Global Fitting of X-ray Spectra

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Correct

Incorrect

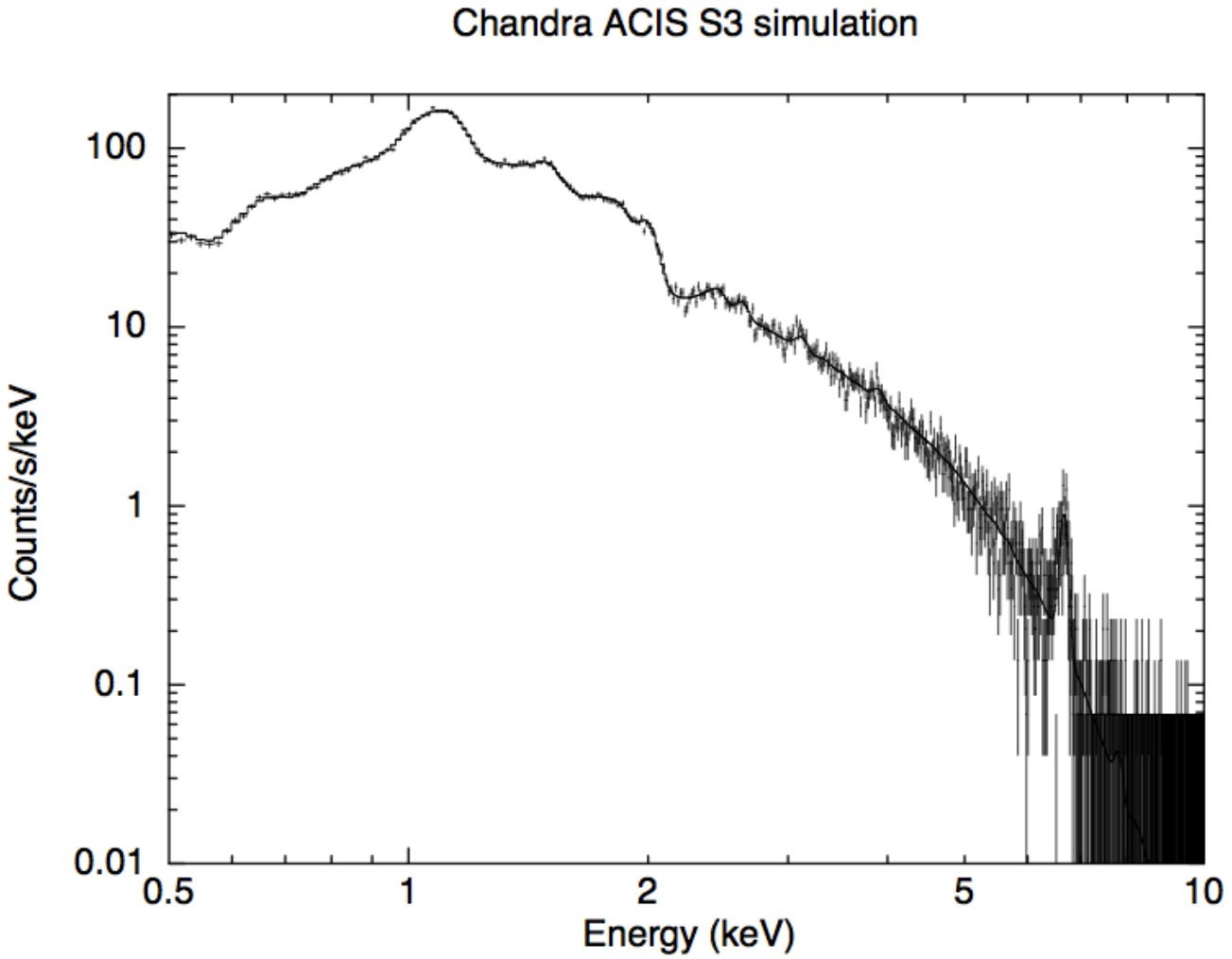
Most X-ray spectra are of moderate or low resolution (eg Chandra ACIS or XMM-Newton EPIC).

However, the spectra generally cover a bandpass of more than 1.5 decades in energy.

Moreover, the continuum shape often provides important physical information.

Therefore, unlike in the UV/optical/IR, most uses of X-ray spectra have involved a simultaneous analysis of the entire spectrum rather than an attempt to measure individual line strengths.

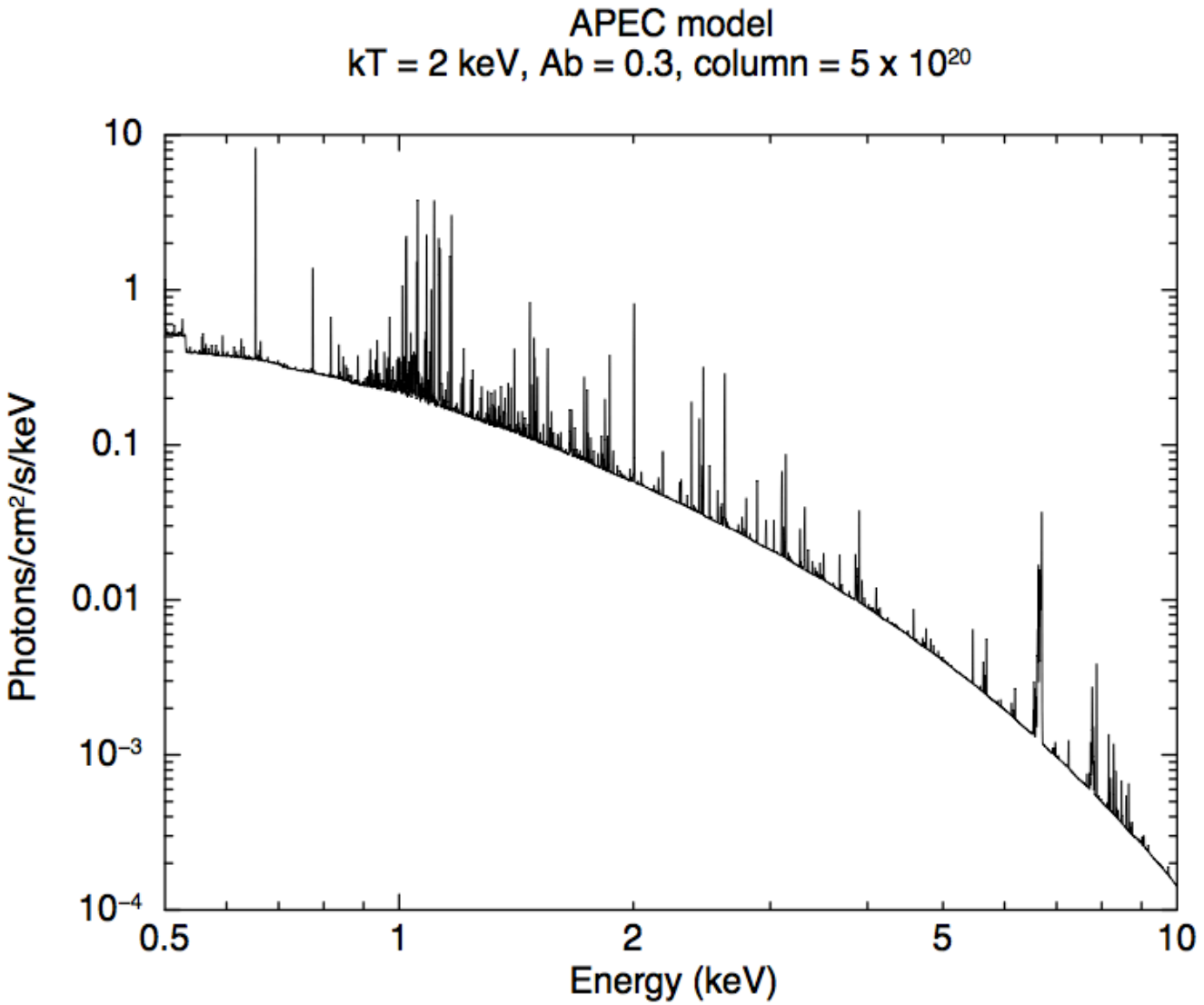
Can we start with this…




```
model phabs(apec)
   0.05
   2.0
   0.3
   0.0
   1.0
fakeit none
   aciss_aimpt_cy16.rmf
   aciss_aimpt_cy16.arf
   y

   aciss_aimpt_cy16.fak
   1000.0
setp energy
cpd /xs
iplot data
  r 0.5 10.0 0.01 200
  view 0.15 0.15 0.85 0.85
  la oy Counts/s/keV
  la y
  la rot
  csize 1.2
```

and infer this




```
model phabs(apec)
   0.05
   2.0
   0.3
   0.0
   1.0
cpd /xs
iplot model
  r 0.5 10.0 1.0e-4 10.0
  view 0.15 0.15 0.85 0.85
  la oy Photons/cm\u2\d/s/keV
  la y
  la rot
  csize 1.2
```

Suppose we observe D(I) counts in channel I (of N) from some source. Then :

$$D(I) = t \int R(I,E)\, A(E)\, S(E)\, dE$$

- S(E) is the source flux at the front of the telescope (in photons/cm^2/s/keV
- A(E) is the energy-dependent effective area of the telescope and detector system (in cm^2)
- R(I,E) is the probability of an incoming photon of energy E being registered in channel I (dimensionless)
- t is the observation length (in seconds)

$$D(I) = t \int R(I,E)\, A(E)\, S(E)\, dE$$

We assume that t, A(E) and R(I,E) are known and want to solve this integral equation for S(E). We can divide the energy range of interest into M bins and turn this into a matrix equation :

$$D_i = t \sum R_{ij}\, A_j\, S_j$$

where S_j is now the flux in photons/cm^2/s in energy bin J. We want to find S_j.

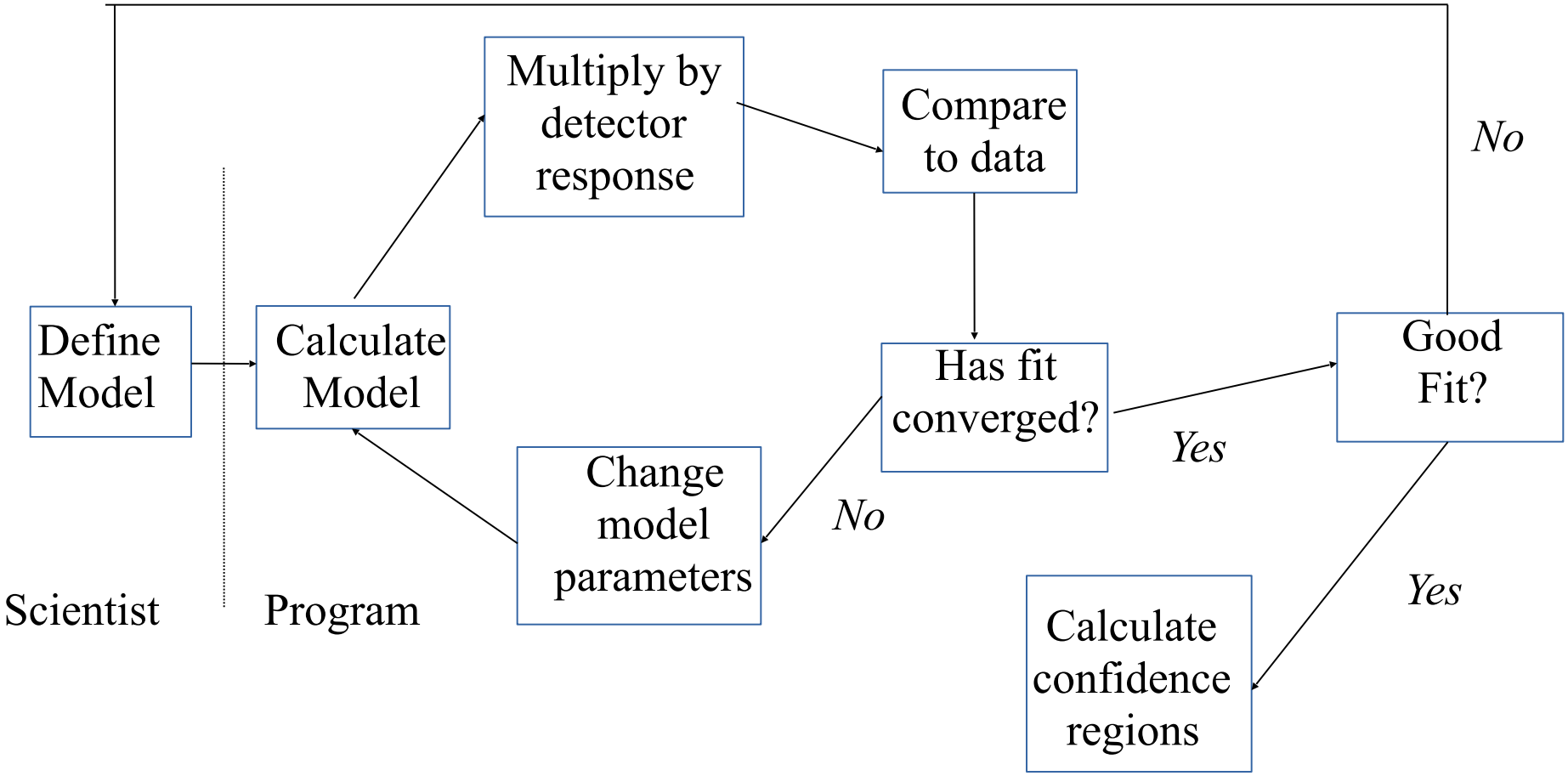
$$D_i = t \sum R_{ij} A_j S_j$$

The obvious tempting solution is to calculate the inverse of R_{ij}, premultiply both sides and rearrange :

$$(1/(t A_j)) \sum (R_{ij})^{-1} D_i = S_j$$

This does not work ! The S_j derived in this way are very sensitive to slight changes in the data D_i. This is a great method for amplifying noise.

(https://en.wikipedia.org/wiki/Tikhonov_regularization)


Define Model
Calculate Model
Multiply by detector response
Compare to data
Has fit converged?
Good Fit?
No
Yes
Change model parameters
No
Yes
Calculate confidence regions
Scientist
Program

o XSPEC - part of HEAsoft. General spectral fitting program with many models available. Python version available as PyXspec.

o Sherpa - part of CIAO (now available standalone). Multi-dimensional fitting program which includes the XSPEC model library. Python interface.

o SPEX - from SRON in the Netherlands. Spectral fitting program specializing in collisional plasmas and high resolution spectroscopy.

o ISIS - from the MIT Chandra HETG group (also includes XSPEC model library). S-lang interface.

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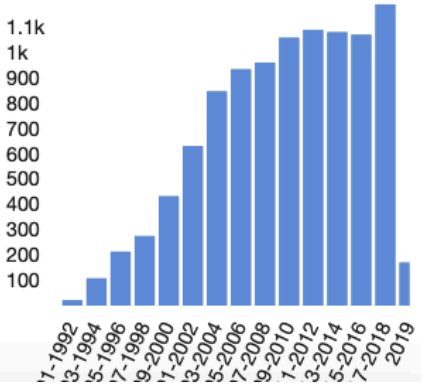

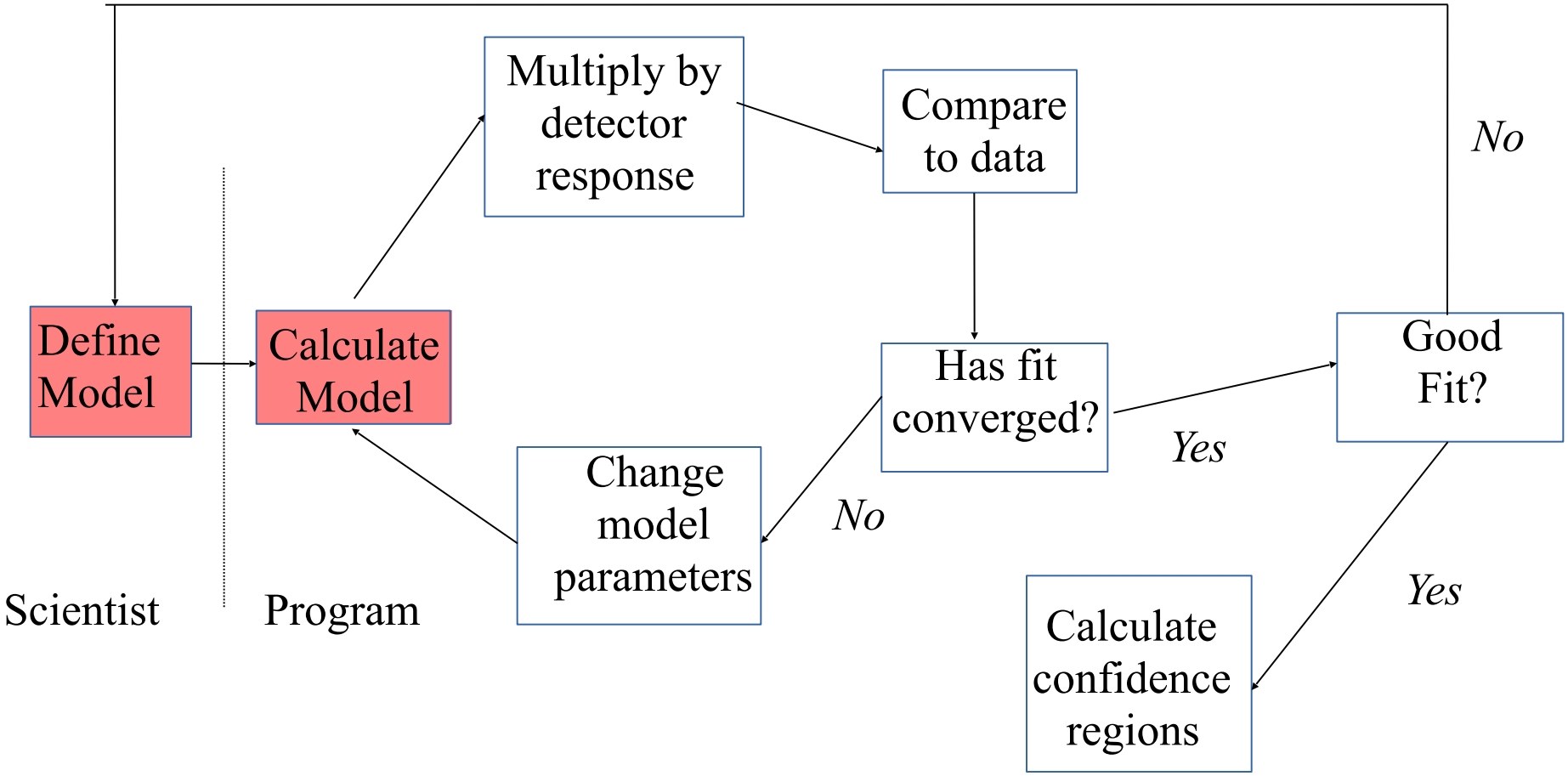
Define Model
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Good Fit?
Change model parameters
Calculate confidence regions
No
Yes
No
Yes
Scientist
Program

All models are wrong, but some are useful - George Box

X-ray spectroscopic models are usually built up from individual components. These can be thought of as two basic types -additive (an emission component e.g. blackbody, line,…) or multiplicative (something which modifies the spectrum e.g. absorption).

$$\text{Model} = M_1 * M_2 * (A_1 + A_2 + M_3 * A_3) + A_4$$

Basic additive (emission) models include :

- blackbody
- thermal bremsstrahlung
- power-law
- collisional plasma (raymond, mekal, apec)
- Gaussian or Lorentzian lines

There are many more models available covering specialised topics such as accretion disks, comptonized plasmas, non-equilibrium ionization plasmas, multi-temperature collisional plasmas…

and multiplicative models include :

- photoelectric absorption due to our Galaxy
- photoelectric absorption due to ionized material
- high energy exponential roll-off.
- cyclotron absorption lines.

Convolution models take as input the current model and manipulate it in some way. Examples are :

- Smoothing with a Gaussian or Lorentzian function (e.g. velocity broadening)
- Compton reflection
- CCD Pile-up

Physical process	XSPEC models
Equilibium Collisional Plasma	(b)(v)apec, (z)(v)bremss, c6(p)(vm|)me)kl, ce(vm|me)kl, equil, (v)meka(l), (v)raymond, smaug
Non-equilibrium Collisional Plasma	(v)(g)nei, (v)(n)pshock, (v)sedov
Photoionized Plasma	absori, redge, swind1, xion, zxipcf
Power-law	bkn2pow, bknpower, cutoffpl, pegpwrlw, plcabs, (z)powerlaw
Black-body	(z)bbody, bbodyrad
Emission Line	(z)gaussian, diskline, kerrdisk, laor(2), lorentz
Compton scattering	bmc, cabs, comp(LS|PS|ST|TT|bb), nthComp, simpl
Accretion disk	disk(bb|ir|m|o|pbb|pn), ezdiskbb, grad, hrefl, kdblur(2), kerr(bb|d|conv), rdblur, sirf, xion
Reflection	(b|p)exr(a|i)v, (i)reflect, refsch
Neutron star atmosphere	nsa(grav|atmos), nsmax
Cooling flow	(mk)(vm)cflow
Gamma-ray burst	grbm
Pair plasma	nteea
Positronium continuum	posm
Synchrotron	srcut, sresc
Photoelectric absorption	absori, edge, partcov, pcfabs, (v)phabs, pwab, smedge, swind1, tb(var)abs, tbgrain, varabs, wndabs, zvfeabs, zxipcf
Cyclotron absorption	cyclabs
Dust scattering	dust
Reddening	redden, uvred, zdust, zsmdust

```
XSPEC12>mo tbabs(apec+phabs(pow))

Input parameter value, delta, min, bot, top, and max values for ...
           1      0.001(      0.01)         0         0     100000      1e+06
1:TBabs:nH>0.05
           1       0.01(      0.01)     0.008     0.008         64         64
2:apec:kT>0.9
           1     -0.001(      0.01)         0         0          5          5
3:apec:Abundanc>0.3
           0      -0.01(      0.01)    -0.999    -0.999         10         10
4:apec:Redshift>
           1       0.01(      0.01)         0         0      1e+20      1e+24
5:apec:norm>1e-5
           1      0.001(      0.01)         0         0     100000      1e+06
6:phabs:nH>0.5
           1       0.01(      0.01)        -3        -2          9         10
7:powerlaw:PhoIndex>1.7
           1       0.01(      0.01)         0         0      1e+20      1e+24
8:powerlaw:norm>1e-4
```

==========

Model TBabs<1>(apec<2> + phabs<3>*powerlaw<4>) Source No.: 1 Active/On

Model par	Model comp	Component	Parameter	Unit	Value	
1	1	TBabs	nH	10^22	5.00000E-02	+/- 0.0
2	2	apec	kT	keV	0.900000	+/- 0.0
3	2	apec	Abundanc		0.300000	frozen
4	2	apec	Redshift		0.0	frozen
5	2	apec	norm		1.00000E-05	+/- 0.0
6	3	phabs	nH	10^22	0.500000	+/- 0.0
7	4	powerlaw	PhoIndex		1.70000	+/- 0.0
8	4	powerlaw	norm		1.00000E-04	+/- 0.0

---

tbvabs Version 2.3
Cosmic absorption with grains and H2, modified from
Wilms, Allen, & McCray, 2000, ApJ 542, 914-924
Questions: Joern Wilms
joern.wilms@sternwarte.uni-erlangen.de
joern.wilms@fau.de

There is a simple XSPEC model interface which enables astronomers to write new models and fit them to their data. You can write your own subroutine (in Fortran, C, C++, or Python) and hook it in - the subroutine takes in the energies on which to calculate the model and the current parameters and writes out the fluxes (in photons/cm^2/s).

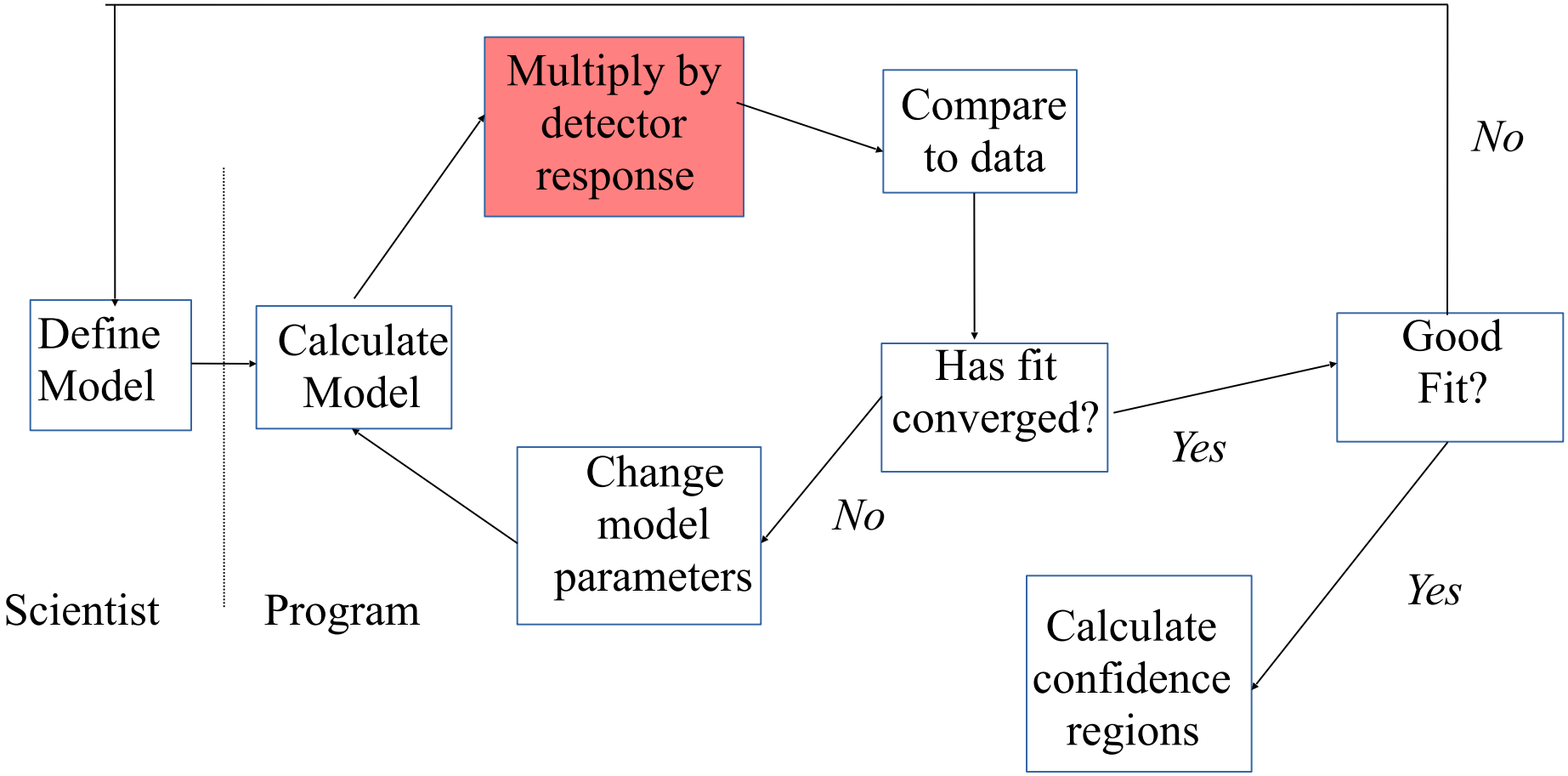
In addition, there is a standard format for files containing model spectra so these too can be fit to data without having to add new routines to XSPEC.

Approximately half the models in XSPEC were written by other scientists for their own research.

The XSPEC mdefine command can be used to define a new model as a simple arithmetic expression which may include other XSPEC models.

For instance, suppose you want a model of the He-like triplet emission line complex (resonance, forbidden and intercombination lines) with two of the parameters being the R = f/i and G = (f+i)/r ratios.

```
mdef triplet gaussian(Ef,sf) + R*gaussian(Ei,si) + (1+R)*gaussian(Er,sr)/G
```


Multiply by detector response
Compare to data
No
Define Model
Calculate Model
Has fit converged?
Good Fit?
Yes
Change model parameters
No
Scientist
Program
Calculate confidence regions
Yes

photons/cm^2/s between energies E_L and E_H at top of telescope

ARF

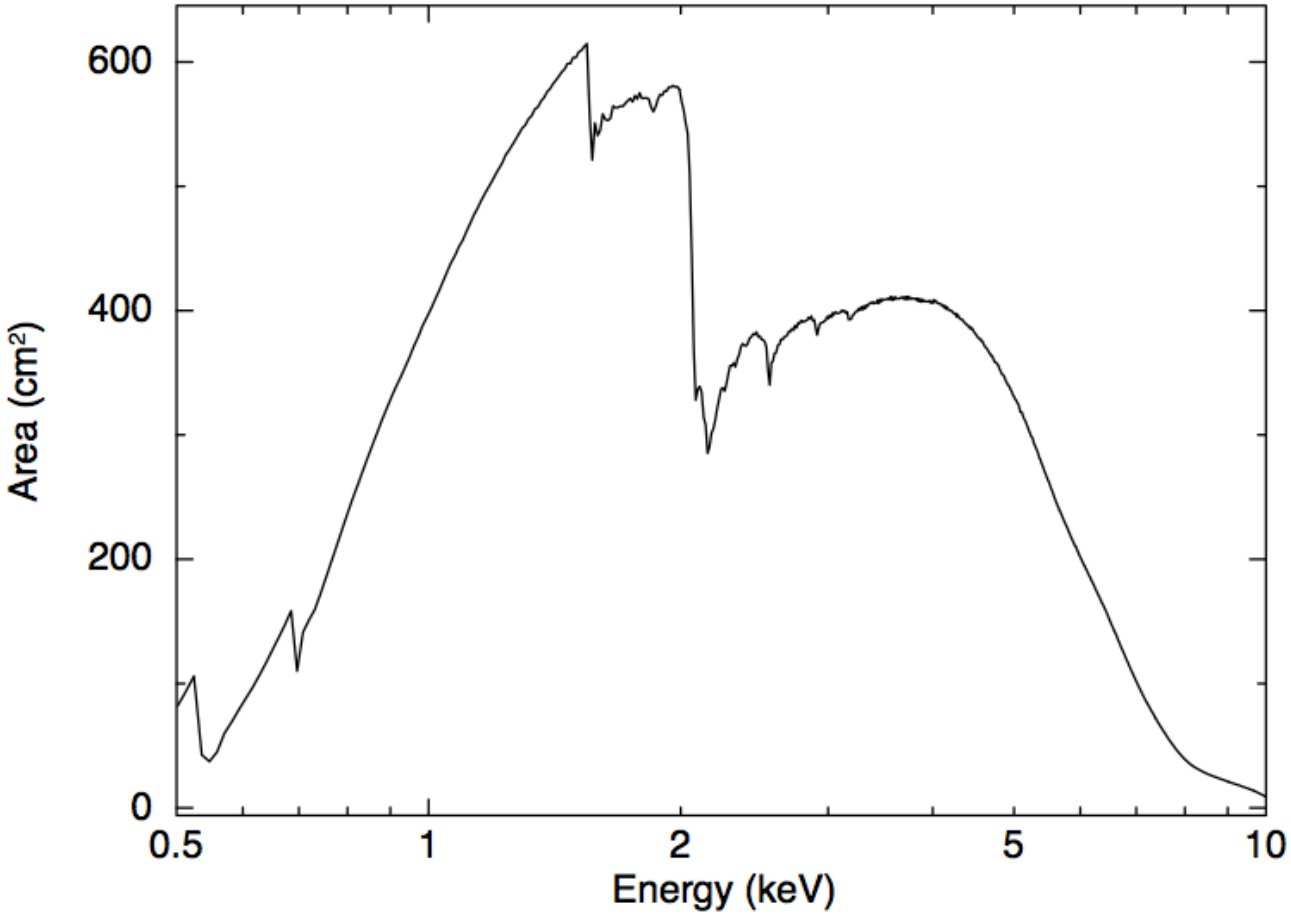
vector

photons/s between energies E_L and E_H at detector

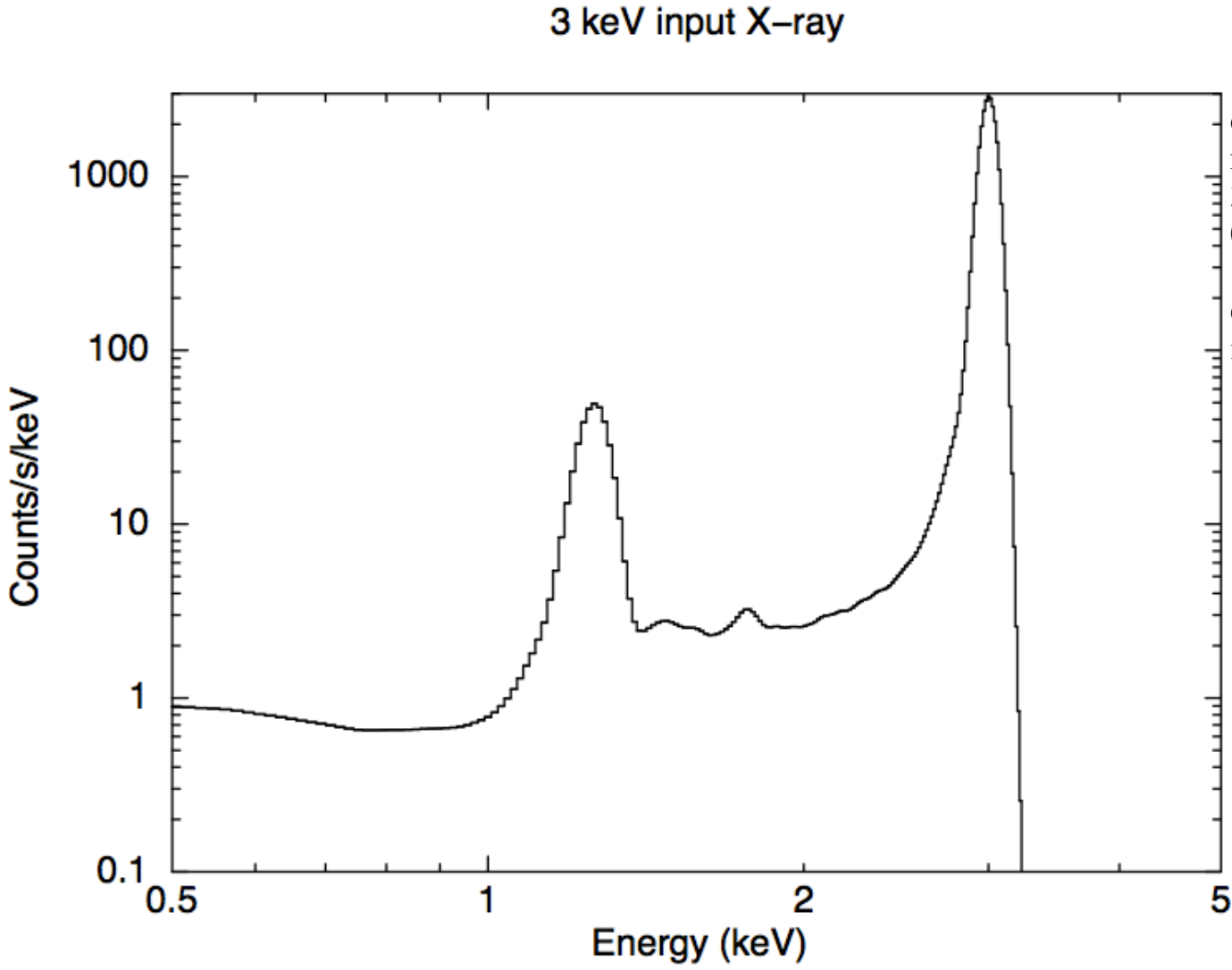
RMF

matrix

counts/s in spectrum channel I of detector




```
data aciss_aimpt_cy16.fak
cpd /xs
iplot eff
  r x 0.5 10.0
  view 0.15 0.15 0.85 0.85
  la oy Area
  la y
  la rot
  lstyle 1 on 1
  lwidth 3 on 1
  csize 1.2
```




```
data aciss_aimpt_cy16.fak
model gauss
3.0
0.0
1.0
cpd /xs
iplot ldata
  col 0 on 1
  r  0.5 10.0 0.1 3000.0
  view 0.15 0.15 0.85 0.85
  la oy Area
  la y
  la rot
  lstyle 1 on 1
  lwidth 3 on 1
  csize 1.2
```

What are the analogs in UV/optical/IR?

An example R(I,E) would be the resolution of a spectrometer. In most UV/optical/IR instruments R(I,E) is simple - a Gaussian or Lorentzian shape.

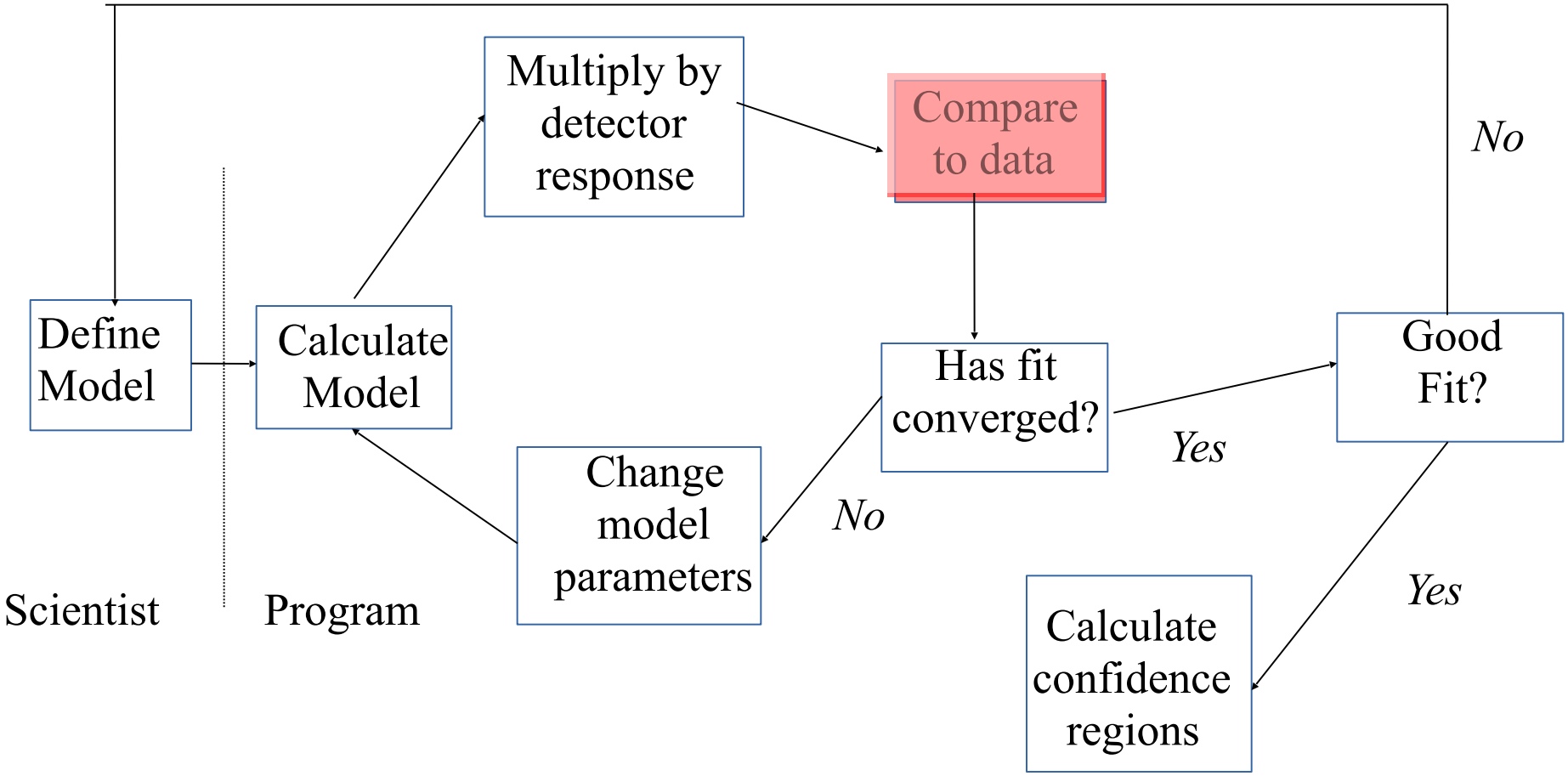
A(E) is the product of telescope reflectivities, detector efficiencies, and filter transmissions. In optical/UV astronomy we usually divide the observed data by this function to obtain the fluxed spectrum.

But can I ignore the response? Sometimes, yes.

If you have proportional counter or CCD spectra you must use the response, R(I,E).

If you have Chandra HETG spectra then you can just about ignore the response (but not A(E)).

But if you try this for XMM-Newton RGS you will get incorrect results. The RGS spectral response has wide wings so line fluxes will be wrong and the continuum level overestimated.


Define Model
Calculate Model
Multiply by detector response
Compare to data
Has fit converged?
Good Fit?
No
Yes
Change model parameters
No
Yes
Calculate confidence regions
Scientist
Program

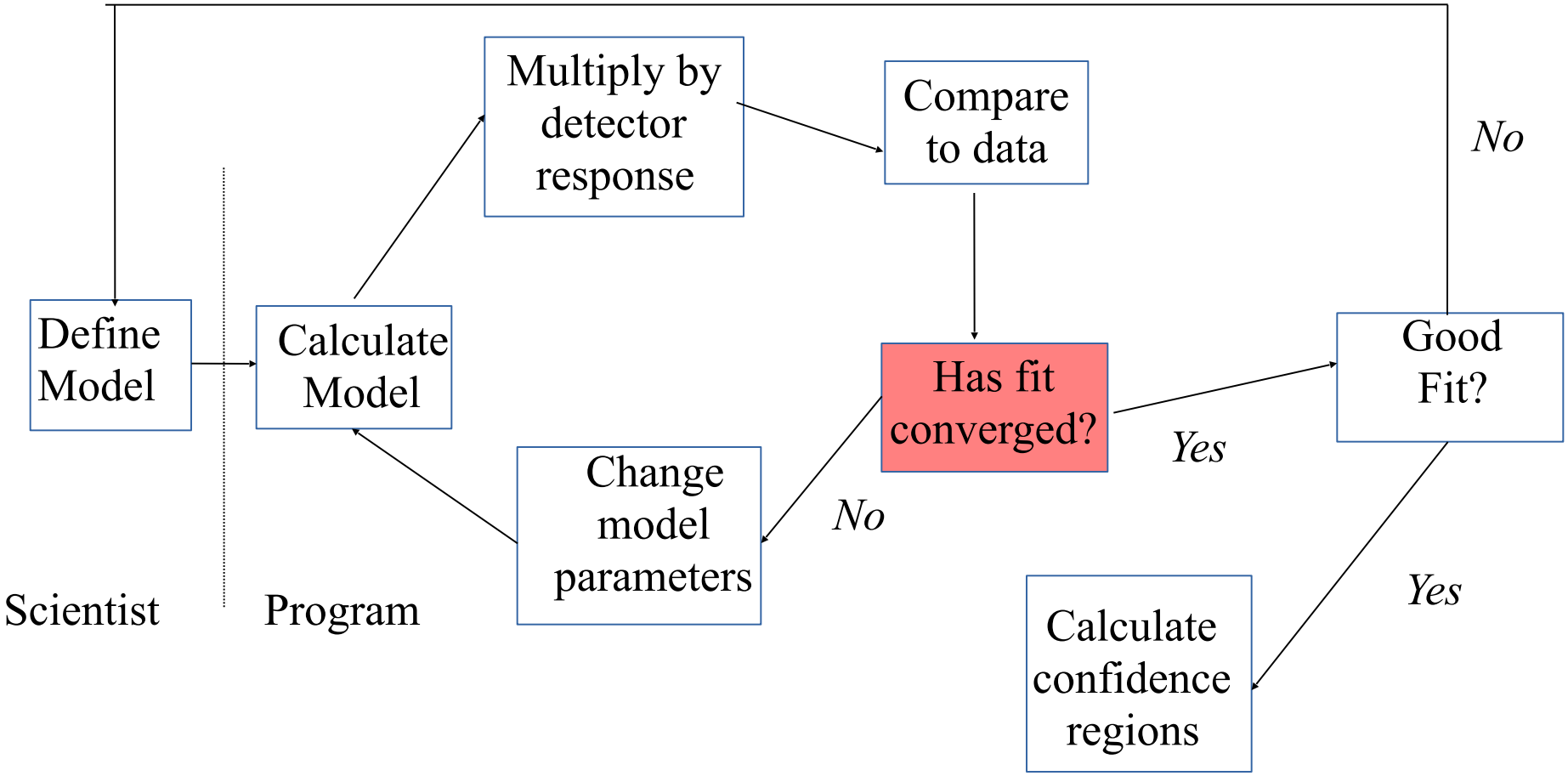
We compare the model to the data using a fit statistic:

$$\text{Fit statistic} = f(\text{data}, \text{model} * \text{response})$$

For fit statistics it is best to use maximum likelihood estimators ie

$$\text{Min} \quad -\log(\text{Probability}(\text{data} \mid \text{model} * \text{response}))$$

while varying the model. Appendix B in the XSPEC manual discusses the statistics which can be used.


Define Model
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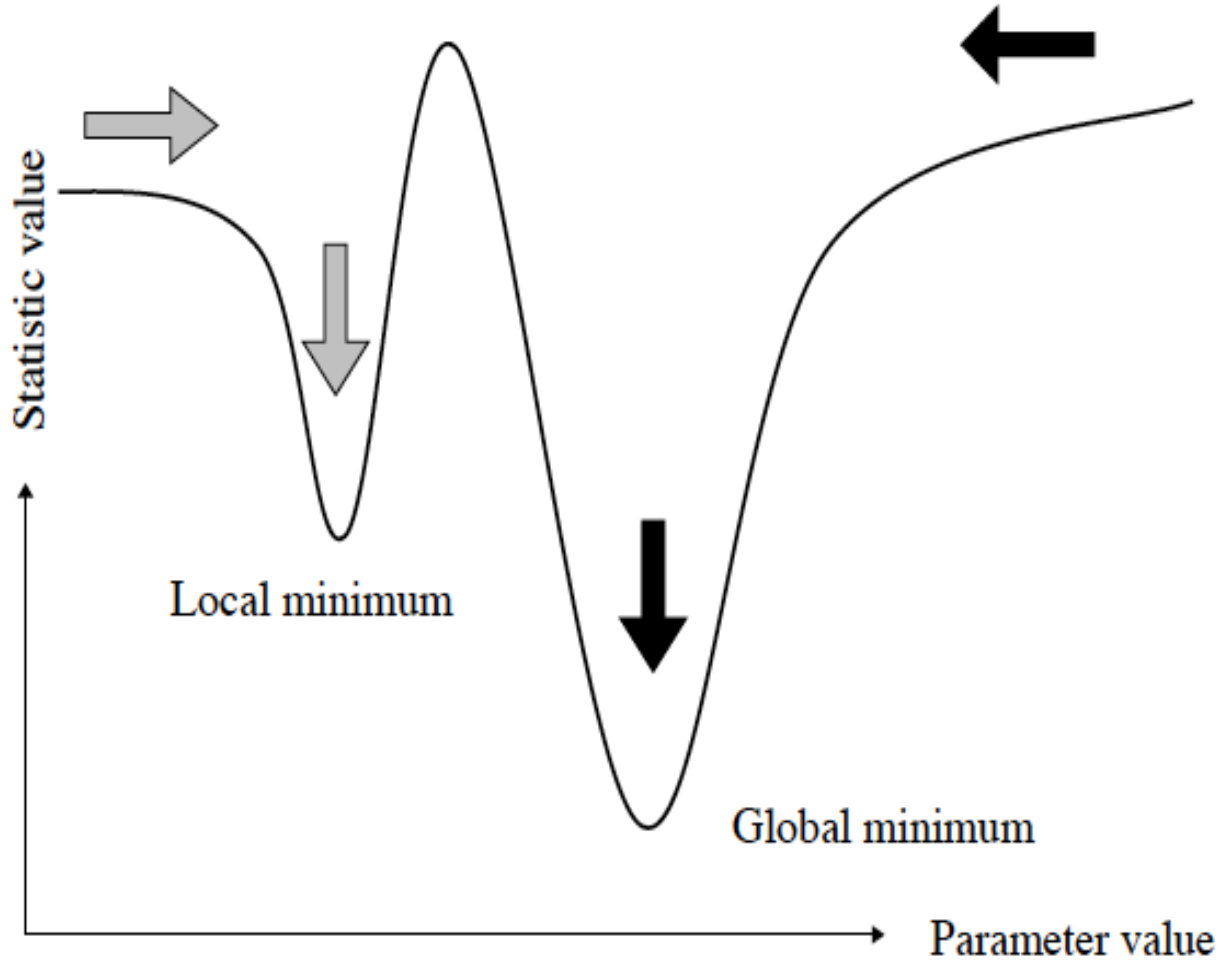
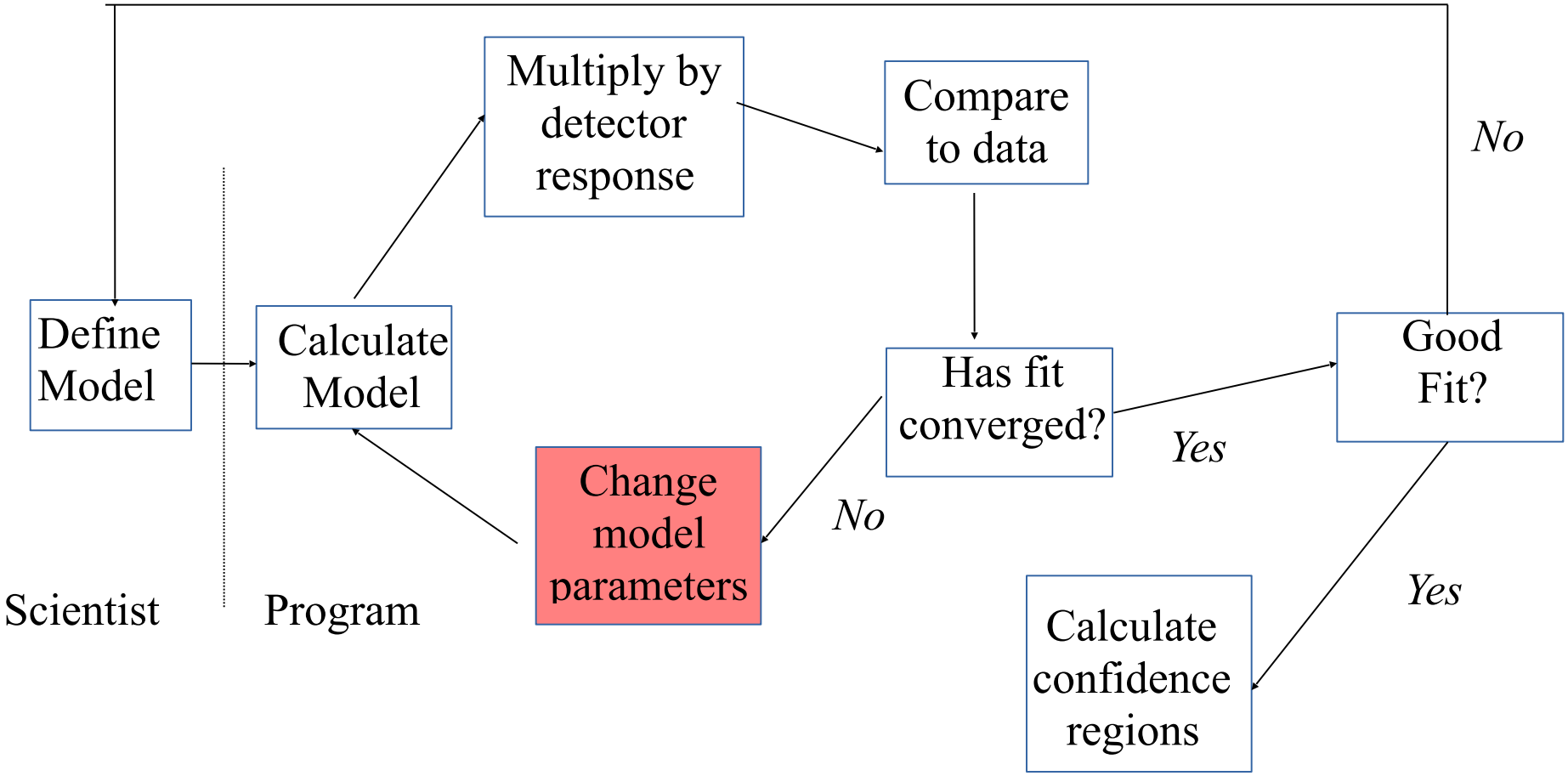
Program

Usual test is whether fit statistic has changed by less than some amount since last iteration. Biggest problem is getting trapped in local minima.




Define Model
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Steepest descent: follow the derivative

Quadratic: assume parameter space is quadratic

Combination: start mostly steepest descent and become more quadratic as best fit approached

Can include probability of choosing parameters which increase statistic as a way of avoiding local minima.

Use approximations to avoid numerical second derivatives.

XSPEC12>fit

		Parameters			
C-Statistic	|beta|/N	Lvl	1:nH	2:kT	5:norm
50923.8	18270.3	-2	0.668253	1.07065	1.61824
39639.9	23950.2	-3	0.598562	1.05858	1.81295
37979.5	8966.3	-4	0.531331	1.06581	1.69958
37541.1	3775.06	-5	0.489487	1.07501	1.59367
36892.3	1818.27	-6	0.456594	1.09010	1.50977
21853.8	10990.7	-7	0.246221	1.36956	0.953106
5301.76	21732.7	-8	0.122799	1.61071	0.985940
1218.88	6525.63	-9	0.0557394	1.86233	0.959554
690.572	1452.38	-10	0.0458976	2.03296	0.949567
687.845	329.137	-11	0.0461829	2.03619	0.954222
687.845	2.13375	-12	0.0461806	2.03620	0.954242

Minimization methods such as those used by the XSPEC fit command (a modified Levenberg-Marquardt) are local. They use some information around the current parameters to find the next set of parameters. For instance, calculate the derivative of the statistic with respect to the parameters then move in the direction of the steepest downward gradient.

These local methods are liable to get stuck in a local minimum. Watch out for this !

The more complicated your model and the more highly correlated the parameters then the more likely that the algorithm will not find the absolute best-fit.

Sometimes you can spot that you are stuck in a local minimum by using the XSPEC error or steppar commands. These both step through parameter values :

- error around the current best-fit
- steppar over a grid you choose

and thus can accidentally find a better fit. Crude but sometimes effective.

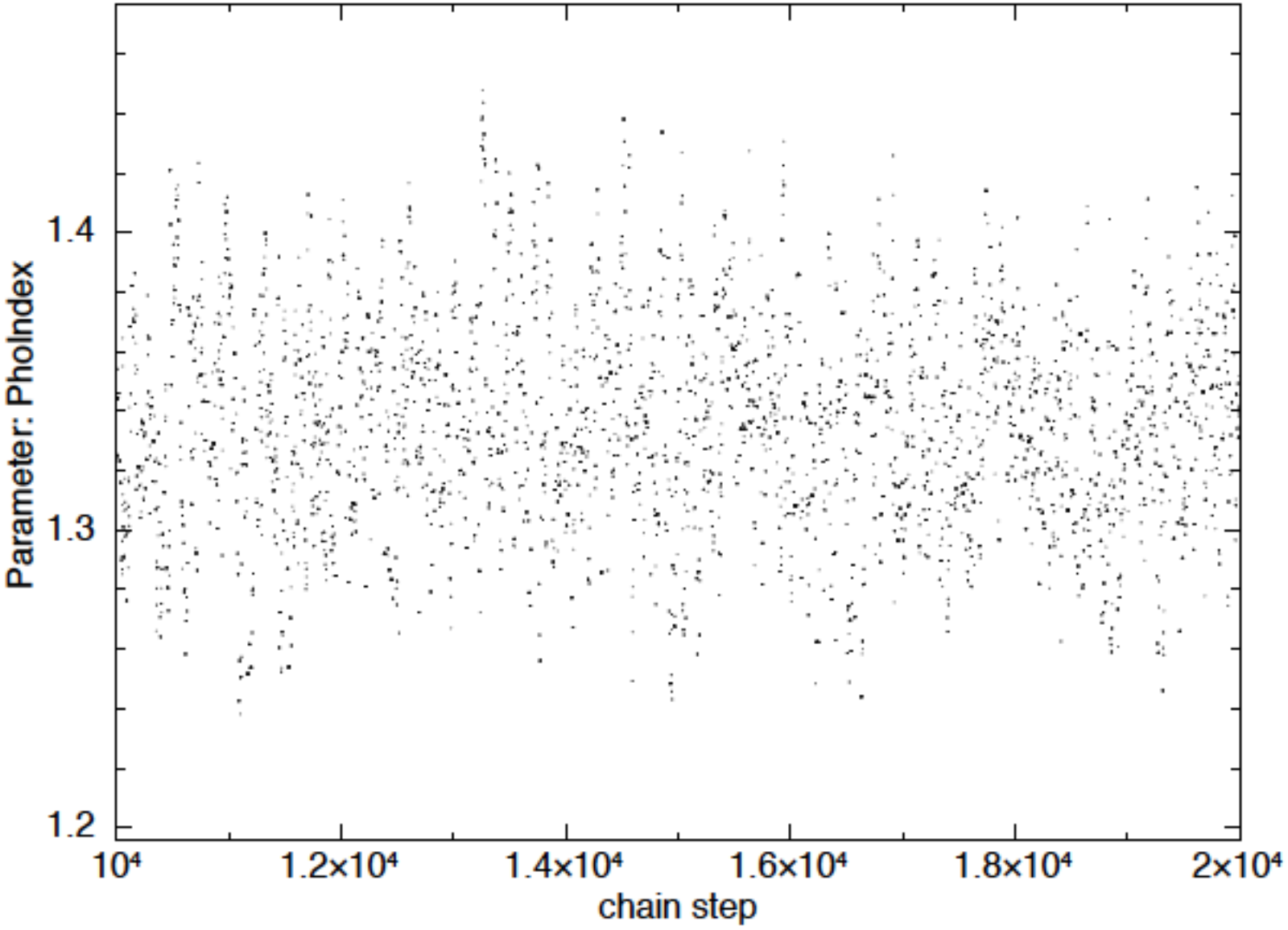
You can do this in a semi-automated fashion by using a local minimization algorithm and following this with the error command with the ability to restart if a new minimum is found during the search.

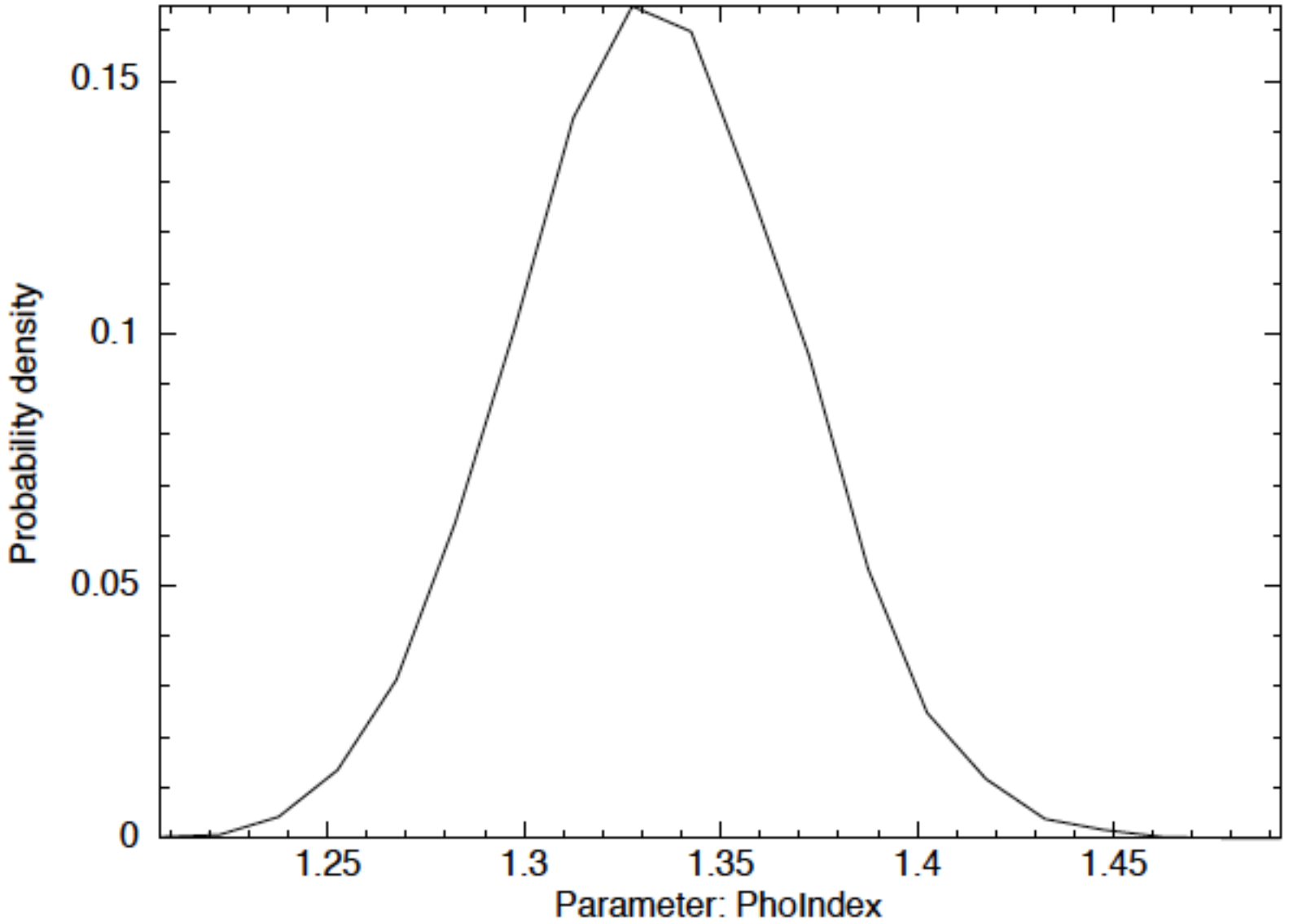
```
XSPEC12>query yes
XSPEC12>error 1 2
```

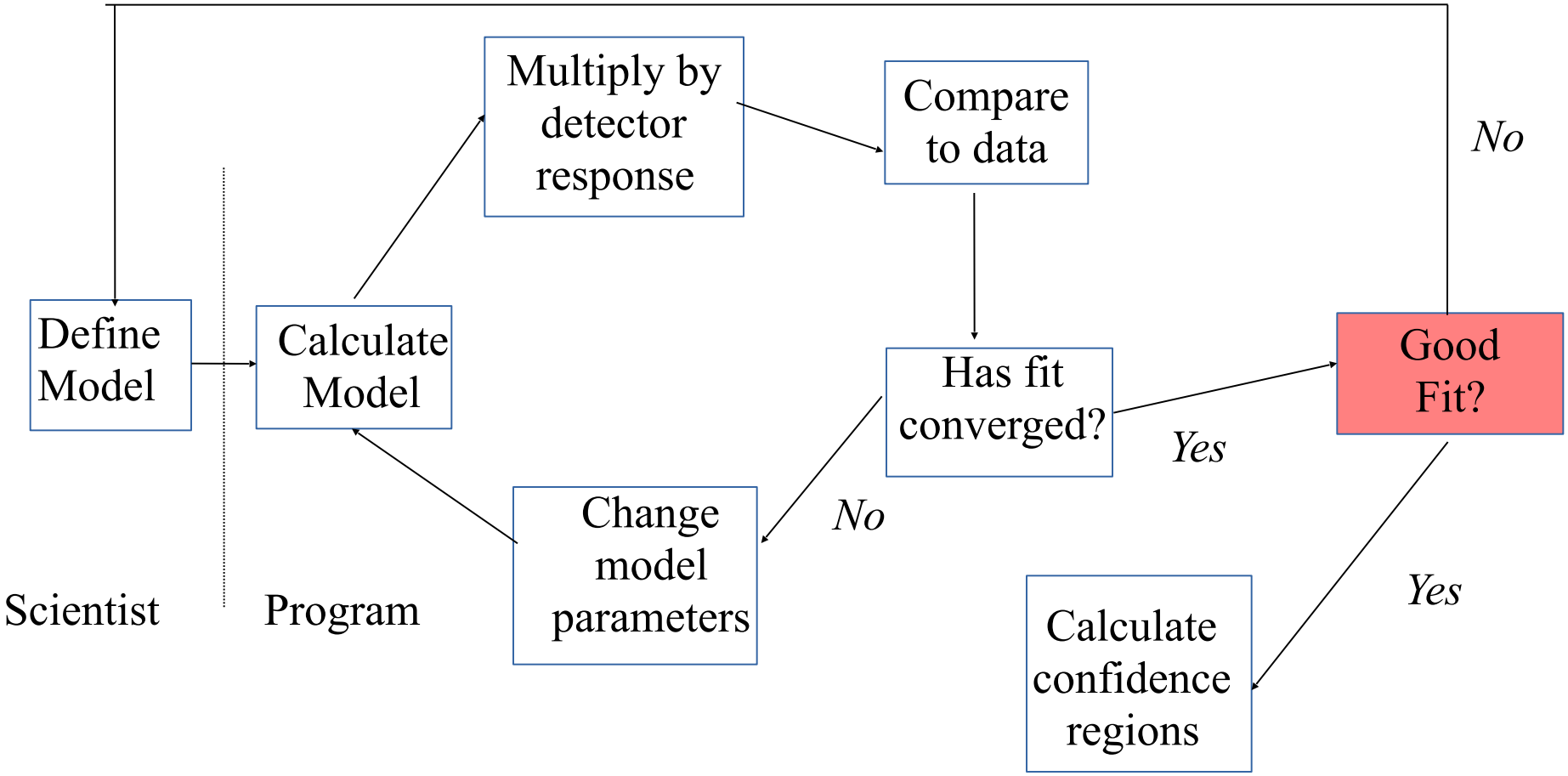
Calculates the error on parameters 1 and 2. If a new minimum is found it will redefine that as the best fit and start again.

There are global minimization methods available - simulated annealing, genetic algorithms, … - but they require many function evaluations (so are slow) and are still not guaranteed to find the true minimum.

The most promising technique, now seeing widespread use in astronomy, is Markov Chain Monte Carlo, which provides an intelligent sampling of parameter space. This is available in XSPEC (via the chain command).


Parameter: PhoIndex
1.4
1.3
1.2
10⁴
1.2×10⁴
1.4×10⁴
1.6×10⁴
1.8×10⁴
2×10⁴
chain step


0.15
0.1
0.05
0
Probability density
1.25
1.3
1.35
1.4
1.45
Parameter: PhoIndex


Define Model
Calculate Model
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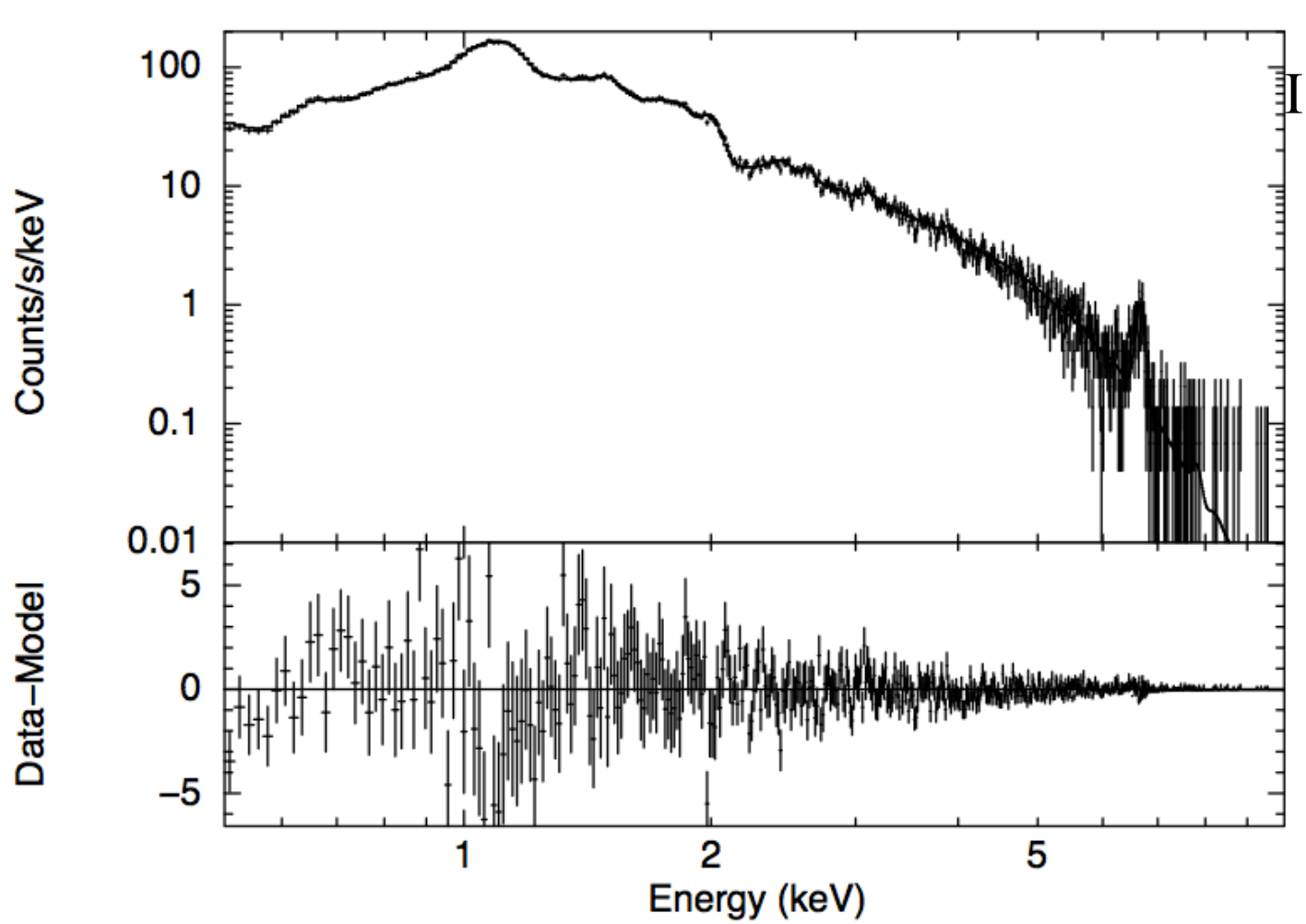
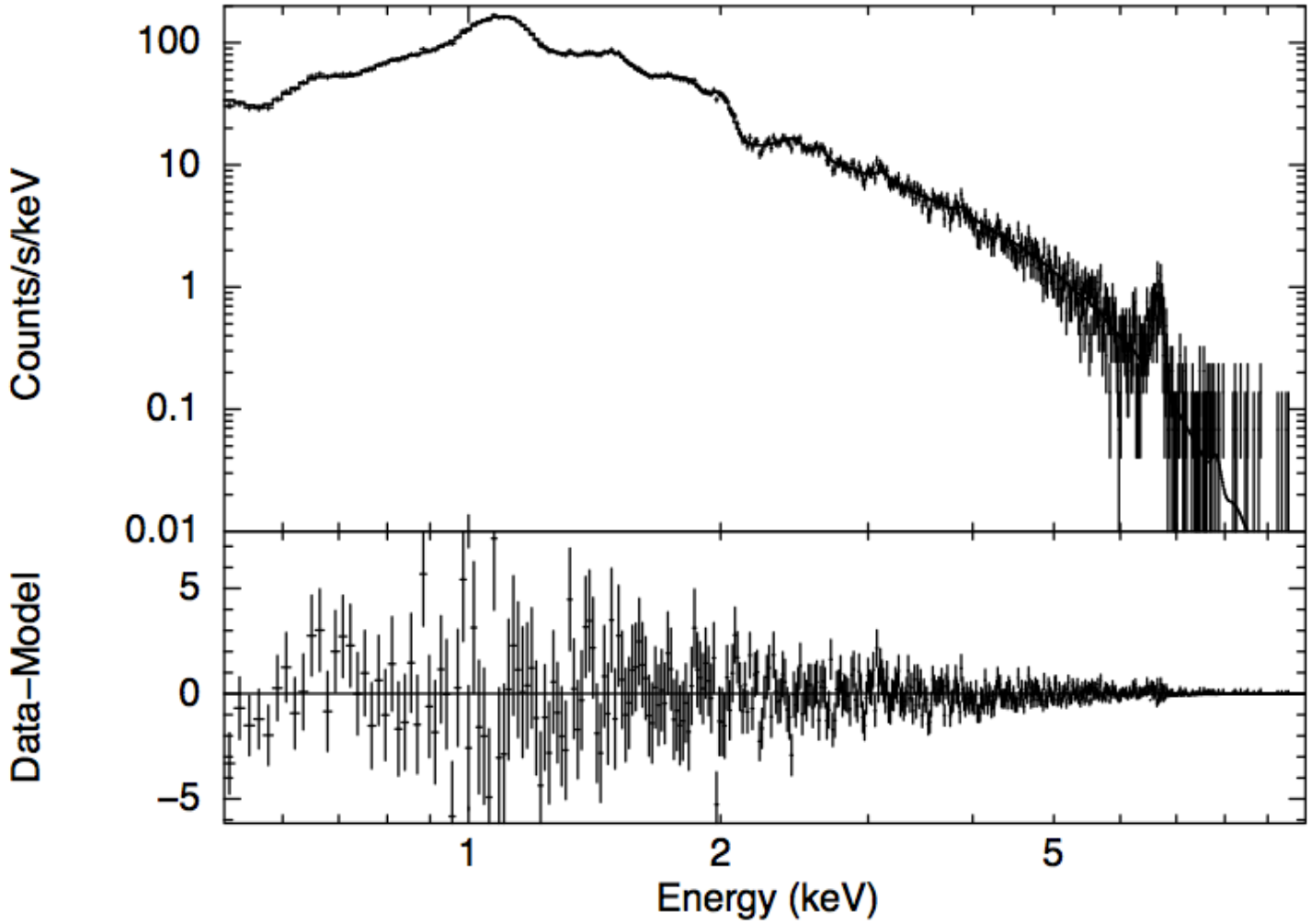
Compare to data
Has fit converged?
Good Fit?
No
Yes
Change model parameters
No
Calculate confidence regions
Yes
Scientist
Program



Is this a good fit ?

```
iplot ldata res
  window 1
  view 0.15 0.4 0.85 0.85
  r y 0.01 200.0
  la t
  la y Counts/s/keV
  window 2
  view 0.15 0.15 0.85 0.4
  la y Data-Model
  csize 1.2
  time off
  lw 3
  lw 3 on 1..4
```

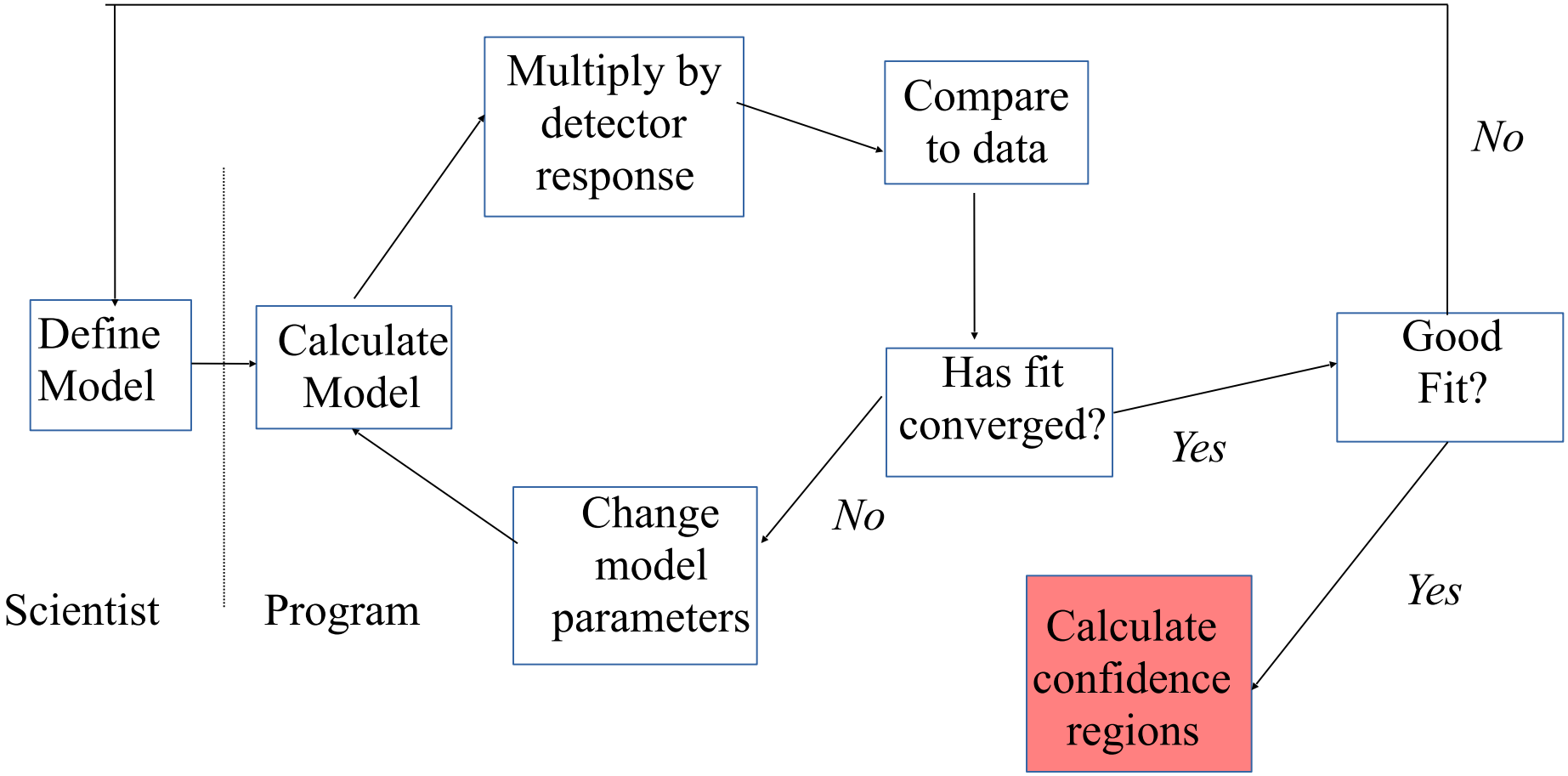
```
XSPEC12>thaw 3
…
XSPEC12>fit
                          Parameters
C-Statistic  |beta|/N    Lvl        1:nH        2:kT    3:Abundanc        5:norm
676.397      100.042      -3     0.0483404      2.00094      0.310125      0.989880
675.537      178.983      -4     0.0485755      1.99874      0.310859      0.991889
675.537      0.423288     -3     0.0485756      1.99873      0.310855      0.991897
…
Model phabs<1>*apec<2> Source No.: 1   Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   phabs      nH         10^22    4.85756E-02  +/-  2.14866E-03
   2    2   apec       kT         keV      1.99873      +/-  1.20435E-02
   3    2   apec       Abundanc            0.310855     +/-  9.21072E-03
   4    2   apec       Redshift            0.0          frozen
   5    2   apec       norm                0.991897     +/-  1.01179E-02
```




```
iplot ldata res
  window 1
  view 0.15 0.4 0.85 0.85
  r y 0.01 200.0
  la t
  la y Counts/s/keV
  window 2
  view 0.15 0.15 0.85 0.4
  la y Data-Model
  csize 1.2
  time off
  lw 3
  lw 3 on 1..4
```

This seems to be the most contentious issue in spectral fitting: we all want a nice simple test for whether we are using the correct model.

Don't use same statistic for testing as fitting.


Define Model
Calculate Model
Multiply by detector response
Compare to data
Has fit converged?
No
Change model parameters
Yes
Good Fit?
No
Yes
Calculate confidence regions
Scientist
Program

The +/- numbers written at the end of the fit are *estimates* of the one sigma error calculated from the second derivatives of the fit statistic with respect to the parameter.

The error command tries different values of the parameter, while minimizing the statistic over all the other parameters, till it finds the required increase in statistic value from the minimum.

The chain command runs MCMC and can be used to produce the complete probability distribution of the parameters (for Bayesians).

Unless you are looking at a bright point source with Chandra you will probably have a background component to the spectrum in addition to the source in which you are interested.

The usual method is to extract a spectrum from another part of the image or another observation. Spectral fitting programs then use both the source and background spectra.

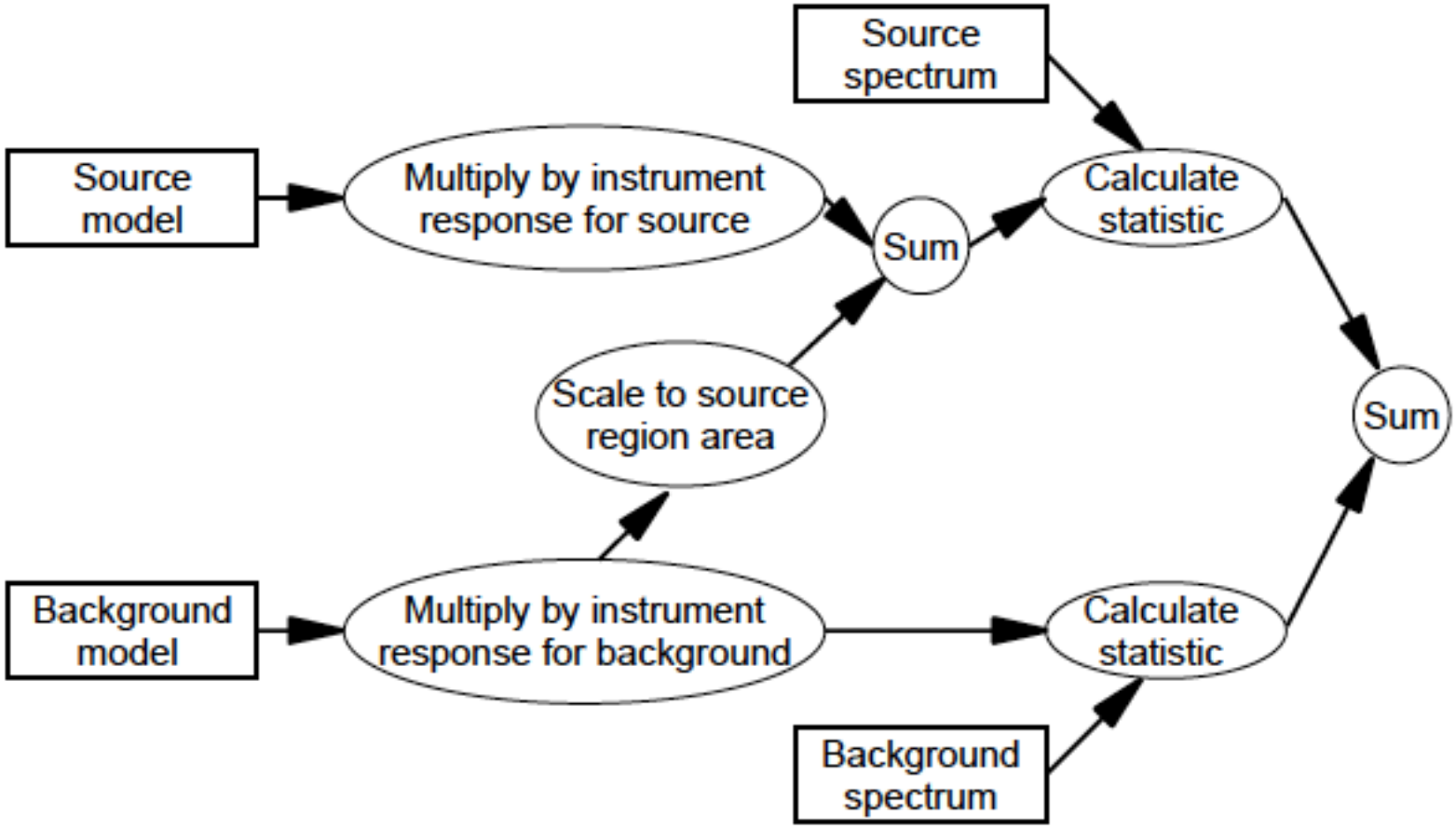
```
XSPEC12>data    mysource.pha
XSPEC12>back    myback.pha
```

If the source and background spectra both have gaussian errors then this is simple but in other cases it is not. XSPEC does attempt to deal with the case of Poisson errors (which is most of X-ray astronomy) but there can be problems.

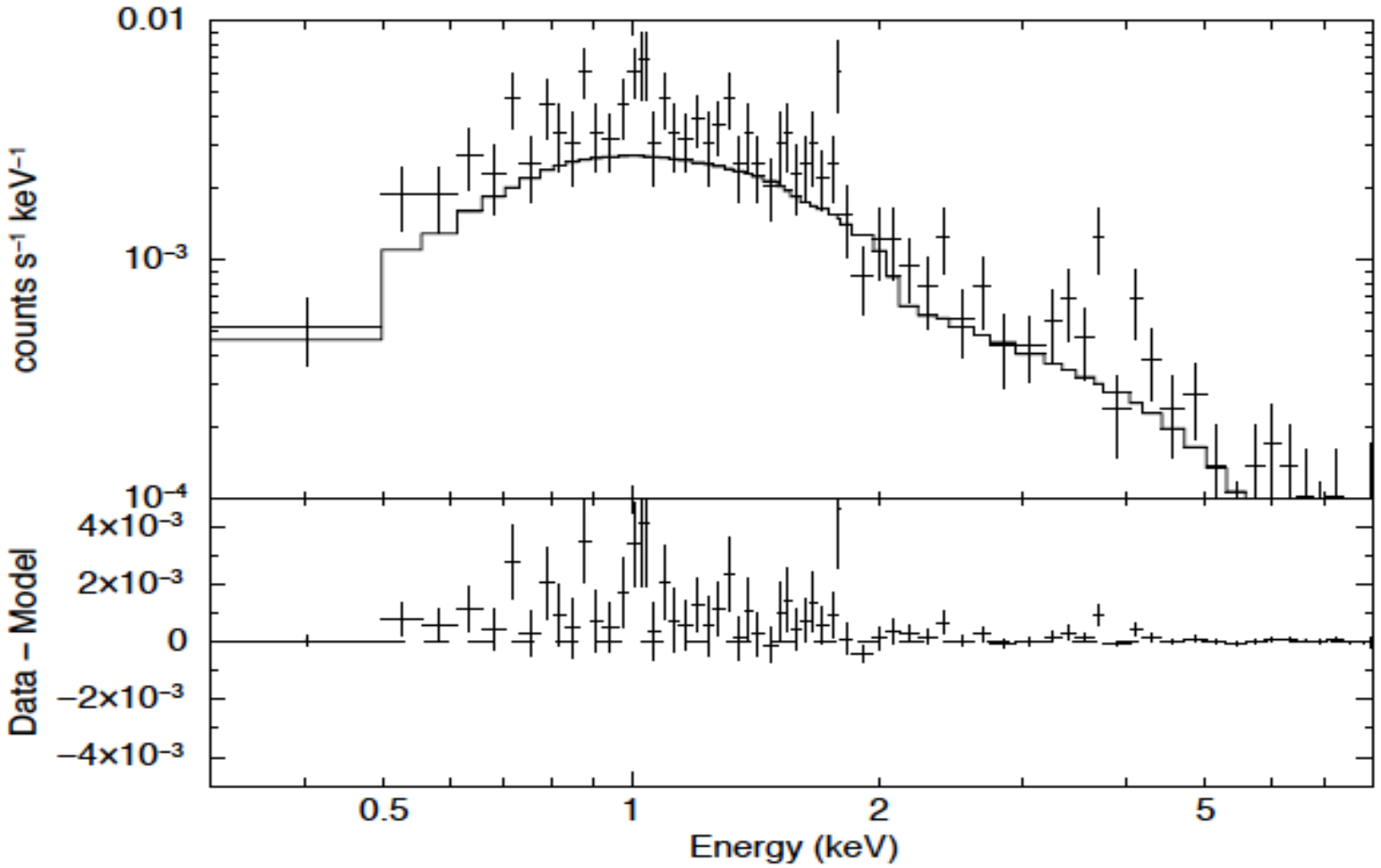
The statistically correct way of dealing with background is to simultaneously fit a model of the source and the background to the source spectrum and a model of the background to the background spectrum. The parameters of the background model are the same for both the source and background observations.

A couple of examples of defining models for the background are in Eckert et al. 2014, A&A 570, 119 and Buchner et al. 2017, MNRAS 464, 454.

Simultaneous fitting of source and background spectra.



Be careful if you have few photons/bin. Chi-squared is biased in this case with fluctuations below the model having more weight than those above, causing the fit model to lie below the true model.



A common solution is to bin up your spectrum so all the bins have > some number of photons. Be careful about this – it can introduce a bias which is difficult to quantify. If you must bin up the data there is an optimal scheme based on the resolution of the detector and the number of counts which is available in eg ftgrouppha.

The best solution is to use the correct maximum likelihood statistic (the "C statistic" - *stat cstat* in XSPEC). If you must use chi-squared then a better method than binning the date is to change the weighting scheme (I like the *weight churazov* option in XSPEC).

More at https://astrophysics.gsfc.nasa.gov/XSPECwiki/low_count_spectra
See also the statistics appendix to the XSPEC manual at https://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/manual/node304.html

The standard XSPEC interface is written in Tcl and is difficult to use for complex scripts. PyXspec is a Python package which provides a way of running XSPEC from the Python interface.

Internal XSPEC data can then be used in other Python packages. For instance plotting can be done using matplotlib.

https://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/python/html

heasp is a new(ish) C++ library and Python package to read, write and manipulate all the file types used by XSPEC.

heasarc.gsfc.nasa.gov/docs/software/lheasoft/headas/heasp/heasp_guide.html

heasptools are a collection of ftools built on top of heasp. These are intended to replace a number of the ftools in the heasarc and caltools packages. They should be more stable and in some cases have additional capabilities. For instance, ftgrouppha is more flexible than grppha.

heasarc.gsfc.nasa.gov/lheasoft/ftools/headas/heasptools.html

Final Advice and Admonitions

Remember that the purpose of spectral fitting is to attain understanding, not fill up tables of numbers.

Try not to bin up your data - especially in a way that is dependent on the data values (eg group min 15).

Try to test whether you really have found the best-fit.

XSPEC: heasarc.gsfc.nasa.gov/docs/xanadu/xspec
heasarc.gsfc.nasa.gov/docs/xanadu/xspec/python
xspec12@bigbang.gsfc.nasa.gov
Facebook group

Sherpa: cxc.harvard.edu/sherpa

ISIS: space.mit.edu/cxc/isis

SPEX: www.sron.nl/astrophysics-spex

Handbook of X-ray Astronomy (Cambridge Observing Handbooks for Research Astronomers 7) 1st Edition, Kindle Edition

by Keith Arnaud (Editor), Randall Smith (Editor), Aneta Siemiginowska (Editor)

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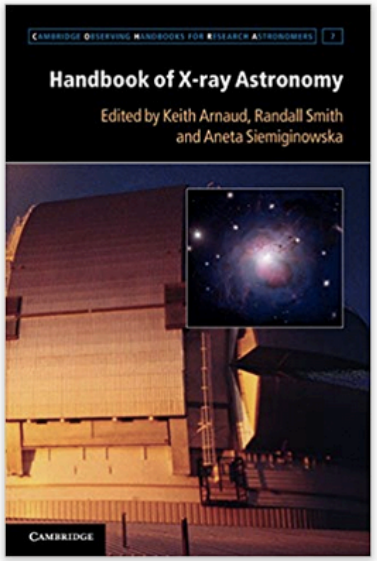

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Congratulations and Best Wishes to Goddard alum Christina Hammock Koch!