AllData* object's \_\_call\_\_ method:

```
AllData("file1 file2 2:3 file3")
```

Note that only the last example allows you to assign multiple data groups, the 3rd spectrum being assigned to data group 2. Also note that in the last example any previously loaded data sets are removed, thus reproducing the behavior of Standard XSPEC's **data** command.

Other ways of removing Spectrum objects (ie. data sets) from the container:

You can check the current state of the *AllData* container at any time by doing:

```
AllData.show()
```

Similarly, to view information about a single *Spectrum* object:

```
s2.show()
```

# 2.1.6 Defining Models

The basic way of defining an XSPEC model is to create an object of the PyXspec class *Model*. Simply pass in a string containing a combination of 1 or more XSPEC model **components**. Since this uses the same syntax as Standard XSPEC's **model** command, component abbreviations are allowed:

```
m1 = Model("wa*po + ga")
```

and to see a complete listing of available XSPEC model components, do:

```
Model.showList()
```

When you define a model like this, PyXspec also automatically adds the new object to the global *AllModels* container. If the model is applied to multiple data groups, object copies are added to the container for each data group.

Similar to the case of spectral data, you can also load models directly into the global container:

```
# Another way to define a new model and create an object for each data group.
AllModels += "wa*po + ga"
# Retrieve the model object assigned to data group 2.
m2 = AllModels(2)
# Various ways to remove all model objects from the container.
AllModels.clear()
AllModels -= "*"
```

To display models and their parameters:

2.1. Quick Tutorial 9

```
# This displays all parameters in all model objects:
AllModels.show()
# While this displays just parameters 1,2,3 and 5:
AllModels.show("1-3, 5")
# This displays a single model object:
m2.show()
```

For defining mulitple (or named) models and assigning multiple sources, please see the *Extended Tutorial* section.

# 2.1.7 Component and Parameter Objects

*Model* objects contain *Component* objects and Component objects contain *Parameter* objects. There are several ways to access and set components and parameters individually (and if you want to change many parameter values at once, it may be faster to use the Model or *AllModels* **setPars** methods described in the next section). Examples of individual Component and Parameter object access:

```
# Component objects are accessible-by-name as Model object attributes:
comp1 = m1.wabs
comp2 = m1.powerlaw
# Parameter objects are accessible-by-name as Component object attributes:
par4 = m1.qaussian.LineE
# ...and we can modify their values:
par4.values = 3.895
m1.wabs.nH = 5.0
comp2.PhoIndex = 1.5
# Can also get a Parameter object directly from a Model, without going
# through a Component. Just pass the Model the Parameter index number:
par5 = m1(5)
# Examples of numerical operations allowed with Parameter objects:
par4 += 0.75
par4 *= 2.0
y1 = m1.wabs.nH \times 100.0
y2 = par4 + par5
```

**Note:** For models with duplicate copies of components, see the *Extended Tutorial* for accessing Component objects by name.

Note that in the above examples, only the parameter's *value* is being accessed or modified. To change all or part of its FULL list of settings including auxiliary values: *value*, *fit delta*, *min*, *bot*, *top*, *max*, you can set its **values** attribute to a tuple or list of size 1-6:

```
par4.values = 4.3, .01, 1e-3
par4.values = [4.3, .01, 1e-3, 1e-2, 100, 200]
```

Or for greater flexibility you can set it to a string using Standard XSPEC's newpar command syntax:

```
# This allows you to set new values non-consecutively.
par4.values = "1.0, -.01,,,,150"
```

A quick way to freeze or thaw a parameter is to toggle its **frozen** attribute:

```
par4.frozen = False
par5.frozen = True
```

To link a parameter to one or more others, set its **link** attribute to a link expression string as you would have with the **newpar** command. To remove the link, set **link** to an empty string or call the parameter's **untie** method:

```
par5.link = "2.3 * 4" # Link par 5 to par 4 with a multiplicative constant.
par5.link = "" # Removes the link.
par5.untie() # Also removes the link.
```

Also ALL linked parameters in a model object can be untied with a single call to the *Model* class **untie** method.

To display a parameter's full set of values (including auxiliary values), just print its values attribute:

```
>>> print(par4.values)
[6.5, 0.05, 0.0, 0.0, 1000000.0, 1000000.0]
```

# 2.1.8 Setting Multiple Parameters At A Time

You can set multiple parameter values with a single call using the *Model* or *AllModels* (see *ModelManager*) **setPars** methods. This may be considerably faster than setting parameters one at a time through the individual *Parameter* objects as shown in the previous section. With **setPars**, the model will be recalculated just ONCE after all the changes have been made. But when setting through individual Parameter objects, the model will be recalculated after EACH parameter change:

```
# For Model object m1, supply 1 or more new parameter values in consecutive order:
m1.setPars(2.5, 1.4, 1.0e3)  # This changes pars 1, 2, and 3.

# Can also change parameter auxiliary values by passing a string using the same
# syntax as with Standard XSPEC's `newpar` command:
m1.setPars(.95, "1.8,,-5,-4,10,10")

# Now set parameters NON-CONSECUTIVELY by passing a Python dictionary object.
# This example changes pars 1, 2, 4, and 6:
m1.setPars(.95, 1.2, {4:9.8, 6:2.0})
```

Parameters can also be initialized by passing values to the *Model* object constructor. You do this by setting the Model constructor's *setPars* keyword argument to a tuple, list, or dictionary (or just a single value or string if only setting the first parameter):

```
# Supply values for parameters 1 and 3, use defaults for the rest.
m = Model("wa*ga", setPars={1:1.5, 3:.2})
# Supply values for 1 and 2, use defaults for the rest.
m = Model("wa*ga", setPars=(1.5, 0.7))
# Supply value only for 1.
m = Model("wa*ga", setPars=1.5)
```

Finally, if you wish to set multiple parameters that belong to *different* model objects, you must use the *AllModels* container's **setPars** method (see *ModelManager*). This follows the same syntax rules as the single Model **setPars**, except that you also supply the Model objects as arguments:

```
# Change pars 1 and 3 in m1, and pars 1 and 2 in m2:
AllModels.setPars(m1, {1:6.4, 3:1.78}, m2, 3.5, 0.99)
```

2.1. Quick Tutorial

# 2.1.9 Fitting

Once data and models are loaded, fitting is performed by calling the **perform** method of the *Fit* global object:

```
Fit.perform()
```

Some of the more frequently modified fit settings are the type of statistic to minimize and the maximum number of fit iterations to perform. These settings are attributes of *Fit*:

```
Fit.nIterations = 100
Fit.statMethod = "cstat"
Fit.statMethod = "chi"
```

Please see FitManager and the Extended Tutorial for Fit's complete functionality.

To display the fit results at any time:

```
Fit.show()
```

# 2.1.10 Plotting

In Standard XSPEC, plot settings are adjusted using the **setplot** command while the plot is displayed through the **plot** command. In PyXspec, all plot settings and functionality is handled through the global *Plot* object (see *PlotManager* for full description). A device must be set before any plots can be displayed, and this done through the **device** attribute:

```
Plot.device = "/xs"
```

The device can also be set to print to an output file in several formats. The list of possible devices is given by the **cpd** command in the Standard XSPEC manual.

A typical setting to adjust is the X-axis units. You can choose to plot channel numbers, or select from various energy and wavelength units. The strings can also be abbreviated. Examples:

```
Plot.xAxis = "channel"
Plot.xAxis = "MeV"
Plot.xAxis = "Hz"
Plot.xAxis = "angstrom"
```

The displays of individual additive components or background spectra is toggled by setting their attributes to a bool:

```
Plot.add = True
Plot.background = False
```

Similarly log/linear settings for data plots (when using energy or wavelength units):

```
Plot.xLog = True
Plot.yLog = False
```

The current plot settings are displayed with:

```
Plot.show()
```

To actually display a plot, send 1 or more string arguments to the *Plot* \_\_call\_\_ method:

```
# Single panel plots
Plot("data")
Plot("model")
Plot("ufspec")
# Multi panel plots
Plot("data chisq")
Plot("data chisq")
Plot("data", "model", "resid")
# Call Plot with no arguments to repeat the previously entered Plot command
Plot()
```

After displaying a plot, you can get an array of the plotted values by calling one of *Plot*'s retrieval methods. All of these functions take an optional plot group number argument for the case of multiple plot groups, and all return the plot values in a Python list:

```
Plot("data")
xVals = Plot.x()
yVals = Plot.y()
yVals2 = Plot.y(2)  # Gets values for data in the second plot group
modVals = Plot.model()
# To get a background array, Plot.background must be set prior to plot
Plot.background = True
Plot("data")
bkg = Plot.backgroundVals()
# Retrieve error arrays
xErrs = Plot.xErr()
yErrs = Plot.yErr()
```

# 2.2 Extended Tutorial

This assumes the user is familiar with the basics of PyXspec as explained in the *Quick Tutorial*.

## 2.2.1 Data

## Background, Response, and Arf

When a *Spectrum* object is created from a spectral data file, PyXspec also reads the file's BACKFILE, RESPFILE, and ANCRFILE keywords and will load the corresponding background, response, and arf files. The spectrum's *Background* and *Response* objects are then available as attributes of the **Spectrum** class, while the arf file name becomes an attribute of the **Response** class:

```
s1 = Spectrum("file1")
b1 = s1.background
r1 = s1.response
arfFileName = r1.arf
```

**Note:** You never create **Background** and **Response** objects directly. They are accessible only through the **Spectrum** class attributes.

These attributes may also be used to add, change, or remove auxiliary files to an existing *Spectrum* object:

```
# Add or replace files:
s1.background = "newBackground.pha"
s1.response.arf = "newArf.pha"
```

```
# Removal examples:
s1.response = None
s1.background = ""
```

*Background* and *Spectrum* store their original file names in their **fileName** attribute. This means that while you SET the Spectrum.background object by assigning it a file name (as shown above), to GET the file name you must access its **fileName** attribute:

Response stores its RMF and optional ARF file names in its rmf and arf attributes respectively:

```
rmfFileName = r1.rmf
arfFileName = r1.arf
```

*Background* objects have some of the same attributes as *Spectrum* objects, such as **areaScale**, **exposure**, **energies**, and **values**. The Spectrum object's **values** array (actually a tuple) does NOT include contributions from the background. Those are stored separately in the associated Background object.

The *Spectrum* class also provides a **multiresponse** array attribute for assigning multiple detectors (or sources) to a spectrum. The standard 0-based Python array indices corresponding to the 1-based XSPEC source numbers:

```
# Set a response for source 2
s1.multiresponse[1] = "resp2.rsp"
# Get the response object for source 2
r2 = s1.multiresponse[1]
# Remove the response from source 2
s1.multiresponse[1] = None
# This is the same as doing s1.response = "resp1.rsp"
s1.multiresponse[0] = "resp1.rsp"
```

The rule is: when doing single-source analysis (typical of most XSPEC sessions) use the **response** attribute, otherwise use the **multiresponse** array.

## Ignore/Notice

To ignore channels for a SINGLE spectrum, call the *Spectrum* object's **ignore** method passing a string following the same syntax as for Standard XSPEC's **ignore** command:

```
s1.ignore("20-30 50-**")
s1.ignore("**-5")
```

Similarly, to notice channels in a single spectrum:

```
s1.notice("10-30,80-**")
s1.notice("all")
```

As with Standard XSPEC, if the **x-axis** plot units are set to energies or wavelengths, **ignore** and **notice** will accept floating-point input assumed to be in those same units:

```
Plot.xAxis = "nm"
# Ignore channel bins corresponding to 15.0 to 20.0 nm wavelengths:
s1.ignore("15.-20.")
```

The currently noticed channel ranges are displayed for each spectrum in the AllData.show() output. You can also get a list of the individual noticed channel numbers from *Spectrum*'s **noticed** attribute:

```
>>> s1.noticed [3,4,5,7,8,10]
```

To apply **ignore** and **notice** commands to ALL loaded spectra, call the methods from the global *AllData* object. To apply to a subset of loaded spectra, add a range specifier to the left of the colon:

```
# These apply to all loaded spectra
AllData.ignore("100-120, 150-200")
AllData.notice("all")
AllData.ignore("bad")
# These apply to a subset of loaded spectra
AllData.ignore("1-3: 60-65")
AllData.notice("2-**:50-60")
```

## 2.2.2 Models

## **Model With Multiple Data Groups**

When a model is defined and spectra are assigned to multiple data groups, PyXspec will generate a *Model* object copy for each data group (assuming the spectra also have responses attached). So if:

```
m1 = Model("wa*ga")
AllData("file1 2:2 file2")
```

then there are  $2 \, Model$  objects for the model definition wabs\*gaussian. The variable ml is set to the object belonging to data group 1, and to get the object for data group 2 do:

```
m2 = AllModels(2)
```

m1 and m2 will each have the same set of Component and Parameter objects.

Parameters can be accessed directly by index from the *Model* objects, and these indices are numbered from 1 to **nParameters** for ALL data group copies. So for the wa\*ga example above:

```
p = m1(2) # Returns the 2nd ('LineE') parameter from the model for data group 1. p = m2(2) # Returns the 2nd ('LineE') parameter from the model for data group 2. p = m2(6) # Wrong!!
```

## **Defining Multiple Models**

Beginning with XSPEC12, it became possible to assign multiple sources to spectra, and each source may have its own model function definition. To keep track of multiple model definitions, XSPEC requires that you assign them names. In PyXspec, the model name and source number are supplied as additional arguments to the *Model* \_\_init\_\_ function:

```
# Define a model named "alpha" assigned to source 1
m_1_1 = Model("wa*po","alpha")
# Define a model named "beta" assigned to source 2
m_2_1 = Model("const*bbody","beta",2)
# (In both of these cases, the returned object belongs to data group 1)
```

**Note:** As with Standard XSPEC, to define a model for source numbers > 1 you first must load a detector response for the source. See "Background, Response, and Arf" in the previous section.

Note that in all previous examples in this tutorial, we have been using unnamed models which were assigned to source 1. Named models and source numbers may also be defined directly into the *AllModels* container by passing in a tuple:

```
# Define a model named "defn1" assigned to source 1
AllModels += ("wa*po", "defn1")
# Define a model named "defn2" assigned to source 2
AllModels += ("const*bbody", "defn2", 2)
# This replaces "defn1" with an unnamed model for source 1
AllModels += "wa*gaussian"
```

and from which *Model* objects can be retrieved:

```
# Get the "defn2" Model object for data group 1
m_2_1 = AllModels(1,"defn2")
# ...and for data group 2
m_2_2 = AllModels(2,"defn2")
```

To view all current source number and model assignments, see the *AllModels.sources* attribute, which displays a dictionary of the [source number]:[model name] pairs.

To remove model definitions:

```
# Remove all data group copies of "defn2"
AllModels -= "defn2"
# Remove all data group copies of the unnamed model (defined above
# as "wa*gaussian")
AllModels -= ""
# Remove all copies of ALL model definitions
AllModels.clear()
```

## **Component And Parameter Access Part 2**

When PyXspec constructs a *Model* object, it immediately adds to it an attribute of type *Component* for every component in the model expression. The attribute has the same (full) name as the component in the original expression, allowing you to access it like:

```
m = Model("wa*pow")
c2 = m.powerlaw
```

However when a model contains multiple copies of the same component, this type of access becomes ambiguous. So to distinguish among copies, for any component making its 2nd or more appearance (from left to right), PyXspec will append \_n to the attribute name where n refers to the component's position in the expression (again from left to right). Or to put it more simply:

```
m = Model("wa*po + po")
# This gets the leftmost powerlaw component
pow1 = m.powerlaw
# This gets the rightmost, which is the 3rd component in the expression.
pow2 = m.powerlaw_3
```

The *Model* object also stores an attribute which is a just a list of the names of its constituent *Component* attributes:

```
>>> m.componentNames
['wabs', 'powerlaw', 'powerlaw_3']
```

This may be useful for example if writing a loop to access each of a model's components. Similarly *Component* objects have a **parameterNames** attribute, listing the names of their constituent *Parameter* attributes:

```
>>> m.powerlaw.parameterNames
['PhoIndex', 'norm']
```

## **Gain Parameters (Response Models)**

Response Models differ from the regular kind in that they act on a Response rather than directly calculate a flux. At present there is only one kind of Response Model in Xspec, and this is **gain**. **gain** is a built-in attribute of all *Response* objects, and is of the class type *RModel*. It has 2 parameters for adjusting the energies of a Response: **slope** and **offset**. Gain parameters are initially off by default, but may be turned on simply by setting either one. For example:

```
s = Spectrum("file1")
# The spectrum's response has a gain attribute that is not in use,
# which is the equivalent of having a slope fixed at 1.0 and offset = 0.0.
r = s.response
# Setting either the slope or offset turns the gain on for this response.
# Both slope and offset will now be fit parameters.
r.gain.slope = 1.05
# The previous setting leaves the offset at 0.0. Now we'll change it.
r.gain.offset = .05
# You can set slope and offset at the same time using Response's setPars method.
r.setPars(.99, .03)
```

**slope** and **offset** are *Parameter* objects and therefore have the same interface as regular model parameters:

```
# Modify the parameter's auxilliary values
r.gain.offset = ".08,,.01,.01,.5,.5"
# Set a parameter link
r.gain.offset.link = ".005*1"
```

To remove the response fit parameters and return the *Response* back to its original state, call the *gain.off()* method:

```
# This deletes the slope and offset parameters.
# Any references to them become invalid.
r.gain.off()
```

#### Flux Calculations

To perform a Standard XSPEC **flux** or **lumin** calculation, call the *AllModels* methods **calcFlux** or **calc-Lumin** respectively:

```
AllModels.calcFlux(".3 1.0")
AllModels.calcFlux(".1 10.0 err")
AllModels.calcLumin(".1 10. .05 err")
```

As in Standard XSPEC the results will be stored with the currently loaded spectra:

```
>>> s1 = AllData(1)
>>> s1.flux
(5.7141821510911499e-14, 0.0, 0.0, 4.0744161672429196e-05, 0.0, 0.0)
>>> s1.lumin
(30.972086553634504, 0.0, 0.0, 0.056670019567301853, 0.0, 0.0)
```

unless there are no spectra, in which case the results are stored with the model object:

```
>>> AllModels(1).flux (5.6336924399373855e-10, 0.0, 0.0, 0.05929616315253175, 0.0, 0.0)
```

## Local Models in C/C++/Fortran

In Standard XSPEC, local model libraries are built with the **initpackage** comamnd and then loaded with **lmod**. The *AllModels* container supplies both of these functions for doing the same thing in PyXspec:

```
AllModels.initpackage("myLocalMods","lmodel.dat")
AllModels.lmod("myLocalMods")
```

By default this looks in the directory set by the LOCAL\_MODEL\_DIRECTORY variable in your ~/.xspec/Xspec.init start-up file. You can override this by giving these functions an absolute or relative path as a dirPath keyword argument (see ModelManager for details).

## **Local Models in Python**

You can also write model functions in Python and insert them into the XSPEC library with the *AllModels* **addPyMod** method. You simply define a function with 3 arguments for energies, parameters, and flux. For example a powerlaw model function might look like:

```
def lpow(engs, params, flux):
    for i in range(len(engs)-1):
        pconst = 1.0 - params[0]
        val = math.pow(engs[i+1],pconst)/pconst - math.pow(engs[i],pconst)/pconst
        flux[i] = val
```

XSPEC will pass **tuples** containing the energy and parameter values to your function. For the flux array, it will pass a **list** pre-sized to nE-1, where nE is the size of the energies array. Your model function should fill in this list with the proper flux values. (For additional optional arguments to your model function, please see the documentation for the **addPyMod** method in *ModelManager*.)

The second thing you must define is a **tuple** containing the parameters' information strings, one string for each parameter in your model. This is equivalent to the parameter strings you would define in a *model.dat* file when adding local models in standard XSPEC, and it requires the same format. (See Appendix C of the XSPEC manual for more details.) So with the powerlaw function above which takes just 1 parameter, you might define a tuple as:

```
powInfo = ("phoIndex \"\" 1.1 -3. -2. 9. 10. 0.01",)
```

Note the need for the trailing comma when there's just one parameter string. This is to let Python know that *powInfo* is a tuple type and not a string.

Once you've defined your function and parameter information, simply call:

```
AllModels.addPyMod(lpow, powInfo, 'add')
```

The 3rd argument tells XSPEC the type of your model function ('add', 'mul', or 'con'). After this call your function will be added to the list of available model components, which you can see by doing *Model.showList()*. Your model will show up with the same name as your original Python function ('lpow'), and is ready for use in future model definitions.

18 Chapter 2. Tutorials

# 2.2.3 Fitting

## **Error**

The **error** command is implemented through *Fit* (see *FitManager*), and the results are stored with the chosen *Parameter* object(s). The **error** attribute stores a tuple containing the low and high range values for the parameter, and the 9-letter status string to report problems incurred during the error calculation.

Example: Estimate the 90% confidence range for the 4th parameter

```
>>> Fit.error("2.706 4")
>>> par4 = AllModels(1)(4)
>>> par4.error
(0.11350354517707145, 0.14372981075906774, 'FFFFFFFFF')
```

## Query

During a *Fit.perform()* operation, the default is to query the user whenever the fit has run the maximum number of iterations, as set by the *Fit.nIterations* attribute. You can change this behavior with the **query** attribute:

```
# When nIterations is reached, continue the fit without stopping to query.
Fit.query = "yes"
# Stop fit at nIterations and do not query.
Fit.query = "no"
# Query the user when nIterations is reached.
Fit.query = "on"
```

## Steppar

The Standard XSPEC **steppar** command is also implemented through the global *Fit* object. You supply it with a string following the same **steppar** command syntax rules. For example:

```
# Step parameters 1 and 2 through the given range values
# over a 10x10 2-D grid.
Fit.steppar("1 20. 30. 10 2 .05 .08 10")
```

## 2.2.4 Fakeit

PyXspec provides access to standard XSPEC's **fakeit** command, which is for creating spectra with simulated data. It is called through the *AllData.fakeit* method:

```
AllData.fakeit(nSpectra=1, settings=None, applyStats=True, filePrefix="")
```

**Note:** If *AllData.fakeit* is run when spectra are currently loaded, it will follow the same rules as the standard XSPEC **fakeit** function: It will REMOVE ALL pre-existing spectra and replace each one with a simulated spectrum (even if *nSpectra* is less than the number originally loaded).

As those familiar with standard **fakeit** know, the user is normally prompted for quite a bit of additional information needed to generate the fakeit files. However the goal here is to have NO additional prompting, and that requires that all information must be entered as arguments to the *AllData* fakeit method call. This is done by passing objects of the *FakeitSettings* class to *AllData.fakeit*, as we'll show further below.

Note: Unless stated otherwise, assume all spectra are OGIP type-1 (1 spectrum per file).

For the simplest of cases, you don't need to create any *FakeitSettings* objects. Just pass in the number of fake spectra you'd like to create:

```
# Create 3 fake spectra using only default settings.
AllData.fakeit(3)
```

The *fakeit* function will then create a default *FakeitSettings* object for each of the 3 spectra. By default, a FakeitSettings object will have empty strings for all of its attributes, and these are handled differently depending on whether the fake spectrum is replacing a currently loaded spectrum, or creating one from scratch.

## From Existing Spectra

When replacing an existing spectrum, *FakeitSettings* attributes with empty strings will simply take their value from the original spectrum. Also note that the **response** and **arf** settings for the original spectrum CANNOT be modified for the fakeit spectrum. If a name is filled in for either of these attributes, it will be ignored. If you wish to modify these, you can make the change to the original spectrum prior to calling fakeit. [The one exception is when the original spectrum has no response, in which case the response attribute MUST be filled in.] If the **fileName** attribute is empty, XSPEC will generate a default output name derived from the original file name.

## **From Scratch**

When creating from scratch, an empty string implies "none" for the arf and background, 1.0 for exposure and correction, and XSPEC's default dummy response for the response attribute. If the fileName attribute is empty, XSPEC will generate a default output file name based on the response name, and it will include an auto-incremented index to prevent multiple output files from overwriting each other.

## **FakeitSettings Objects**

To create a fake spectrum with anything other than default settings, you must supply a *FakeitSettings* object for that spectrum. The FakeitSettings attributes are: response, arf, background, exposure, correction, backExposure, and fileName. All are string types, though exposure, backExposure, and correction can also be entered as floats. Attributes can be set upon object construction, or anytime afterwards:

```
fs1 = FakeitSettings("response1.rsp", exposure = 1500.0)
fs1.background = "back1.pha"
```

A new FakeitSettings object can also be made by copying an existing one:

```
fs2 = FakeitSettings(fs1)
```

And now pass the objects to the fakeit method, either in a list, dictionary, or as a single object:

```
# Apply settings to fakeit spectra 1 and 2:
AllData.fakeit(2,[fs1,fs2])
# Apply setting to fakeit spectrum 1, use defaults for spectrum 2:
AllData.fakeit(2, fs1)
# Apply settings to fakeit spectra 2 and 4, use defaults for 1 and 3:
settingsDict = {2:fs1, 4:fs2}
AllData.fakeit(4, settingsDict)
```

```
# Create 4 fakeit spectra from the same settings object:
settingsList = 4*[fs1]
AllData.fakeit(4, settingsList)
```

The remaining 2 arguments to the *AllData.fakeit* function are for choosing whether to apply statistical fluctuations (default = True), and whether to add an optional prefix string to the names of all output files.

## **OGIP Type-2 Files**

With **OGIP type-2** files, multiple spectra may be placed in a single file. The important thing to recognize when generating type-2 fakeit files is that the **exposure**, **correction**, **backExposure**, and **fileName** attributes apply to the output *files* and not the individual spectra. Therefore these settings will be ignored for all but the first spectrum in a file. For example:

```
# Start with 4 spectra loaded, in 2 type-2 files:
AllData("myDataFile1.pha{1-2} myDataFile2.pha{7-8}")
# Create settings for the 4 fake spectra that will be generated from these:
fs1 = FakeitSettings(background="back1.pha", exposure=250.)
# The exposure setting in fs2 will be ignored!!!
fs2 = FakeitSettings(background="back2.pha", exposure=100.)
fs3 = FakeitSettings(fileName="myFakeitFile_2.pha")
fs4 = FakeitSettings(fs3)
```

# The following change will be ignored!!! fs4.fileName = "myFakeitFile\_3.pha" # Now generate the fakeit files: AllData.fakeit(4, [fs1,fs2,fs3,fs4])

The above will generate 4 fakeit spectra, placed in 2 type-2 files. The exposure setting for spectrum 2 and the fileName setting for spectrum 4 will be ignored. Those values are only set by spectra 1 and 3.

For more fakeit details and examples, please check *FakeitSettings* and the **fakeit** method description in *DataManager*.

## 2.2.5 Monte Carlo Markov Chains (MCMC)

All MCMC operations are handled either by objects of class *Chain*, or the global *AllChains* container object (see the *ChainManager* class description). To create a new chain based on the current fit parameters, simply create a **Chain** object by passing it an output file name:

```
c1 = Chain("chain1.fits")
```

The above call creates the file *chain1.fits*, performs an MCMC run using the default *burn*, *fileType*, *length*, *proposal*, *rand*, *and temperature* values, and automatically places the new object in the *AllChains* container. These default settings are stored as attributes of *AllChains*:

```
# Ensure that new chains will burn the first 100 iterations, will
# have length 1000, and will use the proposal "gaussian fit"
AllChains.defBurn = 100
AllChains.defLength = 1000
AllChains.defProposal = "gaussian fit"
c2 = Chain("chain2.fits")
```

You can also override the *AllChains* default settings by passing additional arguments to *Chain* upon construction:

```
# Length will be 2000 for this chain, use defaults for all other settings.
c3 = Chain("chain3.fits", runLength = 2000)
```

The new chain objects will then store their own settings as attributes:

```
>>> c2.burn
100
>>> c2.runLength
1000
>>> c3.runLength
2000
```

All of a chain object's attributes will be displayed when calling its *show()* method.

To append a new run to an existing chain object, call the object's *run()* method. The appending run will use the object's current attribute settings, and not the *AllChains* default settings:

```
# This will append a run of length 3000 to the c3 chain object, and with a
# Metropolis-Hastings temperature of 50.0:
c3.runLength = 3000
c3.temperature = 50.0
c3.run()
```

Display the new chain length:

```
>>> c3.totalLength
5000
```

To **overwrite** rather than append to an existing chain object, call run with its append argument set to *False*:

```
# This erases the results of any previous runs for object c3.c3.run(False)
```

```
>>> c3.totalLength
3000
```

New chains are loaded into *AllChains* by default, but you can unload or reload them using the *AllChains* arithmetic operators:

```
# Chain c2 may be unloaded by passing its chain index number
AllChains -= 2
# OR by passing the object itself
AllChains -= c2
# 2 ways to remove ALL chains
AllChains -= '*'
AllChains.clear()

# Reload an existing chain object
AllChains += c2
# Load a chain from an existing chain file
AllChains += "earlierChain.fits"
# Create a new chain, to be stored in file "chain4.fits"
AllChains += "chain4.fits"
```

As with Standard XSPEC, unloading a chain will leave the chain's file intact. It merely removes the chain from XSPEC's calculations. To display information about the currently loaded chains, call *AllChains.show()*.

You may also get a chain object from the container at any time by passing it an index number:

```
# Retrieve a chain object for the 4th chain in the container c4 = AllChains(4)
```

22 Chapter 2. Tutorials

# 2.2.6 Plotting

All of the plotting options available in Standard XSPEC's **setplot** command are now implemented as attributes of the *Plot* object. Some of these are mentioned in the *Quick Tutorial*, and please see the *PlotManager* class reference for the complete guide.

One setting of particular interest is the **commands** attribute. This is a tuple of user-entered **PLT** command strings which are added to XSPEC's auto-generated commands when performing a plot, and is modified through *Plot*'s **addCommand** and **delCommand** methods. For example, to enter a PLT command to place an additional label at the specified coordinates on the plot:

```
Plot.addCommand("label 1 pos 10 .05 \"Another Label\"")
```

To view the currently loaded commands:

```
print(Plot.commands)
```

and to remove the 3rd command from the tuple:

```
Plot.delCommand(3)
```

# 2.2.7 XSPEC Settings

Most of the internal switches set through Standard XSPEC's **xset** command are now set through attributes of the global *Xset* object. (See *XspecSettings* for the full class description.)

Examples:

```
Xset.abund = "angr"
Xset.cosmo = "50 .5 0."
Xset.xsect = "bcmc"
```

*Xset* also provides the methods **addModelString** and **delModelString** to set the *<string name>*, *<string value>* pairs which are used by certain models. The *<string name>* argument is case-insensitive:

```
Xset.addModelString("APECROOT","1.3.1")
Xset.addModelString("APECTHERMAL","yes")
Xset.delModelString("neivers")
```

The entire collection of <name>,<value> pairs may be set or retrieved with the Xset.modelStrings attribute:

```
# Replace all previous entries with a new dictionary
Xset.modelStrings = {"neivers":"1.1", "apecroot":"1.3.1"}
# Clear out all entries:
Xset.modelStrings = {}
```

*Xset.show()* will display all of the current settings including the current *<string name>*, *<string value>* pairs.

# 2.2.8 Logging And XSPEC Output

The *Xset* object provides attributes and methods for controlling output chatter level and for creating log files:

```
# Get/Set the console chatter level
ch = Xset.chatter
Xset.chatter = 10
# Get/Set the log chatter level
lch = Xset.logChatter
Xset.logChatter = 20

# Create and open a log file for XSPEC output
# This returns a Python file object
logFile = Xset.openLog("newLogFile.txt")
# Get the Python file object for the currently opened log
logFile = Xset.log
# Close XSPEC's currently opened log file.
Xset.closeLog()
```

# 2.2.9 Exceptions And Error Handling

PyXspec utilizes the standard Python **try/except/raise** mechanism for handling and reporting errors. Currently only exception objects of the class **Exception** are ever raised. In the future other (more specific) error classes may be used, but they should always be derived from **Exception**. So you can catch all PyXspec exceptions with code such as:

```
try:
    # Only 4 spectra are currently loaded
    s = xspec.AllData(5)
except Exception as msg:
    print(str(msg))
```

which will print the error message

Error: Spectrum index number is out of range: 5

PyXspec raises errors in a variety of situations, such as for invalid input argument syntax, or for input which is invalid within the context of the call (as in the example above). It can also raise exceptions if you try to rebind a class attribute when such modification is not permitted.

# 2.2.10 Adding Attributes To PyXspec Objects

A particularly novel feature of Python (in comparison with say C++) is that it allows you to create new attributes "on the fly". The attributes don't have to have been part of the original class definition:

```
class C:
    pass

x = C()
x.pi = 3.1416
```

The downside of course is that spelling or case sensitive errors become much harder to detect. For example, with PyXspec's *Plot* object:

```
Plot.yLog = True # Correct
Plot.ylog = True # Wrong!
```

In the second case, standard Python will simply add a new attribute named *ylog* to *Plot*, and this will have no effect on the actual plot since PyXspec is only looking for an attribute named *yLog*.

So operating under the assumption that this downside outweighs the benefits, we've decided to **disable** the ability to add new attributes to PyXspec class objects. A misspelling or case error will instead raise an **Exception** object. And since some users may genuinely wish to add their own attributes to PyXspec classes, this default behavior may be overridden by toggling the *Xset.allowNewAttributes* flag:

```
s = Spectrum("dataFile.pha")
s.myNewIndex = 10  # Error: Will raise an exception
Xset.allowNewAttributes = True

s.myNewIndex = 10  # OK
  # .
  # .
  # .
  # .
  # . In this section you can now add new attributes to any PyXspec object,
  # . but attribute spelling errors will go undetected.
  # .
  # .

Xset.allowNewAttributes = False
```

# 2.2.11 Using With Other Packages

One of the primary benefits of PyXspec is that it makes it much easier to use XSPEC data and results in 3rd party packages. For example you can bypass XSPEC's built-in plotting functions in favor of a Python plotting library such as Matplotlib:

```
#!/usr/bin/python

from xspec import *
import matplotlib.pyplot as plt

# PyXspec operations:
s = Spectrum("file1.pha")
m = Model("wa*po")
Fit.perform()

# Plot using Matplotlib:
plt.plot(s.noticed, s.values, 'ro', s.noticed, m.folded(1))
plt.xlabel('channels')
plt.ylabel('counts/cm^2/sec/chan')
plt.savefig('myplot')
```

The above code produces a Matplotlib plot of the spectral data and folded model vs. channels (similar to what you get with Standard XSPEC's "plot data" command). It makes use of the *Spectrum* object's **noticed** attribute to pass a list of the channel numbers, and the **values** attribute (a tuple) to pass the spectral data values in counts/cm^2/s. The folded model values are obtained as a list by calling the *Model* object's **folded** method with a spectrum number argument.

26 Chapter 2. Tutorials

# **PYXSPEC CLASS REFERENCE**

# 3.1 Classes

# 3.1.1 Background

class xspec.Background(backTuple, parent)

Background spectral data class.

Attributes (all are get-only)

- •areaScale
- •backScale
- •exposure
- •fileName
- •isPoisson
- •values
- •variance

#### areaScale

The Background area scaling factor (GET only).

This is either a single float (if file stores it as a keyword), or a tuple of floats (if file stores column).

## backScale

The Background back scaling factor (GET only).

This is either a single float (if file stores it as a keyword), or a tuple of floats (if file stores column).

## exposure

The exposure time keyword value [float] (GET only).

#### fileName

The spectrum's file name [string] (GET only).

## isPoisson

Boolean flag, True if spectrum has Poisson errors (GET only).

#### values

Tuple of floats containing the background rates array in counts/cm^2-sec (GET only).

#### variance

Tuple of floats containing the variance of each channel (GET only).

## 3.1.2 Chain

 $\begin{tabular}{ll} \textbf{class} & \texttt{xspec.Chain} & \textit{(fileName, fileType=None, burn=None, runLength=None, proposal=None, rand=None, temperature=None, algorithm=None, walkers=None)} \\ \end{tabular}$ 

#### Monte Carlo Markov Chain class.

#### Methods

- •\_\_init\_\_
- •run
- •show

## **Attributes** ((\*) = get-only)

- •algorithm
- •burn
- •fileName\*
- •fileType\*
- proposal
- rand
- •runLength
- •temperature
- •totalLength\*
- •walkers

The following attribute settings will apply to the NEXT run for this chain: algorithm, runLength, proposal, temperature, burn, rand, walkers.

The algorithm, burn, rand, and walkers settings are irrelevant if run is performing an appending operation.

\_\_init\_\_ (fileName, fileType=None, burn=None, runLength=None, proposal=None, rand=None, temperature=None, algorithm=None, walkers=None)

## Construct a chain object, perform a run, and load into AllChains container.

The only required argument is *fileName*. All other arguments will take their default values from the current settings in the *AllChains* container.

run (append=True)

Perform a new chain run, either appending to or overwriting an existing chain.

#### Args:

*append*: If this is set to True the new run will be appended. If False, the new run will overwrite. Note that the *algorithm*, *burn*, *rand*, and *walkers* settings do not apply when appending.

## show()

Display current settings of Chain object's attributes.

## algorithm

The current chain algorithm. Valid settings are 'gw' (Goodman-Weare) or 'mh' (Metropolis-Hastings).

#### burn

The number of steps that will be thrown away prior to storing the chain [int].

## fileName

Chain output file name.

## fileType

Output format of the chain file [string]. Will be either 'fits' (the default), or 'ascii'.

## proposal

The proposal distribution and source of covariance information to be used for the next run [string].

Examples: 'gaussian fit', 'cauchy fit', 'gaussian chain', etc.

See the 'chain' command in the standard XSPEC manual for more information.

#### rand

Determines whether chain start point will be randomized (True) or taken from the current parameters (False).

## runLength

The length of chain to be added during the next run [int].

#### temperature

The temperature parameter used in the Metropolis-Hastings algorithm for the proposal acceptance or rejection [float].

## totalLength

The cumulative length of the chain [int]. This will increase every time a run is performed.

#### walkers

The number of walkers to be used for 'gw' chains [int].

# 3.1.3 ChainManager

## class xspec. ChainManager

## Monte Carlo Markov Chain container.

PyXspec automatically creates a single object of this class, named *AllChains*.

#### Methods

```
•__call__ (the '()' operator)
```

•\_\_iadd\_\_ (the '+=' operator)

•\_\_isub\_\_ (the '-=' operator)

•clear

•show

•stat

## Attributes

These are the values which will be used when creating new Chain objects, unless they are explicitly overridden as arguments to the Chain class constructor. For more detail, see the descriptions for the corresponding attributes in the Chain class doc.

- •defAlgorithm
- •defBurn
- defFileType
- $\bullet$ defLength
- •defProposal
- defRand
- •defTemperature
- •defWalkers

3.1. Classes 29

```
\_call\_(index)
```

Get a Chain object from the AllChains container.

Args:

*index*: The index of a currently loaded chain file. The list of currently loaded chains can be seen with the AllChains.show() method. The valid range is: 1 <= *index* <= nLoadedChains.

Note that the returned Chain object's modifiable attributes will be initialized with the current AllChains *def*<*attribute*> settings:

```
# Example: Load 2 chains from pre-existing files:
AllChains += "chain1.fits"
AllChains += "chain2.fits"
# and use the __call__ method to retrieve a Chain object
# for the 2nd chain:
c2 = AllChains(2)
```

```
__iadd__(chain)
```

Load a pre-existing chain into the AllChains container.

Args:

chain: may be a currently existing chain object which had been unloaded earlier:

```
>>> AllChains += myChain1
```

the filename of an existing chain file:

```
>>> AllChains += "chainFile.fits"
```

or the filename of a new chain:

```
>>> AllChains += "newChainFile.fits"
```

The last example will also perform a chain run using the default settings.

```
___isub___(chain)
```

Unload one or more chain objects from container.

**Args:** *chain*: may either be a chain object:

```
>>> AllChains -= myChain1
```

a filename:

```
>>> AllChains -= "chainFile.fits"
```

the chain's current index [int] in the AllChains container:

```
>>> AllChains -= 2
```

or a '\*' to unload ALL chains (equivalent to AllChains.clear()):

```
>>> AllChains -= '*'
```

clear()

Unload all chains from container

```
show()
     Display information for current attributes and loaded chains.
stat (parIdx)
     Display statistical information on a particular chain parameter.
         parldx: The parameter index number, including optional model name:
                                                                                    [<modName>:]<idx>.
             May be entered as a string or int (if no model name).
defAlgorithm
     Default chain algorithm (orig = 'gw').
defBurn
     Default burn length for new Chain objects (orig = 0).
defFileType
     Default output file format (orig = 'fits').
defLength
     Default chain length (orig = 100).
defProposal
     Default chain proposal (orig = 'gaussian fit').
defRand
     Default randomization setting (orig = False).
defTemperature
     Default chain temperature (orig = 1.0).
```

# 3.1.4 Component

```
class xspec.Component (compName, parNames)
```

Model component class.

#### **Attributes**

•name The full name of the Component (get only).

Default walkers parameter for 'gw' chains (orig = 10).

•-component contains an attribute of type Parameter for every parameter in the component. The attribute name is the same as the parameter name in xspec.

•parameterNames List of Component's parameter names (get only).

# 3.1.5 DataManager

#### class xspec.DataManager

## Spectral data container.

PyXspec automatically creates a single object of this class, named AllData.

## Methods

- •\_\_call\_\_ (the '()' operator)
- •\_\_iadd\_\_ (the '+=' operator)

3.1. Classes 31

```
•__isub__ (the '-=' operator)
         clear
        diagrsp
        •dummyrsp
        fakeit
        ignore
        notice
        removeDummyrsp
        •show
     Attributes (get-only)
        nGroups
        nSpectra
 call (expr)
     DataManager get or set spectra.
     Args:
         expr:
             Get: An integer referring to the spectrum index number. Returns the spectrum, or raises an
                Exception if the integer is out of range.
             Set: A string following the same syntax rules as Xspec's traditional "data" command handler.
___iadd___(spectra)
     Add 1 spectrum to the data container.
     Args: spectra: The data filename string.
 _isub__(spectra)
     Remove 1 or all spectra from the data container.
     Args:
         spectra: Either a single spectrum index number [int], a single Spectrum object, or the string '*'
             to remove all.
clear()
     Remove all spectra from the data container.
diagrsp()
     Diagonalize the current response matrix for ideal response.
```

All currently loaded responses will be replaced with diagonal response matrices. The energy range and

All currently loaded responses will be replaced with diagonal response matrices. The energy range and channel binning information are retained from the original response, as is the effective area. The channel values are mapped directly into the corresponding energy ranges to simulate a detector with perfect spectral resolution.

To remove diagonal responses and restore the originals, call the *AllData.removeDummyrsp()* method.

Create a dummy response and apply it to all spectra.

**Args:** (all are optional) lowE: Input response energy lower bound, in keV. [float]

highE: Input response energy higher bound, in keV. [float]

nBins: Number of bins into which the energy range is divided [int].

scaleType: 'log' or 'lin' [string]

chanOffset: Starting value of dummy channel energies. [float]

chanWidth: Energy width of the channel bins. [float]

If this is set to 0, the dummy response can only be used for evaluating model arrays, and not for fitting to spectra.

#### Examples:

```
# All values are optional, use keywords to enter values
# non-consecutively. Unspecified values revert to the
# current defaults.
AllData.dummyrsp(.3, 30., 100, chanWidth=.5)
AllData.dummyrsp(highE = 50.)
AllData.dummyrsp(.1,10.,100,"lin",.0, 1.0)
```

Initial defaults: lowE = .1, highE = 50, nBins = 50, scaleType = 'log', chanOffset = .0, chanWidth = .0.

The defaults for *lowE*, *highE*, *nBins*, *scaleType*, and *chanOffset* will be modified for each explicit new entry. *chanWidth* always defaults to 0.

To remove dummy responses and restore actual responses (if any), call the removeDummyrsp() method.

To apply a dummy response to just a single spectrum, use the Spectrum.dummyrsp method.

```
fakeit (nSpectra=1, settings=None, applyStats=True, filePrefix='', noWrite=False) Produce spectra with simulated data using XSPEC's fakeit command.
```

Note that if this method is run when spectra are currently loaded, it will follow the same rule as the standard XSPEC fakeit function: It will REMOVE ALL pre-existing spectra and replace each one with a simulated spectrum (even if *nSpectra* is less than the number originally loaded).

**Args:** (all are optional) *nSpectra*: The number of fake spectra to produce. [int]

If there are nOrig pre-existing spectra loaded at the time this function is called and nSpectra < nOrig, nSpectra will be RESET to nOrig (see note above).

If nSpectra == nOrig, then each of the fake spectra will use the settings from the respective original spectra for their defaults (see the FakeitSettings class description).

If nSpectra > nOrig, then settings for the fake spectra numbered above nOrig will not be based on pre-existing spectra (if any).

settings: A collection of 0 to nSpectra FakeitSettings objects.

This may be entered as a list, a dictionary, a single FakeitSettings object, or None. If *settings* is a dictionary, the key,value pairs should be the spectrum index number (1 is lowest) and the FakeitSettings object.

This function will match up FakeitSettings objects 1-to-1 with the nSpectra fake spectra to be created.

If user provides FEWER than nSpectra FakeitSettings objects, fakeit will generate the necessary additional objects with their default settings.

If MORE than nSpectra FakeitSettings objects are provided, the extra objects will be ignored.

applyStats: If set to True, statistical fluctuations will be included in the generation of fake spectra. [bool]

filePrefix: Optional string to attach as a prefix to default fakeit output file names.

Note that this only applies when using the default file names. If a file name is explicitly entered in the FakeitSettings.fileName attribute, it will not make use of this.

no Write: If set to True, no fakeit output files will be generated. Default is False. [bool]

#### Examples:

```
# Assume no data is loaded, but a model is defined:
AllData.fakeit()
# Creates 1 fake spectrum using the default FakeitSettings object,
# which has all input strings empty. So it will use XSPEC's internal
# dummy response and its output file name will be dummy_rsp_1.fak.
# Now assume AllData contains 2 spectra PRIOR to running EACH of the
# following commands, then:
AllData.fakeit()
# Creates 2 fake spectra with all settings (response, arf,
# background, exposure, corrscale, backExposure, filenames) based
# on the original spectra. The original 2 spectra are removed from
# AllData.
AllData.fakeit(3)
# Creates the first 2 spectra as above. The 3rd fake spectrum is
# based on the default FakeitSettings object and its output filename
# will be dummy_rsp_3.fak
fs = FakeitSettings(background="back1.pha", exposure=2000.0)
sl = 3*[fs]
AllData.fakeit(3, sl)
# Same as above, but all 3 fake spectra will have a background file
# based on back1.pha, and exposure time = 2000.0 sec.
AllData.fakeit(3, sl, False, "my_fake_")
# Same as above, but no statistical fluctuations will be applied to
# fake spectra, and all output files will have the "my_fake_"
# prefix attached.
fs1 = FakeitSettings("resp1.rmf", "arf1.pha", exposure=1500.)
fs2 = FakeitSettings(fs1)
fs2.response = "resp2.rmf"
sd = \{3:fs1, 5:fs2\}
AllData.fakeit(5, sd)
# Creates 5 fake spectra. The first 2 use the settings from the
# originally loaded data. Spectra 3 and 5 use the settings from
# the fs1 and fs2 FakeitSettings objects, which differ only in their
# response names. Spectrum 4 uses the default FakeitSettings object.
```

#### ignore (ignoreRange)

Apply an ingore channels range to multiple loaded spectra.

#### Args:

ignoreRange: String specifying the spectra ranges and/or channel ranges to ignore, or "bad".

This follows the same syntax as used in the standard Xspec "ignore" command, except that the spectrum range always defaults to ALL spectra.

If the channel ranges are floats rather than ints, they will be treated as energies or wavelengths (depending on the *Plot* settings).

### notice (noticeRange)

Apply a notice channels range to multiple loaded spectra.

#### Args:

noticeRange: String specifying the spectra ranges and/or channel ranges to notice.

This follows the same syntax as used in the standard Xspec "notice" command, except that the spectrum range always defaults to ALL spectra.

If the numbers are floats rather than ints, they will be treated as energies or wavelengths (depending on the Plot settings). If the string is 'all', it will notice all channels in all spectra.

#### removeDummyrsp()

Remove all dummy responses, restore original responses (if any).

#### show()

Display information for all loaded spectra.

### nGroups

The number of data groups [int].

#### nSpectra

The number of loaded spectra [int].

## 3.1.6 FakeitSettings

```
class xspec.FakeitSettings (response='', arf='', background='', exposure='', correction='', backEx-
posure='', fileName='')
```

#### Fakeit command settings class.

The AllData.fakeit function will apply 1 FakeitSettings object to every fake spectrum that is to be created. If the user does not explicitly supply their own FakeitSettings objects, AllData.fakeit will create its own as necessary, with default settings.

#### Methods

init

#### **Attributes**

•response Name of detector response file to use for creating the fake spectrum.

When a fake spectrum is based on a pre-existing spectrum which already has a response, this should be left empty. If a name is given it will be IGNORED. However if the pre-existing spectrum has no response, then this MUST be filled.

If the fake spectrum is not based on an existing spectrum, this may be filled or left empty. If it is empty, XSPEC will just use its built-in dummy response.

- •arf Name of optional arf to use with the response. This is ignored if no response is given.
- background Name of optional background file to use when creating the fake spectrum.

If based on an original spectrum, leave this empty to use the original spectrum's background settings.

- •exposure The fake spectrum exposure time.
- •correction Optional correction norm factor.
- •backExposure Optional background exposure time modifier.

For *exposure* and *correction*, if left empty fakeit will use the values from the original spectrum, or 1.0 if not based on an original spectrum. Each of these may be entered as a string or float.

•fileName Optional fake spectrum output file name.

If left empty, fakeit will create a default file name based on the original spectrum, or the response name if no original spectrum. In the latter case, the default names will also have an incremented suffix to prevent file overwriting.

When writing to a multiple-spectrum output file (OGIP type-2), *exposure*, *correction*, *backExposure*, and *fileName* are applied to the entire file rather than a single spectrum. Therefore entries for these attributes will be IGNORED for all but the first fake spectrum in a type-2 output file.

```
__init__ (response='', arf='', background='', exposure='', correction='', backExposure='', file-
Name='')
Create a FakeitSettings object.
```

All arguments are optional, and all may be entered as strings. The *exposure* and *correction* arguments may also be entered as floats.

This can also create a new copy of a pre-existing FakeitSettings object, in which case the pre-existing object should be the only argument entered.

#### Examples:

```
fs1 = FakeitSettings("resp1.pha", exposure=1500.0)
# Reuse fs1's settings, but with a new fileName attribute:
fs2 = FakeitSettings(fs1)
fs2.fileName = "fakeit2.pha"
# Now generate 2 fake spectra
AllData.fakeit(2, [fs1, fs2])
```

## 3.1.7 FitManager

### class xspec.FitManager

### **Xspec fitting class.**

PyXspec automatically creates a single object of this class, named Fit.

### Methods

- •error
- •ftest
- goodness
- •improve
- •perform
- •renorm
- •show
- •steppar
- stepparResults

```
Attributes ((*) = get-only)
         bayes
         covariance*
         •criticalDelta
         •delta
         •dof*
         method
         nIterations
         •query
         statMethod
         •statTest
         •statistic*
         •testStatistic*
         •weight
error (argString)
```

Determine confidence intervals of a fit.

```
argString: A string with identical syntax to the standard interactive XSPEC error command.
    "[[stopat <ntrial> <toler>] [maximum <redchi>] [<delta fit statistic>] [<model param range>...]]"
   where <model param range> =::[<modelName>:]<first param> - <last param>
   See the XSPEC manual for a more detailed description.
```

The results of the error command are stored in the *error* attributes of the individual Parameter objects.

#### Examples:

```
# Estimate the 90% confidence ranges for parameters 1-3
Fit.error("1-3")
# Repeat but with delta fit statistic = 9.0, equivalent to the
# 3 sigma range.
Fit.error("9.0")
# Estimate for parameter 3 after setting the number of trials to 20.
# Note that the tolerance field has to be included (or skipped over).
Fit.error("stop 20,,3")
```

#### ftest (chisq2, dof2, chisq1, dof1)

Calculate the F-statistic and its probability given new and old values of chisq and number of degrees of freedom (DOF).

```
Args: chisq2: [float]
    dof2: [int]
    chisq1: [float]
    dof1: [int]
```

chisq2 and dof2 should come from a new fit, in which an extra model component was added to (or a frozen parameter thawed from) the model which gave *chisq1* and *dof1*. If the F-test probability is low then it is reasonable to add the extra model component.

Warning: It is not correct to use the F-test statistic to test for the presence of a line (see Protassov et al 2002, ApJ 571, 545).

Returns: The F-test probability [float].

```
goodness (nRealizations=100, sim=False)
```

Perform a Monte Carlo calculation of the goodness-of-fit.

**Args:** nRealizations: Number of spectra to simulate [int].

```
sim: flag [bool]
```

If False (default), all simulations are drawn from the best fit model parameter values. If True, parameters will be drawn from a Gaussian centered on the best fit.

### improve()

Try to find a new minimum.

When *Fit.method* is set to one of the MINUIT algorithms, this will run the MINUIT 'improve' command. This does nothing when Fit.method is set to Levenberg-Marquardt.

#### perform()

Perform a fit.

#### renorm (setting=None)

Renormalize the model to minimize statistic with current parameters.

**Args:** *setting*: [string]

If None, this will perform an explicit immediate renormalization. Other options determine when renormalization will be performed automatically. They are the following strings:

- 'auto': Renormalize after a model command or parameter change, and at the beginning of a fit
- 'prefit': Renormalize only at the beginning of a fit.
- 'none': Perform no automatic renormalizations.

### show()

Show fit information.

### steppar (argString)

Perform a steppar run.

Generate the statistic "surface" for 1 or more parameters.

#### Args:

```
argString: [string]
```

This uses identical syntax to the standard interactive XSPEC steppar command. "<step spec> [<step spec> ...]" where:

<step spec> ::= [<loglnolog>] [<currentlbest>] [<modName>:]<param index> <low
value> <high value> <# steps>

See the XSPEC manual for a more detailed description of specs.

### Examples:

```
# Step parameter 3 from 1.5 to 2.5 in 10 linear steps
Fit.steppar("3 1.5 2.5 10")
# Repeat the above but with logarithmic steps
Fit.steppar("log")
# Step parameter 2 linearly from -.2 to .2 in steps of .02
Fit.steppar("nolog 2 -.2 .2 20")
```

### stepparResults(arg)

Retrieve values from the most recent steppar run.

#### **Args:** arg:

argument should either be 'statistic', 'delstat', or a parameter specifier. A parameter specifier should be a string of the form:

```
'[<modName>:]<parNum>'
```

or simply an integer <parNum>.

Returns the requested values as a list of floats.

#### bayes

Turn Bayesian inference on or off [string].

Valid settings are 'on', 'off' (default), or 'cons'. 'cons' turns Bayesian inference on AND gives ALL parameters a constant prior. Priors can be set for parameters individually through the Parameter object's *prior* attribute.

#### covariance

The covariance matrix from the most recent fit [tuple of floats] (GET only).

As with standard XSPEC's "tclout covar", this only returns the diagonal and below-diagonal matrix elements.

#### criticalDelta

Critical delta for fit statistic convergence [float].

The absolute change in the fit statistic between iterations, less than which the fit is deemed to have converged.

#### delta

Set fit delta values to be proportional to the parameter value [float].

**Get:** Returns the current proportional setting, or 0.0 if currently using the fixed fit delta values.

**Set:** Enter the constant factor which will multiply the parameter value to produce a fit delta. A constant factor of 0.0 or negative will turn off the use of proportional fit deltas.

#### dof

The degrees of freedom for the fit [int] (GET only).

#### method

The fitting algorithm to use [string].

Choices are: 'leven', 'migrad', 'minimize', 'monte', 'simplex'. The default is 'leven'.

When setting the method, additional arguments for <nFitIterations> and <fit critical delta> may also be entered. Valid formats for entering multiple arguments are:

```
# Single string
Fit.method = "migrad 100 .05"
# List of strings
Fit.method = ["migrad","100",".05"]
# List of strings and numbers
Fit.method = ["migrad", 100, .05]
```

#### nIterations

The maximum number of fit iterations prior to query [int].

#### query

The fit query setting [string].

•'yes': Fit will continue through query.

•'no': Fit will end at query.

•'on': User will be prompted for "y/n" response.

#### statMethod

The type of fit statistic in use [string].

Valid names: 'chi' | 'cstat' | 'lstat' | 'pstat' | 'pstat' | 'whittle'. To set for individual spectra, add a spectrum number (or range) to the string: ie.

```
>>> Fit.statMethod = "cstat 2"
```

### statTest

The type of test statistic in use [string].

Valid names: 'ad' | 'chi' | 'cvm' | 'ks' | 'pchi' | 'runs'. To set for individual spectra, add a spectrum number (or range) to the string: ie.

```
>>> Fit.statTest = "ad 2"
```

#### statistic

Fit statistic value from the most recent fit [float] (GET only).

#### testStatistic

Test statistic value from the most recent fit [float] (GET only).

### weight

Change the weighting function used in the calculation of chi-sq [string].

Available functions: 'standard', 'gehrels', 'churazov', 'model'

### 3.1.8 **Model**

class xspec.Model (exprString, modName='', sourceNum=1, setPars=None)
 Xspec model class.

#### Methods

- •\_\_init\_\_
- •\_\_call\_\_ (the '()' operator)
- energies
- •folded
- •setPars
- •show
- •showList
- •untie
- values

### **Attributes** (all are get-only)

- •expression The model expression string, using full component names.
- •name The model name, optional in Xspec. This is an empty string for un-named models.
- •<components> Model includes an attribute of type Component for every Xspec component in the model. The attribute name is the same as the full name of the Xspec component (ie. m=Model("po") produces an m.powerlaw attribute).
- •componentNames List of component name strings.

•flux A tuple containing the results of the most recent flux calculation for this model.

The tuple values are: (*value*, *errLow*, *errHigh* (in ergs/cm^2), *value*, *errLow*, *errHigh* (in photons)). This will be filled in after an *AllModels.calcFlux()* call ONLY when no spectra are loaded. Otherwise results are stored in the Spectrum objects.

•lumin Same as flux but for luminosity calculations.

•nParameters Number of parameters in Model object [int].

•startParIndex Global index of the first parameter in this Model object [int].

```
__call__(parIdx)
```

Get a Parameter object from the Model.

**Args:** *parIdx*: The parameter index number.

Regardless of the data group to which the Model object belongs, its parameters are numbered from 1 to *nParameters*.

Returns the specified Parameter object.

```
__init__ (exprString, modName='', sourceNum=1, setPars=None)
Model constructor.
```

New model is automatically added to the *AllModels* container, with one Model object constructed (internally) for each data group to which the model applies. This function returns the Model object corresponding to the lowest numbered data group.

**Args:** *exprString*: The model expression string.

Component names may be abbreviated.

modName: Optional name assigned to model.

Any whitespace in string will be removed. This is required if source number is > 1.

sourceNum: Optional integer for model's source number.

setPars: Optional initial values for the model's parameters.

These may be sent in a tuple, list, or dictionary (or as a single float or string if only setting the first parameter). Examples:

```
# Create a model with all default parameter settings:
m1 = Model("gauss")

# Create wabs*powerlaw and initialize pars 1 and 3 to
# something other than their default values.
m2 = Model("wa*po", setPars={1:5.5, 3:".18,,.01,.02"})

# Create another model named 'b', and reset par 2 to 5.0:
m3 = Model("wa*bbody", "b", setPars={2:5.0})
```

If any mistakes are made with the optional *setPars* parameter arguments, the model will be created using all default values.

You can always reset the parameters later with the *Model.setPars()* method, or directly through the Parameter object's *values* attribute.

#### energies (spectrumIndex)

Get the Model object's energies array for a given spectrum.

Args: spectrumIndex: The spectrum index number.

If this is 0, it will return the energies array used by the default dummy response.

Returns a list of energy array elements, the size will be 1 larger than the corresponding flux array.

This will return the energies array as specified by the *AllModels.setEnergies* function if that has been used to override the response energies array.

#### folded (spectrumIndex)

Get the Model object's folded flux array for a given spectrum.

Args: spectrumIndex: The spectrum index number.

This number should be 0 if model is not presently applied to any spectra (ie. in the "off" state).

Returns a list of folded flux array elements.

### setPars (\*parVals)

Change the value of multiple parameters in a single function call.

This is a quick way to change multiple parameter values at a time since only a SINGLE model recalculation will be performed at the end. In contrast, when parameter values are changed through the individual parameter objects, the model is recalculated after EACH parameter change. (See also *AllModels.setPars()*, for changing multiple parameters belonging to multiple model objects.)

Args: parVals: An arbitrary number of parameter values.

These may be listed singly (as floats or strings), or collected into tuple, list or dictionary containers. Dictionaries must be used if parameters are not in consecutive order, in which case the parameter index number is the dictionary key.

Examples: Assume we have a model object m1 with 5 parameters.

Simplest case: change only the parameter values (and not the auxiliary values, 'sigma', 'min', 'bot', etc.), and change them in consecutive order:

```
# Pass in 1 or more floats
m1.setPars(5.5, 7.83, 4.1e2) # changes pars 1-3
m1.setPars(2.0, 1.3e-5, -.05, 6.34, 9.2) # changes all 5 pars
```

Still changing only the parameter values, but skipping over some:

```
m1.setPars(.02, 4.4, {5:3.2e5}) # changes pars 1-2, 5
m1.setPars({2:3.0, 4:-1.2}) # changes pars 2, 4
m1.setPars({2:1.8}, 9.3, 5.32) # changes pars 2, 3, 4
```

Now also change the auxiliary values for some of the parameters. Pass in a STRING containing "<val>,<sigma>,<min>,<bottom>,<top>,<max>" This uses the same syntax as Standard XSPEC's "newpar" command. Aux values can be skipped by using multiple commas:

```
# This sets a new <val>, <sigma>, and <max> for parameter 1, and
# a new <val> of 5.3 for parameter 2.
m1.setPars(".3,.01,,,,100", 5.3)

# This sets all new auxiliary values for parameter 3.
m1.setPars({3:".8 -.01 1e-4 1e-3 1e5 1e6"})
```

#### show()

Display information for a single Model object.

#### static showList()

Show the list of all available XSPEC model components.

```
untie()
```

Remove links for all parameters in Model object

#### values (spectrumIndex)

Get the Model object's values array for a given spectrum.

**Args:** *spectrumIndex*: The spectrum index number.

This number should be 0 if model is not presently applied to any spectra (ie. in the "off" state).

Returns the values array as a list.

### 3.1.9 ModelManager

#### class xspec. ModelManager

#### Models container.

PyXspec automatically creates a single object of this class, named AllModels.

#### Methods

- •\_\_call\_\_ (the '()' operator)
- •\_\_iadd\_\_ (the '+=' operator)
- •\_\_isub\_\_ (the '-=' operator)
- •addPyMod
- •calcFlux
- •calcLumin
- •clear
- •eqwidth
- initpackage
- •lmod
- •setEnergies
- •setPars
- •show
- •simpars
- •tclLoad

#### Attributes

- •sources (get-only)
- systematic

```
__call__(groupNum, modName='')
```

Get Model objects from the AllModels container.

Args: groupNum: The data group number to which the Model object corresponds.

*modName*: Optional string containing the Model's name (if any).

Returns the Model object.

```
___iadd___(modelInfo)
```

Define a new model and add it to the AllModels container.

This operation is equivalent to the Model class constructor, except that it does not return a Model object.

#### Args:

**modelInfo:** A string containing the model expression (component names may be abbreviated). The model will be unnamed and assigned to source number = 1.

OR

If supplying a model name and a source number, this should be a tuple with:

modelInfo[0] = model expression string

modelInfo[1] = model name string

modelInfo[2] = source number

```
isub (modName)
```

Remove all copies of the given model from the AllModels container.

Args:

**modName:** The name of the model to be removed, or an empty string if the model has no name. If set to "\*", this will behave like the *clear()* function and remove all models.

 $\verb"addPyMod" (func, parInfo, compType, calcsErrors = False, spectrumDependent = False)$ 

Add a user-defined Python model function to XSPEC's models library.

This provides a way to add to XSPEC local models written in Python. It performs the same role as the combination of *initpackage/lmod* commands do for C/C++/Fortran local models. The first 3 arguments (func, parInfo, and compType) are mandatory.

**Args:** func: The user-defined model function (Python type = 'function').

Function must define at least 3 arguments for energies, parameters, and flux.

A optional fourth argument may be added if your model calculates flux errors, and a fifth if your model requires that XSPEC pass it the spectrum number.

parInfo: A tuple of strings.

One string for each parameter your model requires. The format of these strings is identicalto what is placed in a 'model.dat' file (see Appendix C of the XSPEC manual).

*compType*: A string telling XSPEC the type of your model.

Currently allowed types: 'add', 'mul', 'con'

calcsErrors: OPTIONAL bool flag.

If your model function also calculates model errors, set this to True.

spectrumDependent: OPTIONAL bool flag.

Set this to True only if your model function has an explicit dependence on the spectrum.

**Example usage: A local additive model written in Python, named 'myModel',** which takes parameters named 'par1' and 'par2'.

calcFlux (cmdStr)

Calculate the model flux for a given energy range.

Args: cmdStr: string

Should contain the energy limit values and optional error specifiers. This follows the same syntax rules as the standard XSPEC 'flux' command.

The flux will be calculated for all loaded spectra, and the results will be stored in the Spectrum objects' flux attribute. If no spectra are loaded, the flux will be stored in the Model objects' flux attribute.

#### calcLumin (cmdStr)

Calculate the model luminosity for a given energy range and redshift.

**Args:** *cmdStr*: string

Should contain the energy limit values and optional error specifiers. This follows the same syntax rules as the standard XSPEC 'lumin' command.

The lumin will be calculated for all loaded spectra, and the results will be stored in the Spectrum objects' *lumin* attribute. If no spectra are loaded, the flux will be stored in the Model objects' *lumin* attribute.

#### clear()

Remove all models.

eqwidth (component, rangeFrac=None, err=False, number=None, level=None)

Calculate the equivalent width of a model component.

Please see the Standard XSPEC Manual for a discussion on how the eqwidth of a component is calculated.

### Args:

**component:** An integer specifying the model component number for which to calculate the eqwidth (left-most component is 1). If the component belongs to a NAMED model, then this must be a **string** of the form "<modelName>:<compNumber>".

rangeFrac: Determines the energy range for the continuum calculation.

Range will be from E(1-<rangeFrac>) to E(1+<rangeFrac>) where E is the location of the peak of the photon spectrum. The initial default rangeFrac is 0.05. Setting this will change the future default value.

err: Bool flag.

If set to True, errors will be estimated on the equivalent width calculation. This will also require the setting of the "number" and "level" arguments.

number: Only set this if err = True.

This determines the number of sets of randomized parameter values to draw to make the error estimation. [int]

*level*: Only set this if *err* = True.

The error algorithm will order the equivalent widths of the *number* sets of parameter values, and the central *level* percent will determine the error range. [float]

The results of the most recent eqwidth calculation are stored as attributes of the currently loaded Spectrum objects.

 $\verb|initpackage| (packageName, modDescrFile, dirPath=None, udmget=False)|$ 

Initialize a package of local models.

Use this method to compile your local model source code and build a library, which can then be loaded into XSPEC with the *lmod* method.

Args: packageName: The name of the model package [string].

The name should be all lower-case and contain NO numerals or spaces. The local models library file will be based upon this name, and this is also the name you will use when loading the library with the *lmod* method.

modDescrFile: Name of your local model description file [string].

This file is typically named 'lmodel.dat', but you're free to name it something else.

dirPath: Optional directory path to your local models [string].

This may be an absolute or relative path. If you don't enter this argument, XSPEC will look in the directory given by the LOCAL\_MODEL\_DIRECTORY in your Xspec.init start-up file.

udmget: Optional bool flag.

Set this True only when your models need to call XSPEC's udmget function. Udmget is a function for allocating dynamic memory in Fortran routines, and is no longer used within XSPEC itself. If this flag is set to 'True', initpackage will copy the necessary files and build the udmget function within your local models directory.

lmod (packageName, dirPath=None)

Load a local models library.

**Args:** packageName: The name of the model package to be loaded.

This is the same name that is the first argument in the *initpackage* command.

dirPath: An optional string argument.

This should specify the (absolute or relative) path to the local model directory. If this argument is not entered, XSPEC will look in the directory given by the LO-CAL\_MODEL\_DIRECTORY in the Xspec.init start-up file.

```
setEnergies (arg1, arg2=None)
```

Specify new energy binning for model fluxes.

Supply an energy binning array to be used in model evalutations in place of the associated response energies, or add an extension to the response energies.

**Args:** *arg1*: A string containing either:

"<range specifier> [<additional range specifiers>...]"

"<name of input ascii file>"

"extend" [This option also uses arg2]

"reset"

where the first <range specifier> ::= <lowE> <highE> <nBins> logllin

<additional range specifier> ::= <highE> <nBins> logllin

This uses the same syntax as standard XSPEC's 'energies' command. Values can be delimited by spaces or commas.

arg2: String only needed when arg1 is "extend".

This requires an extension specifier string of the form: "lowlhigh <energy> <nBins> logllin"

All energies are in keV. Multiple ranges may be specified to allow for varied binning in different segments of the array, but note that no gaps are allowed in the overall array. Therefore only the first range specifier accepts a <lowE> parameter. Additional ranges will automatically begin at the <highE> value of the previous range.

With the "extend" option, the specifier string supplied to *arg2* will extend the existing response energy array by an additional <nBins> to the new <energy>, in either the high or low direction.

Once an energy array is specified, it will apply to all models and will be used in place of any response energy array (from actual or dummy responses) for calculating and binning the model flux. It will also apply to any models that are created after it is specified. To turn off this behavior and return all models back to using their response energies, set *arg1* to "reset".

*arg1* can also be the name of an ascii text file containing a custom energy array. To see the proper file format, and for more details in general about the 'energies' command, please see the standard XSPEC manual.

#### Examples:

```
# Create an array of 1000 logarithmic-spaced bins, from .1 to 50. keV
AllModels.setEnergies(".1 50. 1000 log")
# Change it to 500 bins
AllModels.setEnergies(",,500")
# Now restore original response energies, but with an extension of the
# high end to 75.0 keV with 100 additional linear bins.
AllModels.setEnergies("extend","high,75.,100 lin")
# Return to using original response energies with no extensions.
AllModels.setEnergies("reset")
```

#### setPars(\*args)

Change the value of multiple parameters from multiple model objects with a single function call.

This is a quick way to change multiple parameter values at a time since only a SINGLE recalculation will be performed at the end. In contrast, when parameter values are changed through the individual parameter objects, the model is recalculated after EACH parameter change. (If all the parameters belong to a single model object, you can also use the *Model.setPars()* function.)

args: An arbitrary number model objects and parameter values.

The first argument must be model object, followed by one or more of its new parameter values. Additional groups of model objects and parameter values may follow.

The parameter values follow the same syntax rules as with the single *Model.setPars()* function. They can be listed singly (as floats or strings), or collected into tuple, list, or dictionary containers. Dictionaries must be used when parameters are not in consecutive order, in which case the parameter index number is the dictionary key.

Parameter indices are local to each model object. That is, they are always numbered from 1 to N where N is the number of parameters in the model object.

#### Examples:

```
# Assume we've already assigned a 3 parameter model to 2 data groups:
m1 = AllModels(1)
m2 = AllModels(2)

# Various ways of changing parameters in consecutive order.

# This changes pars 1-2 in m1 and 1-3 in m2:
AllModels.setPars(m1, .4, "1.3 -.01", m2, "5.3 ,,3.0e-4", 2.2, 1.9)
# ...and these 2 examples do the exact same thing as above:
valList = [.4, "1.3 -.01"]
valTuple = ("5.3 ,,3.0e-4", 2.2, 1.9)
AllModels.setPars(m1, valList, m2, valTuple)
AllModels.setPars(m1, valList, m2,"5.3 ,,3.0e-4", [2.2, 1.9])
```

```
# Parameters in non-consecutive order, must use Python
# dictionaries:

# Change parameter 2 in m1, parameter 1 and 3 in m2:
AllModels.setPars(m1, {2:8.3}, m2, {1:0.99, 3:"7.15 -.01"})
# ...same thing as above:
AllModels.setPars(m1, {2:8.3}, m2, 0.99, {3:"7.15 -.01"})

# Note that identical syntax is used for model objects belonging
# to different sources. All of the above examples are still valid
# had we obtained m1 and m2 like this:

m1 = Model("wabs*pow", "firstMod", 1)
m2 = Model("gauss", "secondMod", 2)
```

#### show (parIDs=None)

Show all or a subset of Xspec model parameters.

#### Args:

*parIDs*: An optional string specifying a range of parameters as with Xspec's "show parameter" function. If no string is supplied, this will show all parameters in all models.

#### simpars()

Create a list of simulated parameter values.

Values are drawn from a multivariate normal distribution based on the covariance matrix from the last fit, or from Monte Carlo Markov chains if they are loaded. This method is identical to doing 'tclout simpars' in standard XSPEC.

Returns a tuple of the simulated parameter values.

### tclLoad (fullLibPath)

Load a local model library by calling Tcl's 'load' command.

This by-passes *lmod* (with its pkgIndex.tcl requirements) and allows the user to load a local model by directly calling Tcl's lower level 'load' command. May also be useful for error diagnostics when *lmod* has failed.

**Args:** *fullLibPath*: The full local model library path and filename.

### sources

A dictionary containing the currently active <source number>:<model name> assignments.

If the model has no name, <model name> will be an empty string. (GET only)

### systematic

The fractional model systematic error.

This will be added in quadrature to the error on the data when evaluating chi-squared. The default value is zero.

#### 3.1.10 Parameter

class xspec.Parameter (parName, parStrategy)

Model or response parameter class.

#### Methods

•untie

```
Attributes ((*) = get-only)
    •error*
    •frozen
    •index*
    •link
    •name*
    prior
    •sigma*
    •unit*
    values
untie()
     Remove parameter link (if any)
error
     A tuple containing the results of the most recent fit error command performed on the parameter (GET
     only). The tuple values are: (<error low bound>, <error high bound>, <error status code string>)
frozen
     Bool, if True then parameter is frozen.
index
     Position of the parameter within the Model object.
     (The first parameter has index = 1) Note that this is the same value that would be used to obtain a Parameter
     object from its Model, ie: par = mod(<index>) (GET only).
link
     Parameter link expression string (empty if not linked).
name
     Name of Parameter (GET only).
prior
     A tuple containing the settings for the prior used when Bayesian inference is turned on.
     Get: Returns a tuple containing: (<pri>riorType>, <optional hyperparameters>)
     Set with: string: <pri><pri><pri>Type></pr>
          or tuple: (<priorType>, <optional hyperparameters>)
          Valid priorTypes are 'cons', 'exp', 'jeffreys', 'gauss'. Hyperparameters should be entered as floats.
sigma
     The Parameter fit sigma (-1.0 when not applicable) (GET only).
unit
     An optional string for the parameter's units (GET only).
values
     List of value floats [val,delta,min,bot,top,max].
     This may be set with: string: x.values = "3.2,,,,1e2, 1e3"
          single float: x.values = 4.1 (sets 'val' only)
          tuple: x.values = 8.2,.02, -10.
```

3.1. Classes 49

Note that Tuple and List input do not allow the use of consecutive commas for argument spacing.

list: x.values = [8.2, .02, -10.]

class xspec.PlotManager (deviceStr)

### 3.1.11 PlotManager

```
Xspec plotting class.
PyXspec automatically creates a single object of this class, named Plot.
Methods
    •__call__ (the '()' operator)
    \bullet add Command\\
    {\color{red}\bullet} background Vals
    •delCommand
    •iplot
    •model
    •noID
    •setGroup
    •setID
    •setRebin
    •show
    \bullet_{\rm X}
    •xErr
    •y
    •yErr
Attributes
    •add
    •area
    •background
    •commands
    device
    •perHz
    •redshift
    •splashPage
    •xAxis
    •xLog
    •yLog
  _call___(*panes)
     Display the plot.
     Input 1 or more plot command strings.
     Examples:
     # Single Plots:
     Plot("data")
     Plot("model")
     Plot("ufspec")
     # Multiple Plots (or single plots taking additional arguments):
     Plot("data", "model", "resid")
     Plot("data model resid")
```

Plot("data", "model m1") # Plots data and a model named "m1".

# To repeat a plot using the previously entered arguments, simply do:

Plot("data, model, resid")

Plot()

#### addCommand (cmd)

Add a plot command [string] to the end of the plot commands list.

#### backgroundVals (plotGroup=1, plotWindow=1)

Return a list of background data values for a plot group and plot window

Background value arrays only exist for data plots when the *Plot.background* flag is set to True.

#### delCommand (num)

Remove a plot command by (1-based) number [int].

This is intended for removal of single commands. To remove ALL commands, set the *Plot.commands* attribute to an empty tuple, ie:

```
>>> Plot.commands = ()
```

#### iplot (\*panes)

Display the plot and leave it in interactive plotting mode.

This function takes the same arguments and syntax as when displaying plots in the regular mode (through Plot's \_\_call\_\_ method). Examples:

```
Plot.iplot("data") # 1-panel data plot
Plot.iplot("data model") # 2-panel data and model
Plot.iplot() # Repeats the previous plot.
```

#### model (plotGroup=1, plotWindow=1)

Return a list of Y-coordinate model values for a plot group and plot window

#### noID()

Turn off the plotting of line IDs.

#### setGroup (groupStr)

Define a range of spectra to be in the same plot group.

Input argument is a string specifying one or more ranges, delimited by commas and/or spaces. Examples:

```
# Spectra 1-3 in plot group 1, 4-6 in group 2.
Plot.setGroup("1-3 4-6")

# Spectra 1, 2, and 4 are each now in their own group.
Plot.setGroup("1,2 4")

# All spectra are in a single plot group.
Plot.setGroup("1-**")

# If input argument is Python's 'None' variable, all
# plot grouping will be removed.
Plot.setGroup(None)
```

### **setID** (temperature=None, emissivity=None, redshift=None)

Switch on plotting of line IDs.

All input arguments are floats and are optional. If they are omitted they will retain their previous values.

- •temperature: Selects the temperature of the APEC line list.
- •emissitivity: Only lines with emissivities above this setting will be displayed.
- •redshift: Line display will be redshifted by this amount.

To turn off plotting of line IDs, use the *noID()* function.

```
setRebin (minSig=None, maxBins=None, groupNum=None, errType=None)
```

Define characteristics used in rebinning the data (for plotting purposes ONLY).

All input arguments are optional. If they are omitted they will retain their previous values.

- •minSig: Bins will be combined until this minimum significance is reached (in units of sigma). [float]
- •maxBins: The maximum number of bins to combine in attempt to reach minSig. [int]
- groupNum: The plot group number to which this setting applies. If number is negative, it will apply to ALL plot groups. [int]
- •errType: Specifies how to calculate the error bars on the new bins. Valid entries are "quad", "sqrt", "poiss-1","poiss-2", "poiss-3". [string] See the "setplot" description in the XSPEC manual for more information.

#### show()

Display current plot settings

#### $\mathbf{x}$ (plotGroup=1, plotWindow=1)

Return a list of X-coordinate data values for a plot group and plot window

### xErr (plotGroup=1, plotWindow=1)

Return a list of X-coordinate errors for a plot group and plot window

### y (plotGroup=1, plotWindow=1)

Return a list of Y-coordinate data values for a plot group and plot window

#### yErr (plotGroup=1, plotWindow=1)

Return a list of Y-coordinate errors for a plot group and plot window

#### add

Turn on/off the display of individual additive components [bool].

### area

Toggle displaying the data divided by the response effective area for each channel [bool].

#### background

Toggle displaying the background spectrum (if any) when plotting data [bool].

#### commands

### Custom plot commands to be appended to Xspec-generated commands.

Get: Returns a tuple of the currently entered command strings.

Set: Replaces all commands with the new tuple of strings.

#### To remove ALL plot commands, set to an empty tuple, ie:

```
>>> Plot.commands = ()
```

For inserting and deleting individual commands, use addCommand and delCommand functions.

#### device

The plotting device name [string].

### perHz

Toggle displaying Y-axis units per Hz when using wavelength units for X-axis [bool].

#### redshift

Apply a redshift to the X-axis energy or wavelength values [float].

This will multiply X-axis energies by a factor of (1+z) to allow for viewing in the source frame. Y-axis values will be equally affected in plots which are normalized by energy or wavelength. Note that this is not

connected in any way to redshift parameters in the model (or the setplot id redshift parameter) and should only be used for illustrative purposes.

### splashPage

When set to False, the usual XSPEC version and build data information will not be printed to the screen when the first plot window is initially opened [bool].

#### xAxis

X-Axis Units [string].

Valid options are: "channel", (energies) "keV", "MeV", "GeV", "Hz", (wavelengths) "angstrom", "cm", "micron", nm"

These are case-insensitive and may be abbreviated.

This setting also affects the ignore/notice range interpretation.

### xLog

Set the x-axis to logarithmic or linear for energy or wavelength plots [bool].

*xLog* has no effect on plots in channel space. *xLog* and *yLog* will not work for model-related plots (eg. *model*, *ufspec*, and their variants) as their axes are always set to log scale.

#### yLog

See xLog.

### 3.1.12 Response

class xspec.Response (parent, respTuple)

Detector response class.

#### Methods

setPars

show

**Attributes** (get-only unless stated otherwise)

- •arf Get/Set the arf filename string. Enter None or empty string to remove an existing arf.
- •chanEnergies Tuple of floats, the detector channel energies in keV. These are the energies normally stored in the EBOUNDS extension.
- •energies Tuple of floats, the photon energies in keV. These are the energies normally stored in the MATRIX extension.
- •gain A response model object (class RModel) for applying a shift in response file gain.

(Also see Response.setPars() for setting multiple gain parameters at a time.)

When gain is turned ON, it creates two variable fit Parameter object members:

```
>>> gain.slope # (default = 1.0)
>>> gain.offset # (default = 0.0)
```

To turn gain ON simply assign a value to EITHER parameter, ie.:

```
>>> gain.slope = 1.05
```

This automatically also creates a *gain.offset* parameter with default value 0.0, which you may want to re-adjust. Examples:

```
>>> gain.offset = .02
>>> gain.offset.values = ".015,.001,,,,0.1"
```

*slope* and *offset* are of the same type as regular model parameters, and therefore have the same functions, attributes, and syntax rules for setting values. (See the Parameter class help for more details.)

To turn gain OFF, call its off() method:

```
>>> gain.off()
```

gain.off() restores the response to its original state, and renders the slope and offset parameters inaccessible.

•rmf The response file name string.

•sourceNumber The 1-based source number for which the response is assigned. This is normally always 1 unless multiple sources are loaded for multiple-model evaluation.

```
setPars (*seqPars)
```

Set multiple response parameters with a single function call.

Similar to the *Model.setPars()* function, this allows multiple response parameters to be changed with just a SINGLE recalculation performed at the end.

#### Args:

**seqPars:** An arbitrary number of CONSECUTIVE parameter values to be matched 1-to-1 with the response model's parameters.

Currently just 1 response model is available (gain), which has 2 response parameters (slope and offset).

### Examples:

```
s = Spectrum("file1")
resp = s.response
# 'gain' is off by default and response parameters don't yet exist.
   The following call automatically turns 'gain' on and creates
   both 'slope' and 'offset' parameters even though it is only
   assigning to 'slope'. 'offset' will retain its default value
   of 0.0.
resp.setPars(1.05) # Equivalent to doing: resp.gain.slope = 1.05
# This is equivalent to: resp.gain.slope = .995
                        resp.gain.offset = .08
   except that the recalculation is only performed at the end
   rather than after each parameter is changed:
resp.setPars(.995, .08)
# Can also assign auxiliary values by passing 1 or 2 string
# arguments.
resp.setPars("1.1,,.02,.02,1.8,1.8","-.05,,-2,-2")
# Remove gain and restore response to original state:
resp.gain.off()
```

#### show()

Display response information including (optional) response parameters.

### 3.1.13 RModel

class xspec.RModel (resp, parNames, rmodName)

### Response Model class.

Response models are functions which act upon the detector RMF. XSPEC currently has just one response model: *gain*, which is a built-in attribute of the Response class. RModel objects are not intended for stand-alone creation: its \_\_init\_\_ function should be considered private.

#### **Attributes**

•**exparameters>** When RModel is ON, it contains an attribute of type Parameter for every parameter in the model. An RModel is turned ON by a 'set' operation on ANY of its parameters. For example with the *gain* RModel:

```
>>> resp.gain.offset = .03
```

automatically creates *offset* AND *slope* parameters if they don't already exist (*slope* would be initialized to its default value of 1.0). The shift is then applied immediately to the Response object *resp*.

When RModel is OFF (see the *RModel.off()* method), the parameters are not accessible.

•isOn Boolean flag showing the On/Off status of the RModel (get only).

•parameterNames List of the response model's parameter names (get only).

off()

Remove response parameters and turn the model OFF.

The Response is restored to its original state.

is0n

On/Off indicator for RModel object.

### 3.1.14 Spectrum

```
class xspec.Spectrum(dataFile)
```

Spectral data class.

#### Methods

- •\_\_init\_\_
- •dummyrsp
- •ignore
- •ignoredString
- notice
- noticedString
- •show

### **Attributes** ((\*) = get-only)

- •areaScale\*
- •background
- •backScale\*
- •cornorm
- correction
- •dataGroup\*
- •energies\*
- eqwidth\*

```
•exposure*
•fileName*
•fileName*
•flux*
•ignored*
•index*
•isPoisson*
•lumin*
•multiresponse
•noticed*
•rate*
•response
•values*
•variance*
_init___(dataFile)
Construct a Spectrum object.
```

Read in a spectrum and any associated background, response and arf files. Spectrum is automatically added to the *AllData* container.

**Args:** dataFile: Spectral data filename [string].

```
dummyrsp(lowE=None, highE=None, nBins=None, scaleType=None, chanOffset=None, chan-
Width=None, sourceNum=1)
```

Create a dummy response for this spectrum only.

```
Args (all are optional): lowE: Input response energy lower bound, in keV. [float]
```

```
highE: Input response energy higher bound, in keV. [float]
```

*nBins*: Number of bins into which the energy range is divided. [int]

```
scaleType: 'log' or 'lin'. [string]
```

chanOffset: Starting value of dummy channel energies. [float]

chanWidth: Energy width of the channel bins. [float]

If *chanWidth* is set to 0, the dummy response can only be used for evaluating model arrays, and not for fitting to spectra.

sourceNum: Optional source number for the dummy response. [int]

### Examples:

```
# All values are optional, use keywords to enter values
# non-consecutively. Unspecified values revert to the
# current defaults.
s = Spectrum("dataFile.pha")
s.dummyrsp(.3, 30., 100, chanWidth=.5)
s.dummyrsp(highE = 50., sourceNum = 2)
s.dummyrsp(.1,10.,100,"lin",.0, 1.0, 1)
```

Initial defaults: lowE = .1, highE = 50., nBins = 50, scaleType = "log" chanOffset = .0, chanWidth = .0, sourceNum = 1

The defaults for *lowE*, *highE*, *nBins*, *scaleType*, and *chanOffset* will be modified for each explicit new entry. *chanWidth* always defaults to 0 and *sourceNum* always defaults to 1.

To remove the spectrum's dummy response(s) and restore actual responses (if any), call *All-Data.removeDummyrsp()*.

#### ignore (ignoreRange)

Ignore a range of the spectrum by channels or energy/wavelengths.

Args: ignoreRange: String specifying the channel range to ignore.

This follows the same syntax as used in the standard Xspec "ignore" command. If the numbers are floats rather than ints, they will be treated as energies or wavelengths (depending on the *Plot* settings).

Note that "bad" will not work from here, as it can only be applied to ALL of the loaded spectra.

To apply range(s) to multiple spectra, use the *AllData* ignore function.

#### ignoredString()

Return a string of ignored channel ranges.

This produces a string in compact (hyphenated) form, which can be used as input to a subsequent 'ignore' command. Example:

If ignored channels are [1,3,4,5,7], this function will output "1 3-5 7".

#### notice (noticeRange)

Notice a range of the spectrum by channels or energy/wavelengths.

**Args:** *noticeRange*: String specifying the channel range to notice.

This follows the same syntax as used in the standard Xspec "notice" command. If the numbers are floats rather than ints, they will be treated as energies or wavelengths (depending on the *Plot* settings). If the string is "all", it will notice all channels in spectrum.

To apply range(s) to multiple spectra, use the AllData notice function.

#### noticedString()

Return a string of noticed channel ranges.

This produces a string in compact (hyphenated) form, which can be used as input to a subsequent 'notice' command. Example:

If noticed channels are [1,3,4,5,7], this function will output "1 3-5 7".

#### show()

Display information for this Spectrum object

#### areaScale

The Spectrum area scaling factor.

This is either a single float (if file stores it as a keyword), or a tuple of floats (if file stores column).

#### backScale

The Spectrum background scaling factor.

This is either a single float (if file stores it as a keyword), or a tuple of floats (if file stores column).

### background

Get/Set the spectrum's background.

**Get:** Returns the Background object associated with the Spectrum. If Spectrum has no background object, this will raise an Exception.

**Set:** Supply a background filename [string]. This will become the new background to the Spectrum object, and any previously existing background will be removed. If string is empty, all whitespace, or the Python None variable, the background (if any) will be removed.

#### cornorm

Get/Set the normalization of a spectrum's correction file. [float]

#### correction

Get/Set the correction file.

**Get:** Returns the Spectrum's current correction information as an object of class Background. This raises an Exception if Spectrum has no correction.

**Set:** Enter the filename string for the new correction. This will remove any previously existing correction. Returns the new correction info as an object of class Background. If string is "none", empty, or all whitespace, the current correction will be removed and this will return None.

#### dataGroup

The data group to which the spectrum belongs [int].

### energies

Tuple of pairs of floats (also implemented as tuples) giving the E\_Min and E\_Max of each noticed channel.

#### eqwidth

Tuple of 3 floats containing the results of the most recent eqwidth calculation for this spectrum (performed with the *AllModels.eqwidth* method).

The results are stored as: [0] - eqwidth calculation

- [1] eqwidth error lower bound
- [2] eqwidth error upper bound

The error bounds will be 0.0 if no error calculation was performed, and all will be 0.0 if eqwidth wasn't performed for this spectrum.

#### exposure

The exposure time keyword value [float].

#### fileName

The spectrum's file name [string].

#### flux

A tuple containing the results of the most recent flux calculation for this spectrum.

The tuple values are: (value, errLow, errHigh (in ergs/cm<sup>2</sup>), value, errLow, errHigh (in photons)) for each model applied to the spectrum.

### ignored

A list of the currently ignored (1-based) channel numbers.

#### index

The spectrum's current index number within the AllData container [int].

#### isPoisson

Boolean flag, true if spectrum has Poisson errors.

#### lumir

Similar to flux, the results of the most recent luminosity calculation.

#### multiresponse

Get/Set detector response ARRAY elements when using multiple sources.

This is for use only when assigning multiple responses to a spectrum, for multi-source/multi-model analysis. For standard single-source analysis, use the *response* attribute instead.

You must provide an array index for all *multiresponse* get/set operations. Note that array indices ARE 0-BASED, so multiresponse[0] corresponds to source 1. Examples:

```
# Get the response assigned to source 1.
# This particular call is the same as doing
# "r1 = s.response"
r1 = spec.multiresponse[0]

# Get the response for the second source.
# Can only do this with multiresponse.
r2 = spec.multiresponse[1]

# Define a third source by adding a new response:
spec.multiresponse[2] = "myResp3.pha"

# Now remove the response for the second source:
spec.multiresponse[1] = None
```

#### noticed

A list of the currently noticed (1-based) channel numbers.

#### rate

A tuple containing the total Spectrum rates in counts/sec.

The tuple consists of: [0] - current net rate (w/ background subtracted),

- [1] net rate variance,
- [2] total rate (without background),
- [3] predicted model rate

#### response

Get/Set the detector response.

Use this for standard SINGLE-SOURCE analysis. To add other responses for multi-source and multi-model analysis, use the *multiresponse* attribute.

Get: Returns a Response object, or raises an Exception if none exists

Set: Supply a response filename string. To remove a response, supply an empty string or None.

#### values

Tuple of floats containing the spectrum rates for noticed channels in counts/cm<sup>2</sup>-sec.

#### variance

Tuple of floats containing the variance of each noticed channel.

# 3.1.15 XspecSettings

#### class xspec.XspecSettings

Storage class for Xspec settings.

PyXspec automatically creates a single object of this class, named Xset.

#### Methods

- •addModelString
- •closeLog
- delModelString
- •openLog
- restore

•save

#### **Attributes** ((\*) = get-only)

- •abund
- •allowNewAttributes
- •allowPrompting
- •chatter
- logChatter
- •cosmo
- •log\*
- modelStrings
- parallel
- •seed
- version\*
- xsect

### addModelString(key, value)

Add a key, value pair of strings to XSPEC's internal database.

This database provides a way to pass string values to certain model functions which are hardcoded to search for "key". (See the XSPEC manual description for the "xset" command for a table showing model/key usage.)

If the key, value pair already exists, it will be replaced with the new entries.

#### closeLog()

Close XSPEC's current log file.

#### delModelString(key)

Remove a key, value pair from XSPEC's internal string database.

### openLog(fileName)

Open a file and set it to be XSPEC's log file.

**Args:** *fileName*: The name of the log file.

If Xspec already has an open log file, it will close it. Returns a Python file object for the new log file.

Once opened, the log file object is also stored as the *Xset.log* attribute.

**Note:** To ensure proper cleanup and file flushing, it is recommended that you call *Xset.closeLog(fileName)* before exiting PyXspec.

#### restore(fileName)

Restore the data/model configuration and settings.

This will restore the data, models, and settings from a previous PyXspec session, as saved in file generated by the *Xset.save()* function.

**Args:** *fileName*: The output file from a previous *Xset.save* command.

#### save (fileName, info='a')

Save the data and model configuration and XSPEC settings

**Args:** *fileName*: The name of the output file.

If the file name has no extension, '.xcm' will be appended.

info: A flag specifying which information to save:

• 'a' = save all (the default)

- 'f' = only save the data files information
- 'm' = only save the model information

#### abund

Get/Set the abundance table used in the plasma emission and photoelectric absorption models [string].

```
Valid tables: 'angr', 'aspl', 'feld', 'aneb', 'grsa', 'wilm', 'lodd', 'file <filename>'
```

#### allowNewAttributes

Get/Set the flag which allows the setting of new instance attributes for ALL PyXspec classes [bool].

This is False by default, and is intended to catch the user's attention if they misspell an attribute name when attempting to set it. Under normal Python behavior, a misspelling would simply create a new attribute and issue no warnings or errors.

You must make sure this flag is set to True if you genuinely wish to add new attributes.

#### allowPrompting

Get/Set flag determining whether user prompting occurs.

Get/Set whether user will be prompted in situations where XSPEC may require additional information to complete a task. Default is 'True'. [bool]

#### chatter

Get/Set the console chatter level [int].

#### cosmo

Get/Set the cosmology values.

### Get: Returns a tuple of floats containing (H0, q0, l0), where

- H0 is the Hubble constant in km/(s-Mpc),
- q0 is the deceleration parameter, and
- 10 is the cosmological constant.

Set: Enter a single string containing one or more of H0, q0, 10.

#### Examples:

```
Xset.cosmo = "100" # sets H0 to 100.0
Xset.cosmo = ",0" # sets q0 to 0.0
Xset.cosmo = ",0.7" # sets 10 to 0.7
Xset.cosmo = "50 .5 0." # sets H0=50.0, q0=0.5, 10=0.0
```

#### log

Get only: Returns the currently opened log file object, or None if no log file is open (also see the *openLog* and *closeLog* methods).

### logChatter

Get/Set the log chatter level [int].

### modelStrings

XSPEC's internal database of <string\_name>, <string\_value> pairs for settings which may be accessed by model functions.

**Get:** Returns a tuple of tuples, the inner tuples being composed of <string\_name>,<string\_value> string pairs.

**Set:** Replaces ENTIRE database with user-supplied new database. Input may be a dictionary of <a href="mailto:<a href="mailto:string\_name">string\_value</a> entries, or a tuple of (<a href="mailto:string\_name">string\_value</a>) tuples.

For inserting and deleting INDIVIDUAL string name and value pairs, use the *addModelString* and *delModelString* methods.

#### parallel

An attribute for controlling the number of parallel processes in use during various XSPEC contexts.

### Examples:

```
# Use up to 4 parallel processes during
# Levenberg-Marquardt fitting.
Xset.parallel.leven = 4

# Use up to 4 parallel processes during
# Fit.error() command runs.
Xset.parallel.error = 4

# Reset all contexts to single process usage.
Xset.parallel.reset()
```

#### seed

Re-seed and re-initialize XSPEC's random-number generator with the supplied integer value (SET only).

#### version

The version strings for PyXspec and standard XSPEC.

GET only, this returns a tuple containing:

(<PyXspec version string>,<standard XSPEC version string>)

#### xsect

Get/set the photoelectric absorption cross-sections in use [string].

Available options: 'bcmc', 'obcm', 'vern'

**CHAPTER** 

### **FOUR**

### **NOTES**

### 4.1 Release Notes

# 4.1.1 Version 2.0.0 Nov 2016 [XSPEC 12.9.1]

(\*) = previously available as XSPEC patches

#### **New Features**

- Now compatible with Python 3.x. (No longer compatible with Python versions prior to 2.5.)
- Added Xset.save() and restore() functions for saving and recovering the state of a PyXspec session.
- New adjustable attributes for the Chain class: walkers and algorithm.\*
- AllModels.tclLoad() method added to provide a lower-level alternative to the lmod() local model loading scheme.\*
- *Xset.allowPrompting* attribute provides option for turning on/off XSPEC prompting. This can be useful in iPython environments where certain contexts can lead to infinite prompting loops.
- PyXspec manuals have been converted from Doxygen-generated to Sphinx-generated HTML and PDF.

#### **Fixes**

• Was previously unable to unlink a linked parameter in a Python-coded local model.\*

### 4.1.2 Version 1.1.0 Jul 2015 [XSPEC 12.9.0]

#### **New Features**

- Local models may now be written in Python and inserted into XSPEC's models library with new *AllModels.addPyMod()* function.
- The plot array retrieval interface (ie. *Plot.x()*, *Plot.y()*) has been expanded to allow retrieval from secondary plot panels in a mulit-panel plot.
- New Parameter.index attribute.
- New backscale attribute for Spectrum and Background classes.
- Added new function *Fit.stepparResults()* for retrieving results of most recent steppar run. (Previously available as a patch)

• New *noWrite* option added to *AllData.fakeit* (Previously available as patch)

#### **Fixes**

- The *Model.\_\_call\_\_* function now returns Parameter objects by reference rather than by value. This is to allow the returned object to retain any custom attributes the user may have added.
- Improved handling of Ctrl-c breaking in several prompting contexts.

### 4.1.3 Version 1.0.4 Jul 2014 [XSPEC 12.8.2]

- Added Fit.testStatistic attribute for retrieving the test statistic value from the most recent fit.
- Added compiler macros for switching to <Python/Python.h> include paths when building on Mac platforms.
- Bug fix for get/set Spectrum.correction files on OS X Mavericks.

## 4.1.4 Version 1.0.3 Aug 2013 [XSPEC 12.8.1]

- The *Fit.statMethod* and *statTest* attributes can now be set for a range of individual spectra rather than only applying to all.
- Bug fix to the RModel class (ie. the class of the *Response.gain* attribute). If the user assigned multiple RModel objects to point to the same underlying XSPEC response gain, changes made through one object weren't necessarily showing up in the other objects. This also fixes a related bug created in Xspec patch 12.8.0l that caused a list of error messages to appear (only) in Python versions 2.6.x.

#### 4.1.5 Version 1.0.2 Jan 2013

- Added Xset.parallel attribute, with options 'leven' and 'error' for setting parallel processes.
- Added Fit.statTest attribute for getting/setting the XSPEC test statistic.

### 4.1.6 Version 1.0.1 Dec 2012 [XSPEC 12.8.0]

• 2 additions to the Spectrum class: an *ignored* attribute and an *ignoredString()* function. The former returns a Python list object containing every ignored channel number. The latter returns the same information in convenient string form, which can be reused as input to a future *ignore* or *notice* command.

# 4.1.7 Version 1.0 Feb 2012 [XSPEC 12.7.1]

Changes relative to the PyXspec Beta version:

**Warning:** Two Backwards-Incompatible Changes:

• When using **multiple data groups**, the Model objects assigned to the higher-numbered groups now all have their parameters indexed from **1 to nPar**. For example with a 3 parameter model applied to 2 data groups, you would now access the first parameter in the 2nd model object with mod2(1) rather than mod2(4).

Chapter 4. Notes

• The *Model.setPars()* function (introduced with patch 12.7.0f) used the **p**'n' keyword argument syntax to set non-consecutive parameters. This has been replaced. with the use of Python **dictionaries**. For example, *m.setPars(p2=.3, p4=1.1)* should now be *m.setPars(f2:.3, 4:1.1)*.

#### **New Features**

- Added Standard XSPEC's *gain* command functionality. This is implemented with the new *gain* attribute for Response classes. *Response.gain* is a class of type RModel, and has two Parameter objects: *slope* and *intercept*.
- New AllModels.setPars() function for changing multiple parameters in multiple Model objects with a single call.
- Now compatible with Cygwin.

Features Previously Added As Patches To XSPEC 12.7.0

- AllModels.initpackage() for building local models inside the Python shell.
- Bayesian inference provided through the *Fit.bayes* and *Parameter.prior* attributes.
- *Fit.goodness()* and *Fit.improve()* functions.
- Model.setPars() function for changing multiple parameters with a single call.
- AllModels.simpars() function to do the equivalent of Standard XSPEC's tclout simpars.
- Fit.covariance attribute for retrieving the covariance matrix from the most recent fit.
- Model.expression attribute which stores the model expression string.
- AllModels.sources attribute which stores a map of source number and model name assignments.

#### **Fixes**

- All PyXspec bug fixes previously released as patches to XSPEC 12.7.0 are included.
- Now handles model component-by-name access when the component is a table model whose name includes whitespace.

# 4.2 What's Missing

Python equivalents for these standard XSPEC commands are not yet implemented:

- hardcopy
- · identify
- · margin
- · mdefine
- Tcl script commands: addline, lrt, modid, multifake, rescalecov, simftest, writefits

The following commands perform functions which are not applicable to the currently intended design and usage of PyXspec, and therefore are not likely to be implemented in the near future:

- addcomp
- autosave
- delcomp
- editmod

4.2. What's Missing 65

• script

66 Chapter 4. Notes

### **CHAPTER**

# **FIVE**

# **AUTHORS**

PyXspec was developed by Craig Gordon and Keith Arnaud HEASARC Software Development, Astrophysics Science Division, Code 660.1, NASA/GSFC, Greenbelt MD 20771

Please send questions, comments, and bug reports to xspec12@athena.gsfc.nasa.gov

68 Chapter 5. Authors

Symbols	calcLumin() (xspec.ModelManager method), 45
call() (xspec.ChainManager method), 29call() (xspec.DataManager method), 32call() (xspec.Model method), 41call() (xspec.ModelManager method), 43	Chain (class in xspec), 28 ChainManager (class in xspec), 29 chatter (xspec.XspecSettings attribute), 61 clear() (xspec.ChainManager method), 30 clear() (xspec.DataManager method), 32
call() (xspec.PlotManager method), 50 iadd() (xspec.ChainManager method), 30 iadd() (xspec.DataManager method), 32 iadd() (xspec.ModelManager method), 43 init() (xspec.Chain method), 28	clear() (xspec.ModelManager method), 45 closeLog() (xspec.XspecSettings method), 60 commands (xspec.PlotManager attribute), 52 Component (class in xspec), 31
init() (xspec.FakeitSettings method), 36 init() (xspec.Model method), 41 init() (xspec.Spectrum method), 56 isub() (xspec.ChainManager method), 30 isub() (xspec.DataManager method), 32	cornorm (xspec.Spectrum attribute), 57 correction (xspec.Spectrum attribute), 58 cosmo (xspec.XspecSettings attribute), 61 covariance (xspec.FitManager attribute), 39 criticalDelta (xspec.FitManager attribute), 39
isub() (xspec.ModelManager method), 44	D
abund (xspec.XspecSettings attribute), 61 add (xspec.PlotManager attribute), 52 addCommand() (xspec.PlotManager method), 50 addModelString() (xspec.XspecSettings method), 60 addPyMod() (xspec.ModelManager method), 44 algorithm (xspec.Chain attribute), 28 allowNewAttributes (xspec.XspecSettings attribute), 61 allowPrompting (xspec.XspecSettings attribute), 61 area (xspec.PlotManager attribute), 52 areaScale (xspec.Background attribute), 27 areaScale (xspec.Spectrum attribute), 57	dataGroup (xspec.Spectrum attribute), 58 DataManager (class in xspec), 31 defAlgorithm (xspec.ChainManager attribute), 31 defBurn (xspec.ChainManager attribute), 31 defFileType (xspec.ChainManager attribute), 31 defLength (xspec.ChainManager attribute), 31 defProposal (xspec.ChainManager attribute), 31 defRand (xspec.ChainManager attribute), 31 defTemperature (xspec.ChainManager attribute), 31 defWalkers (xspec.ChainManager attribute), 31 defWalkers (xspec.ChainManager attribute), 31 delCommand() (xspec.PlotManager method), 51 delModelString() (xspec.XspecSettings method), 60 delta (xspec.FitManager attribute), 39
Background (class in xspec), 27 background (xspec.PlotManager attribute), 52 background (xspec.Spectrum attribute), 57 backgroundVals() (xspec.PlotManager method), 51	device (xspec.PlotManager attribute), 52 diagrsp() (xspec.DataManager method), 32 dof (xspec.FitManager attribute), 39 dummyrsp() (xspec.DataManager method), 32 dummyrsp() (xspec.Spectrum method), 56
backScale (xspec.Background attribute), 27 backScale (xspec.Spectrum attribute), 57 bayes (xspec.FitManager attribute), 39 burn (xspec.Chain attribute), 28	energies (xspec.Spectrum attribute), 58 energies() (xspec.Model method), 41 eqwidth (xspec.Spectrum attribute), 58
C	eqwidth() (xspec.ModelManager method), 45 error (xspec.Parameter attribute), 49
calcFlux() (xspec.ModelManager method), 44	· · · · · · · · · · · · · · · · · · ·

error() (xspec.FitManager method), 37 exposure (xspec.Background attribute), 27 exposure (xspec.Spectrum attribute), 58	noID() (xspec.PlotManager method), 51 notice() (xspec.DataManager method), 35 notice() (xspec.Spectrum method), 57 noticed (xspec.Spectrum attribute), 59 noticedString() (xspec.Spectrum method), 57
fakeit() (xspec.DataManager method), 33	nSpectra (xspec.DataManager attribute), 35
FakeitSettings (class in xspec), 35	_
fileName (xspec.Background attribute), 27	O
fileName (xspec.Chain attribute), 28	off() (xspec.RModel method), 55
fileName (xspec.Spectrum attribute), 58 fileType (xspec.Chain attribute), 28	openLog() (xspec.XspecSettings method), 60
FitManager (class in xspec), 36	Р
flux (xspec.Spectrum attribute), 58	parallel (xspec.XspecSettings attribute), 62
folded() (xspec.Model method), 42	Parameter (class in xspec), 48
frozen (xspec.Parameter attribute), 49	perform() (xspec.FitManager method), 38
ftest() (xspec.FitManager method), 37	perHz (xspec.PlotManager attribute), 52
C	PlotManager (class in xspec), 50
G	prior (xspec.Parameter attribute), 49
goodness() (xspec.FitManager method), 37	proposal (xspec.Chain attribute), 28
I	Q
ignore() (xspec.DataManager method), 34	query (xspec.FitManager attribute), 39
ignore() (xspec.Spectrum method), 56	D
ignored (xspec.Spectrum attribute), 58	R
ignoredString() (xspec.Spectrum method), 57	rand (xspec.Chain attribute), 29
improve() (xspec.FitManager method), 38 index (xspec.Parameter attribute), 49	rate (xspec.Spectrum attribute), 59
index (xspec.1 arameter attribute), 49	redshift (xspec.PlotManager attribute), 52
initpackage() (xspec.ModelManager method), 45	removeDummyrsp() (xspec.DataManager method), 35 renorm() (xspec.FitManager method), 38
iplot() (xspec.PlotManager method), 51	Response (class in xspec), 53
isOn (xspec.RModel attribute), 55	response (xspec.Spectrum attribute), 59
isPoisson (xspec.Background attribute), 27	restore() (xspec.XspecSettings method), 60
isPoisson (xspec.Spectrum attribute), 58	RModel (class in xspec), 55
1	run() (xspec.Chain method), 28
L	runLength (xspec.Chain attribute), 29
link (xspec.Parameter attribute), 49	C
lmod() (xspec.ModelManager method), 46	S
log (xspec.XspecSettings attribute), 61	save() (xspec.XspecSettings method), 60
logChatter (xspec.XspecSettings attribute), 61 lumin (xspec.Spectrum attribute), 58	seed (xspec.XspecSettings attribute), 62
iumin (xspec.spectrum attribute), 56	setEnergies() (xspec.ModelManager method), 46
M	setGroup() (xspec.PlotManager method), 51 setID() (xspec.PlotManager method), 51
method (xspec.FitManager attribute), 39	setPars() (xspec. Model method), 42
Model (class in xspec), 40	setPars() (xspec.ModelManager method), 47
model() (xspec.PlotManager method), 51	setPars() (xspec.Response method), 54
ModelManager (class in xspec), 43	setRebin() (xspec.PlotManager method), 51
modelStrings (xspec.XspecSettings attribute), 61	show() (xspec.Chain method), 28
multiresponse (xspec.Spectrum attribute), 58	show() (xspec.ChainManager method), 30
N	show() (xspec.DataManager method), 35
	show() (xspec.FitManager method), 38
name (xspec.Parameter attribute), 49	show() (xspec.Model method), 42
nGroups (xspec.DataManager attribute), 35 nIterations (xspec.FitManager attribute), 39	show() (xspec.ModelManager method), 48 show() (xspec.PlotManager method), 52
micrations (Aspecti invialiant) attilude 1, 17	

70 Index

```
show() (xspec.Response method), 54
show() (xspec.Spectrum method), 57
showList() (xspec.Model static method), 42
sigma (xspec.Parameter attribute), 49
simpars() (xspec.ModelManager method), 48
sources (xspec.ModelManager attribute), 48
Spectrum (class in xspec), 55
splashPage (xspec.PlotManager attribute), 53
stat() (xspec.ChainManager method), 31
statistic (xspec.FitManager attribute), 40
statMethod (xspec.FitManager attribute), 40
statTest (xspec.FitManager attribute), 40
steppar() (xspec.FitManager method), 38
stepparResults() (xspec.FitManager method), 38
systematic (xspec.ModelManager attribute), 48
Т
tclLoad() (xspec.ModelManager method), 48
temperature (xspec.Chain attribute), 29
testStatistic (xspec.FitManager attribute), 40
totalLength (xspec.Chain attribute), 29
U
unit (xspec.Parameter attribute), 49
untie() (xspec.Model method), 43
untie() (xspec.Parameter method), 49
V
values (xspec.Background attribute), 27
values (xspec.Parameter attribute), 49
values (xspec.Spectrum attribute), 59
values() (xspec.Model method), 43
variance (xspec.Background attribute), 27
variance (xspec.Spectrum attribute), 59
version (xspec.XspecSettings attribute), 62
W
walkers (xspec.Chain attribute), 29
weight (xspec.FitManager attribute), 40
X
x() (xspec.PlotManager method), 52
xAxis (xspec.PlotManager attribute), 53
xErr() (xspec.PlotManager method), 52
xLog (xspec.PlotManager attribute), 53
xsect (xspec.XspecSettings attribute), 62
XspecSettings (class in xspec), 59
Υ
y() (xspec.PlotManager method), 52
yErr() (xspec.PlotManager method), 52
yLog (xspec.PlotManager attribute), 53
```

Index 71