

X-RAY SPECTROSCOPY: PART II - FITTING DATA

MICHAEL A. NOWAK

(MIT-CHANDRA X-RAY SCIENCE CENTER)

-WITH HELP OVER THE YEARS FROM-

JÖRN WILMS, JOHN DAVIS, JOHN HOUCK,

DAVE HEUNEMOERDER, MIKE NOBLE

OUTLINE (PART II):

- THE DEFINITION OF THE FIT EQUATION
 - THE DANGERS OF INVERTING THE EQUATION
- THE FORWARD FOLDING PARADIGM
 - DEFINING A MODEL & SETTING PARAMETERS
- STRATEGIES FOR FITTING - A WORKED EXAMPLE
- SAVING YOUR FITS
- ADVANCED STUFF

SOLVING THE FIT EQUATION:

$$C(h) = \int_0^{\infty} \sum_i R_i(h, E) A_i(E) S_i(E) dE dT + B(h)$$

REALLY JUST A MATRIX EQUATION-

$$C_h = T \sum_i \sum_E R_{hE}^i A_E^i S_E^i dE + B_h$$

CAN'T WE INVERT IT?

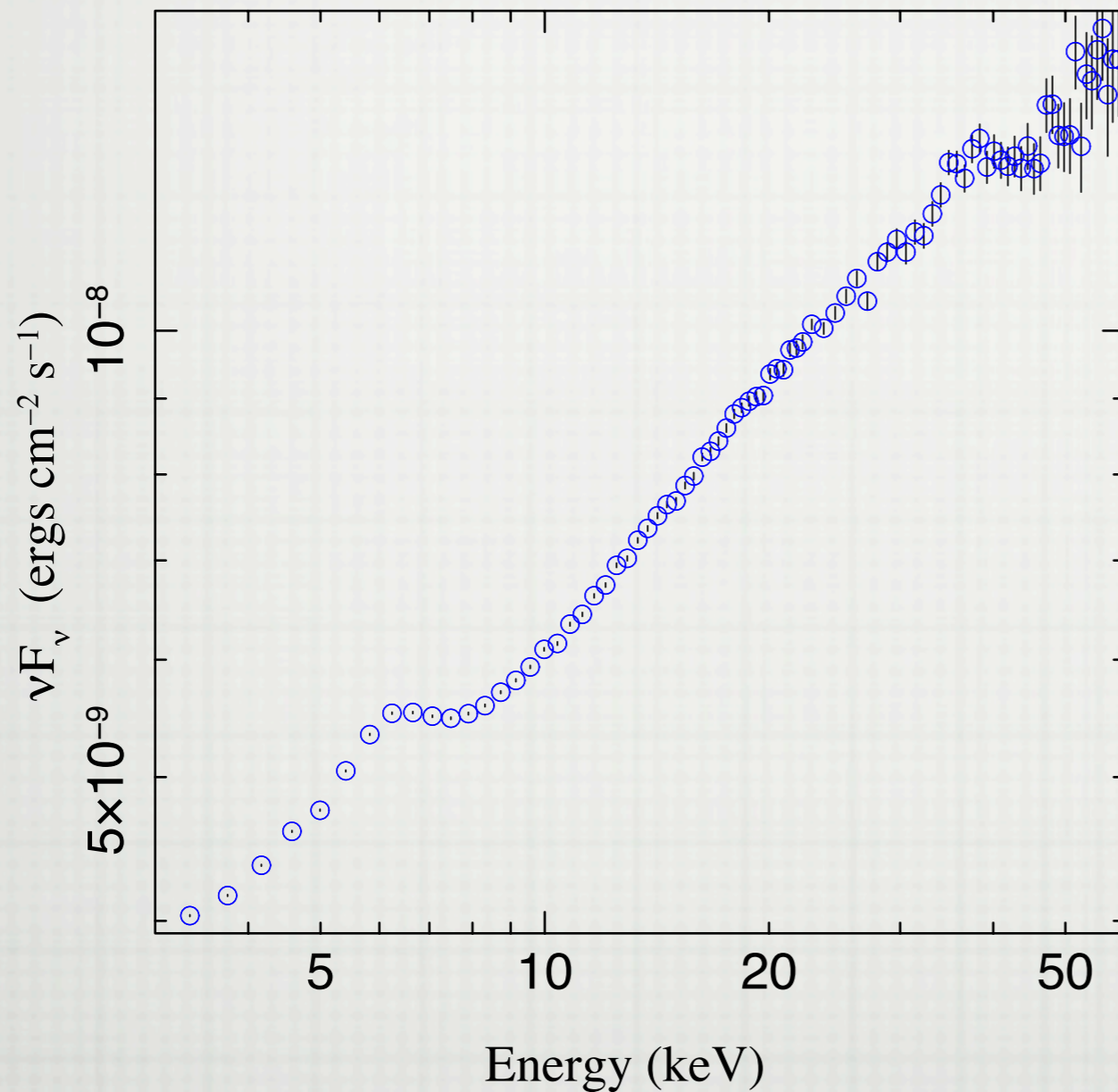
NO!
HORRIBLY
UNSTABLE!

$$R_{hE}^{-1} \frac{(C_h - B_h)}{T A_E} = S_E dE$$

NOISE

UNCERTAINTIES

WHAT ABOUT "UNFOLDING" THE SPECTRUM? DANGEROUS!!!

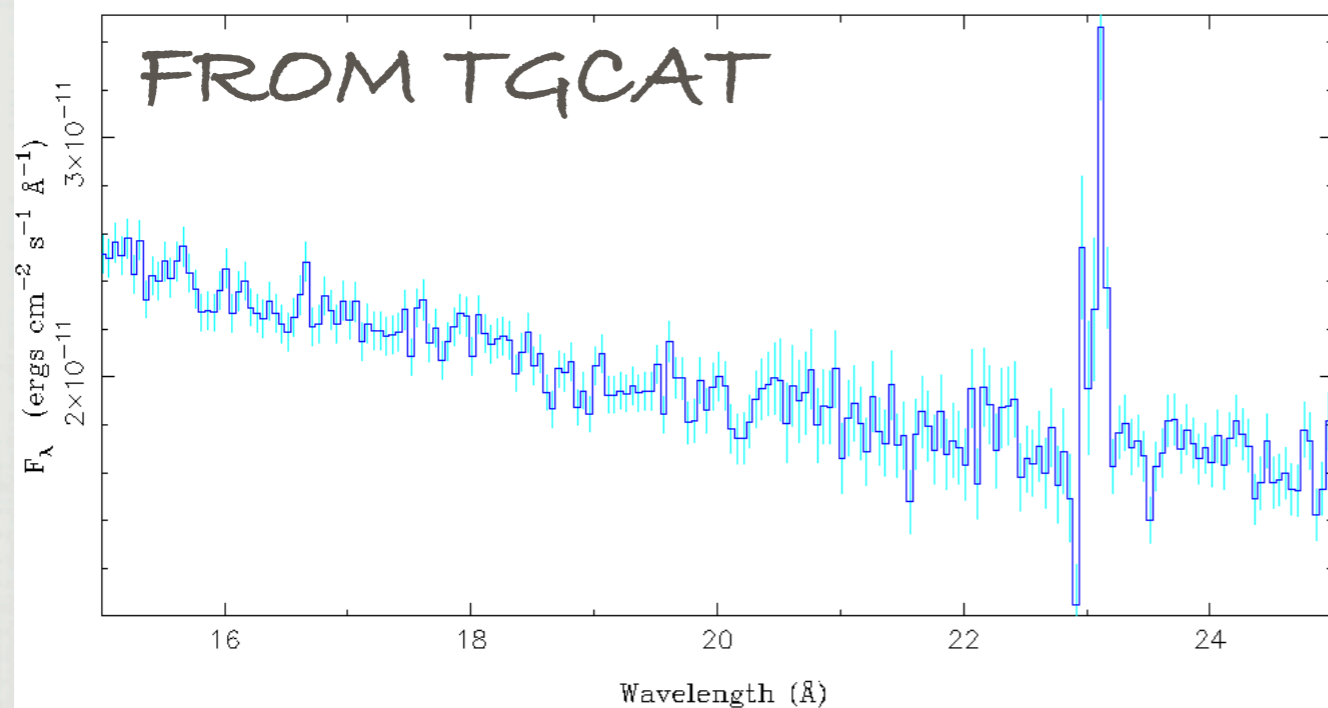


$$\mathcal{F}(h) = \frac{C(h) - B(h)}{T \sum_E R_{hE} A_E}$$

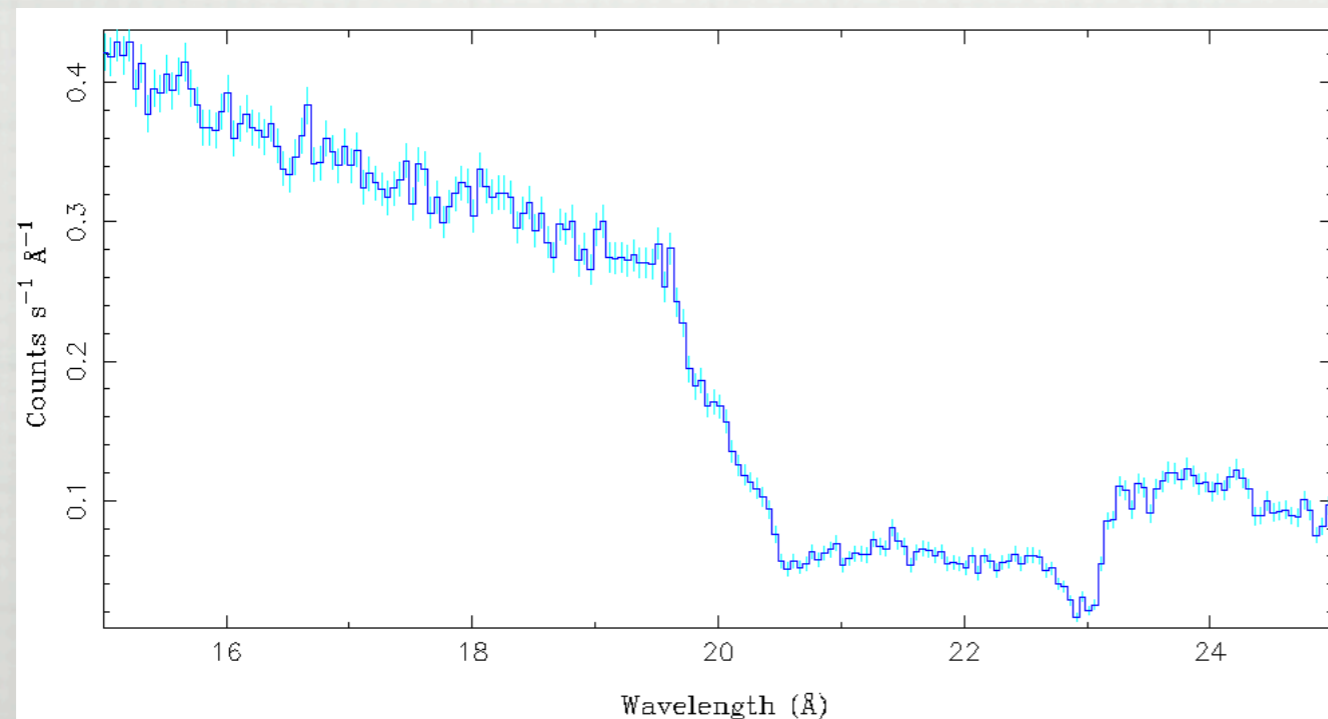
MOST "UNFOLDED"
SPECTRA IN THE
LITERATURE HAVE
NOT BEEN DONE
THIS WAY!
(THEY'RE EVEN MORE
DANGEROUS!)

```
isis> fancy_plot_unit("kev", "ergs");  
isis> plot_unfold(pca; dsym=4, dcol=4, xrng={3, 60});
```

UNFOLDED SPECTRA CAN BE VERY MISLEADING



THIS LOVELY
"EMISSION
LINE" IN
XTE J1118+480



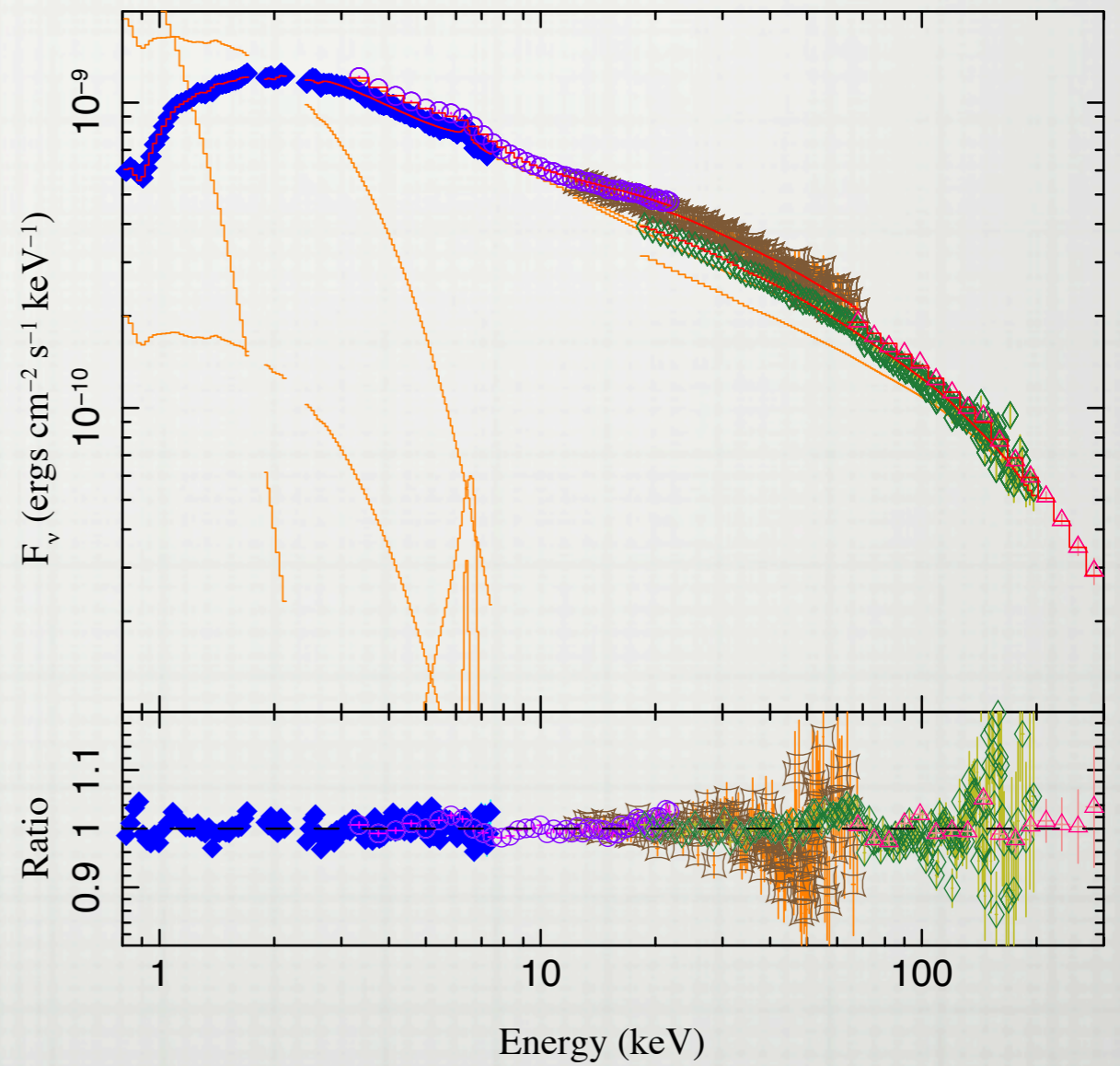
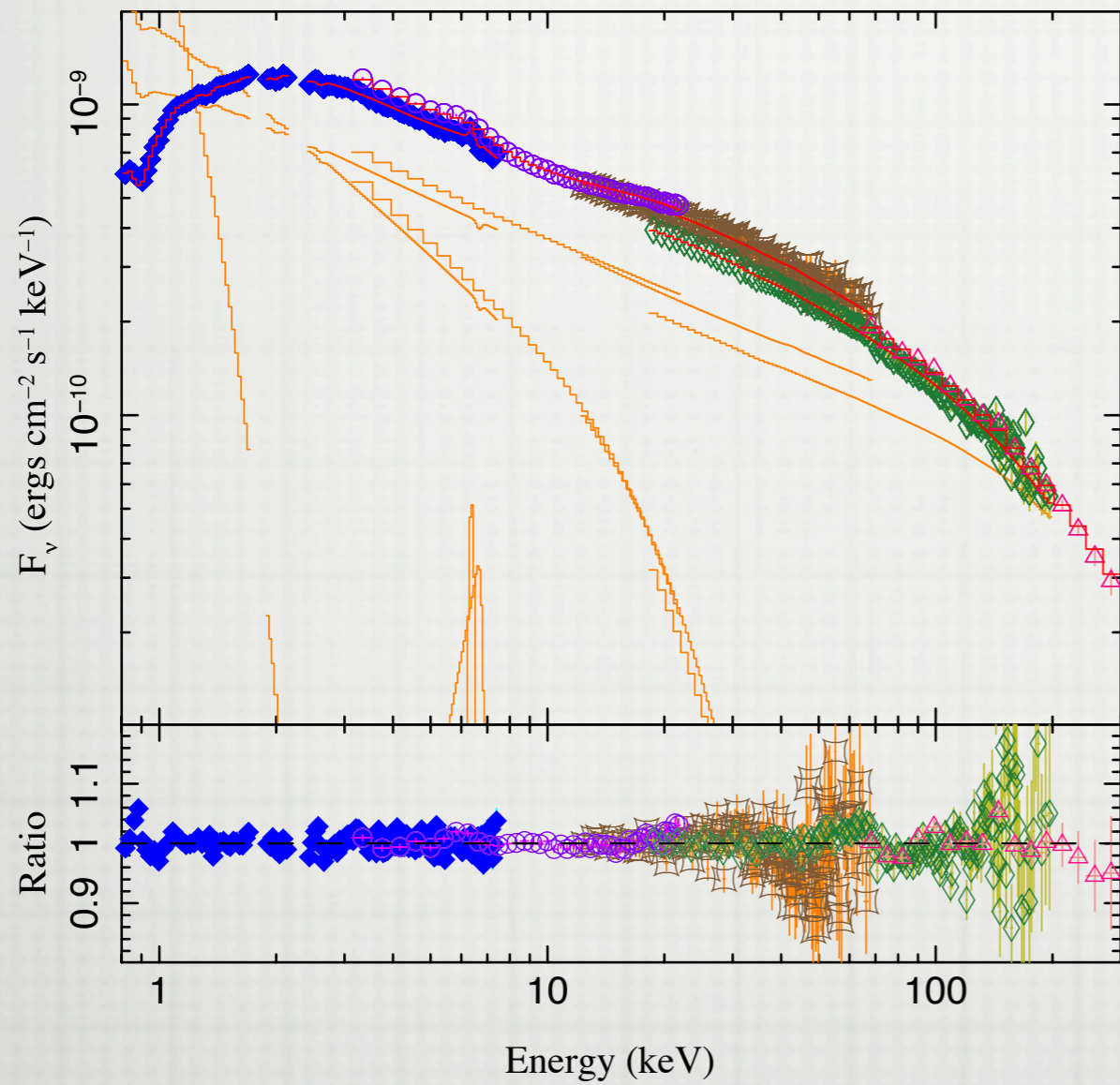
IS REALLY A
DETECTOR
FEATURE

SOLVING THE FIT EQUATION:

$$\sum_h \frac{[C_h - B_h - T \sum_i \sum_E R_{hE}^i A_E^i \mathcal{F}_E(M_p)]^2}{\sigma_h^2}$$

- "FORWARD FOLDING" - VARY A SET OF MODEL PARAMETERS, CALCULATING COUNTS/BIN, AND MINIMIZE A STATISTIC - TYPICALLY χ^2
- THIS IS ALSO NOT "UNIQUE"! DIFFERENT MODELS CAN YIELD NEARLY IDENTICAL FIT STATISTICS.

IDENTICAL DATA, DIFFERENT FITS, SIMILAR STATISTICS



STEPS FOR PERFORMING A SUCCESSFUL X-RAY ANALYSIS

- LOAD THE DATA - CHECK THAT IT IS WHAT YOU WANT!
- PLOT THE DATA - *SEE* THAT IT IS WHAT YOU WANT!
- GROUP & NOTICE THE DATA OF INTEREST. PLOT!
- DEFINE A MODEL. PUT IN "REASONABLE" STARTING PARAMETERS. *EVALUATE THE MODEL*, AND PLOT!
- THINK! REASONABLE? IF NOT, ITERATE!

STEPS FOR PERFORMING A SUCCESSFUL X-RAY ANALYSIS

- FIT THE DATA. PLOT THE RESULTS. LOOK AT PARAMETERS.
- THINK! REASONABLE? IF NOT, ITERATE!
- SEARCH FOR ERROR BARS. LOOK AT RESULTS.
- THINK! REASONABLE? IF NOT, ITERATE!
- TRY OTHER MODELS. DO THEY WORK AS WELL? DO THEY ALSO MAKE PHYSICAL SENSE?

GROUPING & NOTICING

- WE SET SYSTEMATIC ERRORS, & GROUP THE DATA

```
isis> set_sys_err_frac(pca,Double_Type[129]+0.005);  
isis> group(pca;min_sn=5,bounds=3,unit="kev");  
isis> notice_values(pca,3,20;unit="kev");
```

- GROUP CAN GET FANCY FOR DATA ON THE SAME GRID:

```
isis> group([1,2];min_sn={5,8},min_chan={1,4},  
           bounds={3,15},unit="kev",sn_data=1);  
isis> notice_values([1,2],3,5,8,20;unit="kev");
```

- EXCLUDE/INCLUDE DATA WITHOUT CHANGING BINS"

```
isis> exclude(1); % ignore dataset #1  
isis> include(1); % bring back with previous binning
```

AREN'T SYSTEMATIC ERRORS EVIL?

- YES! BUT SOMETIMES IT'S ALL WE'VE GOT.
- PEOPLE ARE WORKING ON FANCY METHODS WITH BAYESIAN STATS, MARKOV CHAIN MONTE CARLO, ...
- USEFUL IN SOME SITUATIONS, BUT ...
- THEY PRESUME A "DEFINABLE", CORRELATED BUT RANDOM UNCERTAINTY
- PRESUME FITS TO AN ISOLATED DATA SET
- NEITHER IS TRUE FOR PCA+HEXTE: SYSTEMATICS DOMINATE THE FIRST, BUT NOT THE LATTER

HOW DOES THE FIT FUNCTION WORK IN ISIS?

```
fit_fun("convolution(#, funct1(#)*(funct2(#)+funct3(#))  
+ funct4(#)+...");
```

- ISIS TREATS FUNCTIONS AS VECTORS OF VALUES. ANYTHING THAT MAKES MATH SENSE "WORKS".
- MODELS ARE (USUALLY) COUNTS/BIN, SO MATH SENSE IS NOT NECESSARILY PHYSICAL SENSE!

HOW DOES THE FIT FUNCTION WORK IN ISIS?

```
fit_fun("convolution(#, funct1(#)*(funct2(#)+funct3(#))  
+ funct4(#)+...");
```

- #'S ARE USED TO IDENTIFY AN "INSTANCE" OF A MODEL. THUS YOU CAN HAVE GAUSSIAN(1), GAUSSIAN(5), THE NUMBERS KEEP THE INSTANCES DISTINCT. EACH CAN HAVE THEIR OWN PARAMETERS.
- "WILD CARD" CHARACTERS CAN BE USEFUL HERE:

```
set_par("gaussian(*).Sigma", 0.1, 0, 0, 0.5);
```
- PARAMETER NAMES ARE CASE SENSITIVE!

DEFINING THE FIT FUNCTION

```
isis> fit_fun("phabs(1)*powerlaw(1)");
isis>
isis> list_par; % Or just list_free to see the unfrozen parameters.
phabs(1)*powerlaw(1)
  idx  param                tie-to  freeze  value  min  max
   1  phabs(1).nH            0      0      1     0  100000  10^22
   2  powerlaw(1).norm       0      0      1     0    1e+10
   3  powerlaw(1).PhoIndex   0      0      1    -2     9
isis>
isis> % Could use edit_par; to use an editor window, or, on the command line ...
isis> set_par(1,0.6,-1); % Or: set_par("phabs(*).nH",0.6,-1);
isis> set_par(3,1.7,0,1,3);
isis>
isis> () = renorm_counts;
Parameters[Variable] = 3[1]
      Data bins = 45
      Chi-square = 2210.172
      Reduced chi-square = 50.23119
```

- USE YOUR KNOWLEDGE OF PHYSICS AND THE PROPERTIES OF THE SOURCE TO GUIDE YOUR INITIAL PARAMETER GUESSES!

HOW DOES THE FIT FUNCTION WORK IN ISIS?

```
fit_fun("convolution(#, funct1(#)*(funct2(#)+funct3(#))  
+ funct4(#)+...");
```

- YOU CAN RENAME ANY MODEL WITH: `alias_fun("old", "new");`
- CONVOLUTION MODELS HAVE A UNIQUE SYNTAX.
- REFLECTION, RELATIVISTIC SMEARING = CONVOLUTION
- THE UNIQUE ISIS VARIABLE, `Isis_Active_Dataset`, CAN BE USED TO IDENTIFY & ISOLATE MODEL "INSTANCES".
- `Isis_Active_Dataset = #` OF DATA SET BEING EVALUATED.
- `gaussian(Isis_Active_Dataset) = gaussian(1)` FOR DATA SET 1, `= gaussian(2)` FOR DATA SET 2, ETC.

HOW DOES THE FIT FUNCTION WORK IN ISIS?

```
fit_fun("convolution(#, funct1(#)*(funct2(#)+funct3(#))  
+ funct4(#)+...");
```

- THE FUNCTIONS WILL BE EVALUATED ON THE *INTERNAL* ARF GRID (USUALLY FINER THAN THAT FOR PHA).
- YOU CAN FORCE ISIS TO USE ANY GRID & REBIN TO ARF
- ISIS WILL LOOK AT THE RMF AND ONLY EVALUATE AT ENERGIES WHERE E->PHA BINS THAT ARE "NOTICED".
- YOU CAN FORCE ISIS TO EVALUATE A WIDER RANGE - SOMETIMES NECESSARY FOR CONVOLUTION MODELS.
- ISIS EVALUATES WHOLE MODEL FOR *EACH* DATA SET

THINGS YOU CAN DO WITH PARAMETERS

- YOU CAN FREEZE OR THAW ANY FIT PARAMETER:

```
isis> set_par("phabs(1).nH",0.6,1);           % 1 Freezes
isis> set_par("phabs(1).nH",0.6,0);           % 0 Thaws
isis> freeze("phabs(1).nH"); freeze(1);      % Either works
isis> thaw("phabs(1).nH"); thaw(1);          % Either works
```

- YOU CAN TIE PARAMETER VALUES TOGETHER.

```
isis> tie(1,2,3,4);                          % Tie parameters 2-4 -> 1
isis> untie(2,3,4);                          % Untie parameters 2-4
```

THINGS YOU CAN DO WITH PARAMETERS

- ANY PARAMETER CAN BE MADE AN ARBITRARY FUNCTION OF ANY OTHER PARAMETER(S)!

```
isis> set_par_fun("phabs(1).nH", "sin(powerlaw(1).norm)+2");  
isis> set_par_fun(1, "sin(_par(2))+2");  
isis> set_par_fun(1, NULL);      % That was stupid, let's not!
```

- USE CONSTANT AS A CONVENIENT DUMMY PARAMETER

```
isis> fit_fun("gaussian(1)+gaussian(2)+0*constant(1)");  
isis> set_par_fun("gaussian(2).LineE",  
                 "gaussian(1).LineE+constant(1).factor");
```

GETTING ON WITH THE FITTING

- START OFF WITH "LEAST IMPORTANT" AND "NARROW BAND" PARAMETERS FROZEN.
- LIMIT PARAMETER RANGES TO "SENSIBLE" VALUES.
- TRY AN OVERALL RE-NORMALIZATION FIRST.
- FIT! CHOOSE FROM SEVERAL OPTIMIZATION METHODS:

```
isis> set_fit_method("lmdif");           % Default. Good & fast.
isis> set_fit_method("marquardt");      % Sometimes works better
isis>                                   % than lmdif. Fast.
isis> set_fit_method("subplex");        % Very slow, but can find
isis>                                   % minima that others miss
isis> set_fit_method("plm");            % parallelized Levenberg-
                                         % Marquardt for multi-core
                                         % machines
```

THINGS TO KNOW ABOUT FITTING METHODS

```
isis> set_fit_method("lmdif");  
isis> set_fit_method("marquardt");
```

- LEVENBERG-MARQUARDT METHODS EXPECT CHI²-TYPE STATISTICS, I.E.: $\sum_i (D_i - M_i)^2 / \sigma_i^2$

```
isis> set_fit_method("subplex");
```

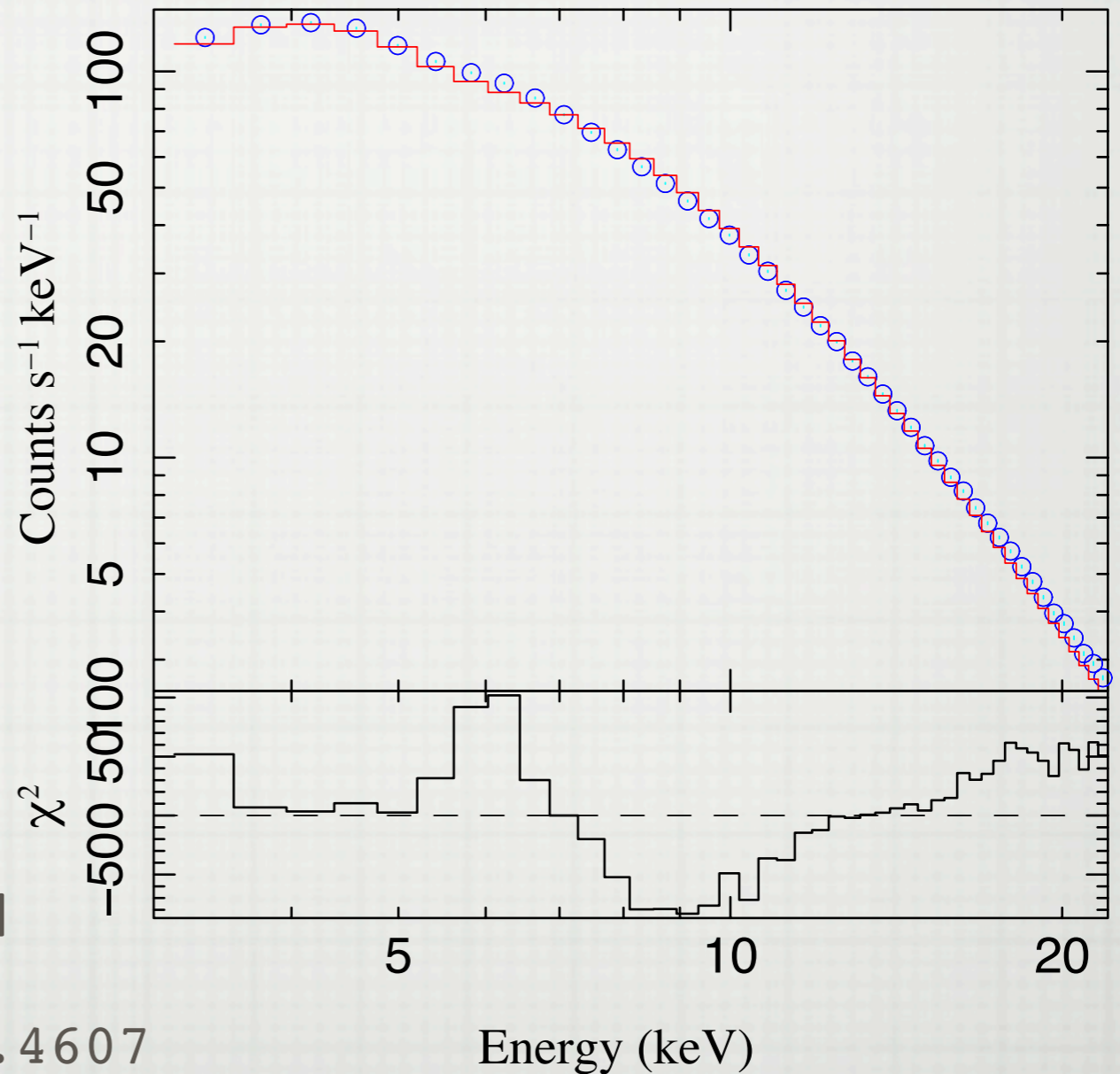
- SUBPLEX CAN BE USED ON CASH STATISTICS.
(NOTE- ISIS CASH IS THE SAME AS XSPEC/
SHERPA CSTAT.)

GETTING ON WITH THE FITTING

UNTIL YOU
REALLY KNOW
WHAT YOU'RE DOING,
PLOT RESIDUALS
WITH χ^2 !

```
isis> () = fit_counts;  
Parameters[Variable] = 3[2]  
Data bins = 45  
Chi-square = 672.4607  
Reduced chi-square = 15.63862
```

```
isis> plot_data(pca; dsym=4, dcol=4, decol=5, xrng={3, 22}, res=2);
```

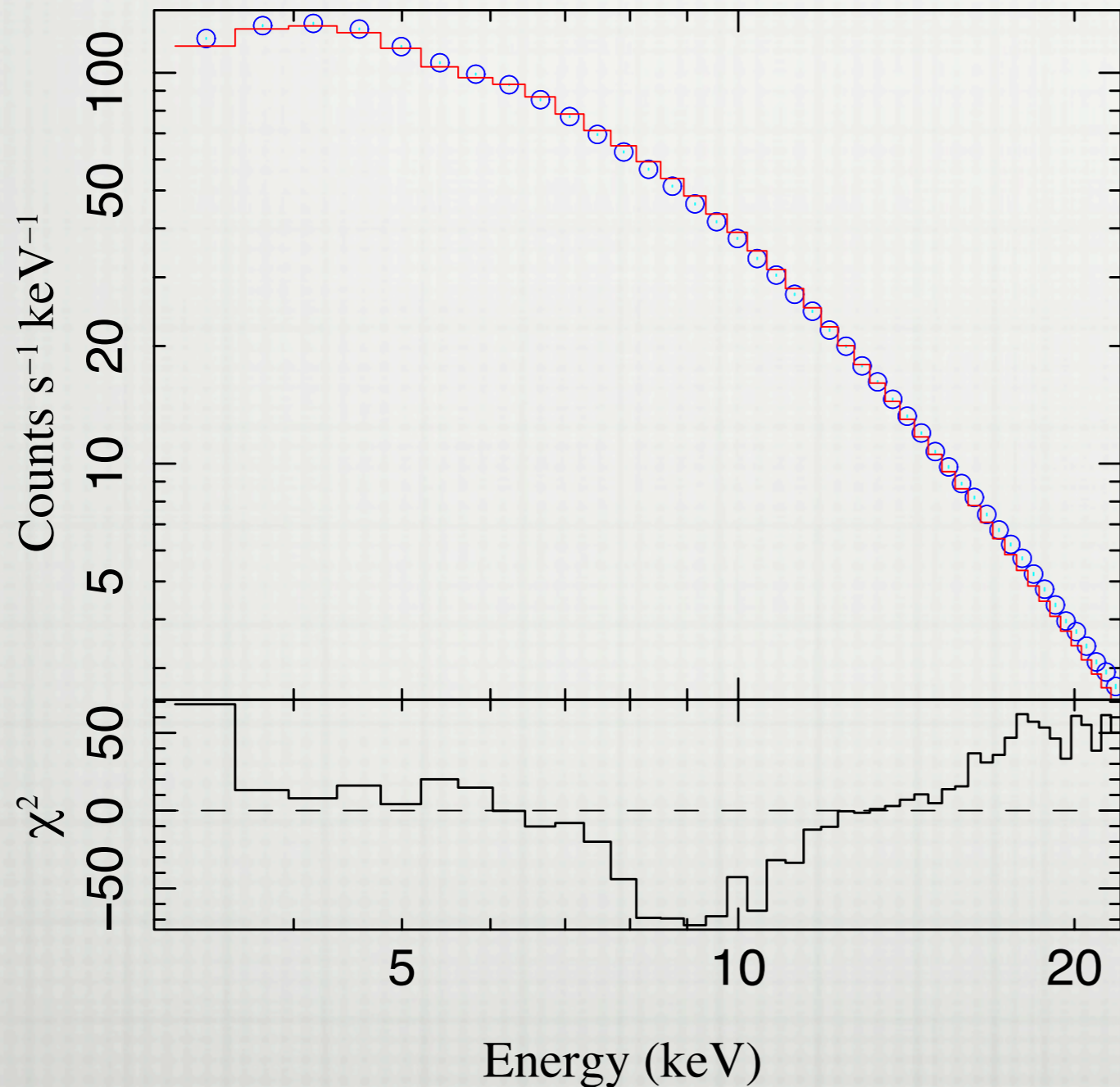


LINE? ADD ONE AND REFIT

```
isis> fit_fun("phabs(1)*(powerlaw(1)+gaussian(1))");
isis> list_par;
phabs(1)*(powerlaw(1)+gaussian(1))
  idx  param                tie-to  freeze      value      min      max
  ---  ---                ---    ---      ---      ---      ---
  1    phabs(1).nH          0      1         0.6        0      100000  10^22
  2    powerlaw(1).norm     0      0        1.539388   0       1e+10
  3    powerlaw(1).PhoIndex 0      0        1.588304   1         3
  4    gaussian(1).norm     0      0         1          0       1e+10
  5    gaussian(1).LineE    0      0         6.5        0      1000000  keV
  6    gaussian(1).Sigma    0      0         0.1        0         10     keV

isis> set_par("gaussian(1).LineE",6.4,1,6,7);
isis> set_par("gaussian(1).norm",0.1,0,0,1);
isis> () = fit_counts;
Parameters[Variable] = 6[3]
      Data bins = 45
      Chi-square = 623.9285
      Reduced chi-square = 14.85544
isis> thaw(6);
isis> () = fit_counts;
Parameters[Variable] = 6[4]
      Data bins = 45
      Chi-square = 618.4107
      Reduced chi-square = 15.08319
isis> plot_data(pca;dsym=4,dcol=4,decol=5,xrng={3,22},res=2);
```

SOME, BUT NOT ENOUGH, IMPROVEMENT



THE RESIDUALS
SEEM TO INDICATE
THAT A BREAK IN
THE POWERLAW
WOULD IMPROVE
THE FIT.

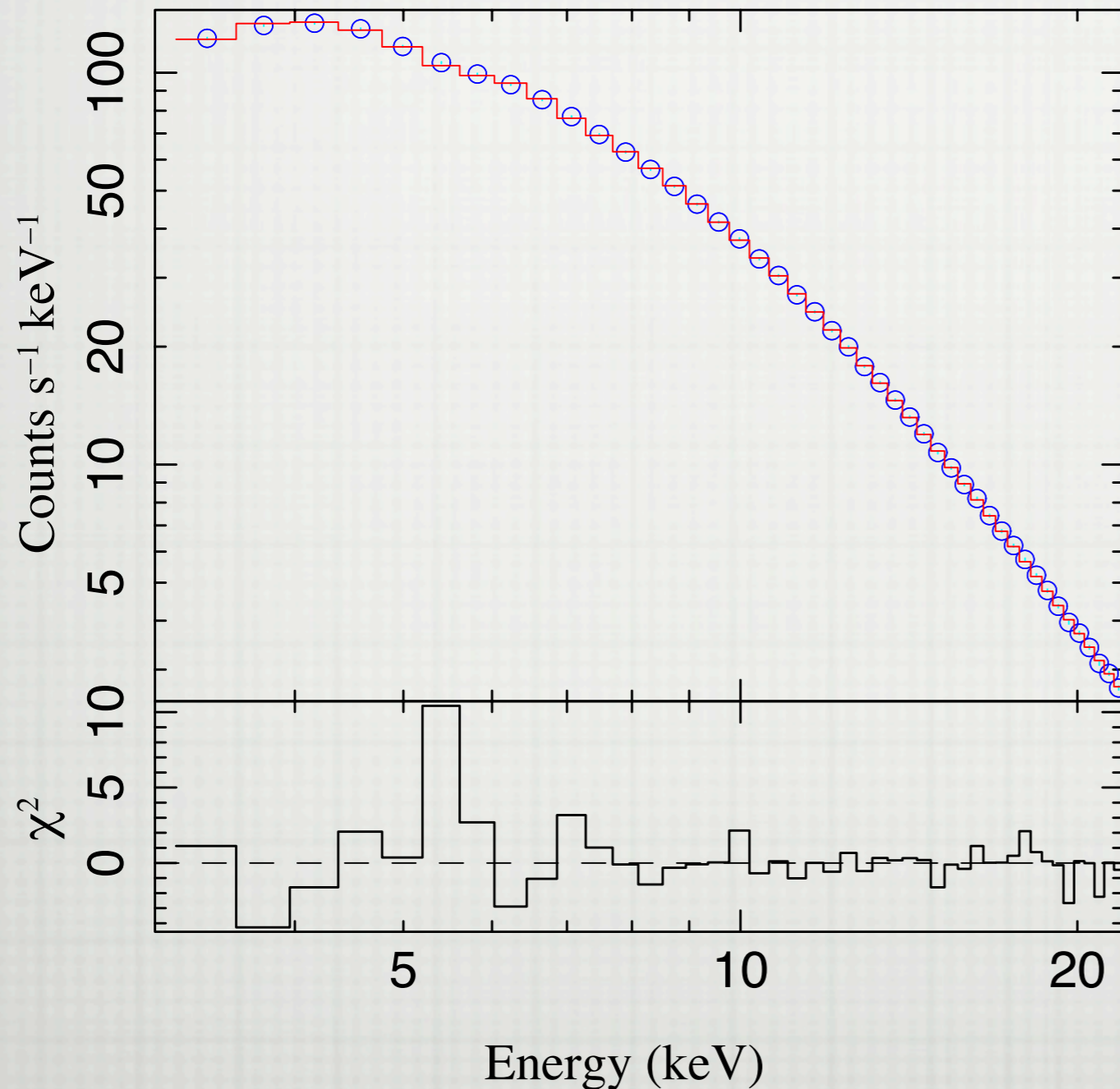
LET'S ADD ONE.

```

isis> fit_fun("phabs(1)*(bknpower(1)+gaussian(1))");
isis> list_par;
phabs(1)*(bknpower(1)+gaussian(1))
  idx  param                tie-to  freeze      value      min      max
  1  phabs(1).nH              0      1         0.6         0      100000  10^22
  2  bknpower(1).norm         0      0          1          0      1e+10
  3  bknpower(1).PhoIndx1     0      0          1         -2         9
  4  bknpower(1).BreakE       0      0          5         0.01     1000000  keV
  5  bknpower(1).PhoIndx2     0      0          2         -2         9
  6  gaussian(1).norm         0      0    0.006378002  0         1
  7  gaussian(1).LineE        0      1          6.4         6         7  keV
  8  gaussian(1).Sigma        0      0    5.283852e-05  0         1  keV
isis>
isis> set_par(2,1.5,0,0.1,10); % bknpower has same normalization as powerlaw
isis> set_par(3,1.6,0,1,3); % slope wasn't too far off
isis> set_par(4,10,0,8,13); % break looks to be around 9 or 10 keV
isis> set_par(5,1.4,0,1,3); % second power law looks "harder"
isis>
isis> () = renorm_counts;
Parameters[Variable] = 8[1]
      Data bins = 45
      Chi-square = 397.054
      Reduced chi-square = 9.023955
isis>
isis> () = fit_counts;
Parameters[Variable] = 8[6]
      Data bins = 45
      Chi-square = 23.81623
      Reduced chi-square = 0.6106725
isis> plot_data(pca;dsym=4,dcol=4,decol=5,xrng={3,22},res=2);

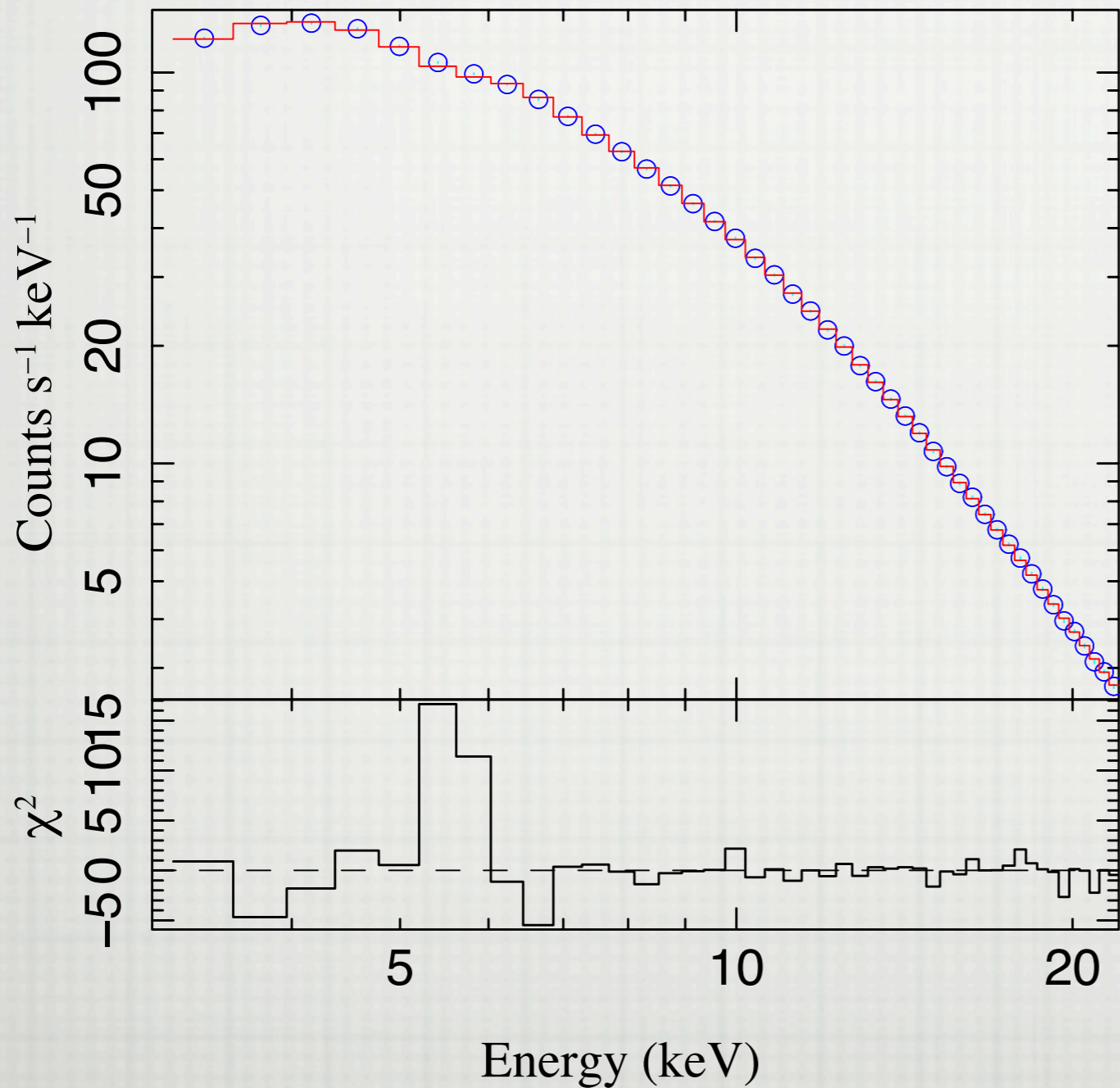
```


GETTING THERE, BUT WE MAY BE STUCK IN A LOCAL MINIMUM



ERROR BAR
SEARCHES ARE
OFTEN A GOOD WAY
TO GET "UNSTUCK"

MUCH IMPROVEMENT, BUT SOME RESIDUALS REMAIN



WE HAD FROZEN
THE ENERGY OF THE
LINE. IMPROVEMENT
IF WE LET IT GO
FREE?

```

isis> thaw("gaussian(1).LineE");
isis> () = fit_counts;
Parameters[Variable] = 8[7]
      Data bins = 45
      Chi-square = 23.81605
      Reduced chi-square = 0.6267381
isis> list_free;
phabs(1)*(bknpower(1)+gaussian(1))
idx  param                tie-to  freeze      value          min          max
  2  bknpower(1).norm        0      0          1.77756        0.1          10
  3  bknpower(1).PhoIndx1    0      0          1.677097        1            3
  4  bknpower(1).BreakE      0      0          9.76005         8           13 keV
  5  bknpower(1).PhoIndx2    0      0          1.408868        1            3
  6  gaussian(1).norm        0      0          0.008118369    0            1
  7  gaussian(1).LineE       0      0           6.4            6            7 keV
  8  gaussian(1).Sigma       0      0          5.283852e-05   0            1 keV
isis>
isis> set_fit_method("subplex");
isis> () = fit_counts;
Parameters[Variable] = 8[7]
      Data bins = 45
      Chi-square = 20.52235
      Reduced chi-square = 0.5400618
isis>
isis> set_fit_method("lmdif");
isis> () = fit_counts;
Parameters[Variable] = 8[7]
      Data bins = 45
      Chi-square = 20.39472
      Reduced chi-square = 0.5367033
isis> plot_data(pca;dsym=4,dcol=4,decol=5,xrng={3,22},res=2);

```

```

isis> conf(8); % Can search for error bars individually
**** Parameter range endpoint 0 is inside the confidence limit
**** Lower confidence limit didn't converge[8]: allow wider parameter ranges?
Found improved fit, stat= 15.072 for param[8] = 0.500079
**** Found improved fit
0.500079
0.500079
isis>
isis> (,) = conf_loop(,1,0.1;save,prefix="bknpower_gaussian.");
Found improved fit, stat= 14.6825 for param[2] = 1.76451
**** Found improved fit
Parameters[Variable] = 8[7]
      Data bins = 45
      Chi-square = 14.62909
      Reduced chi-square = 0.3849759
isis>
isis> !more bknpower_gaussian.save
phabs(1)*(bknpower(1)+gaussian(1))

```

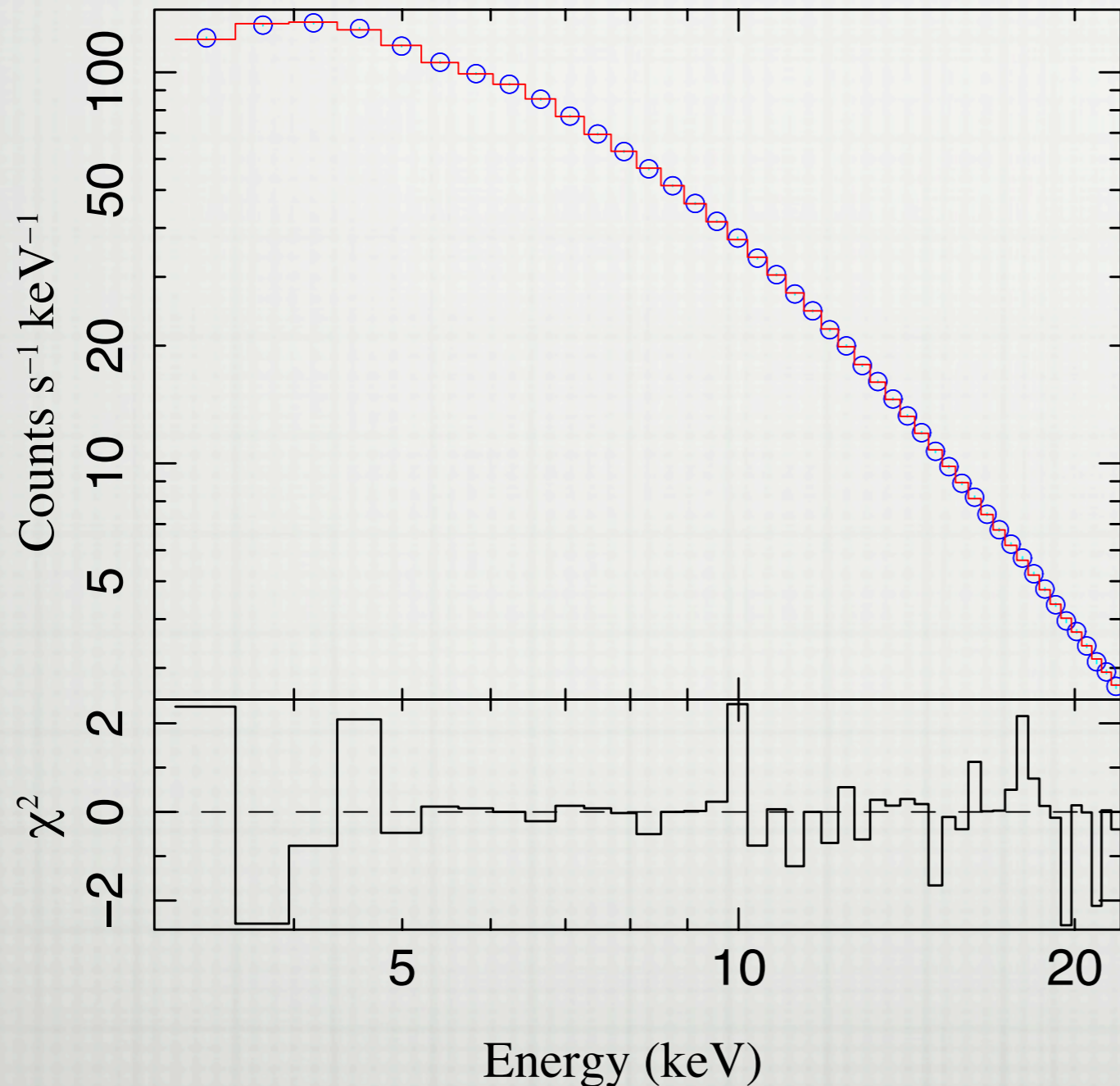
idx	param	tie-to	freeze	value	min	max	
1	phabs(1).nH	0	1	0.6	0	100000	10^22
2	bknpower(1).norm	0	0	1.769163	1.736502	1.803789	
3	bknpower(1).PhoIndx1	0	0	1.676277	1.664857	1.688937	
4	bknpower(1).BreakE	0	0	9.626676	9.136459	10.09752	keV
5	bknpower(1).PhoIndx2	0	0	1.410334	1.393771	1.426189	
6	gaussian(1).norm	0	0	0.01083106	0.008576826	0.01347842	
7	gaussian(1).LineE	0	0	6.160142	6.028331	6.29854	keV
8	gaussian(1).Sigma	0	0	0.4182171	0.192534	0.6204544	keV

```

isis>
isis> plot_data(pca;dsym=4,dcol=4,decol=5,xrng={3,22},res=2);

```

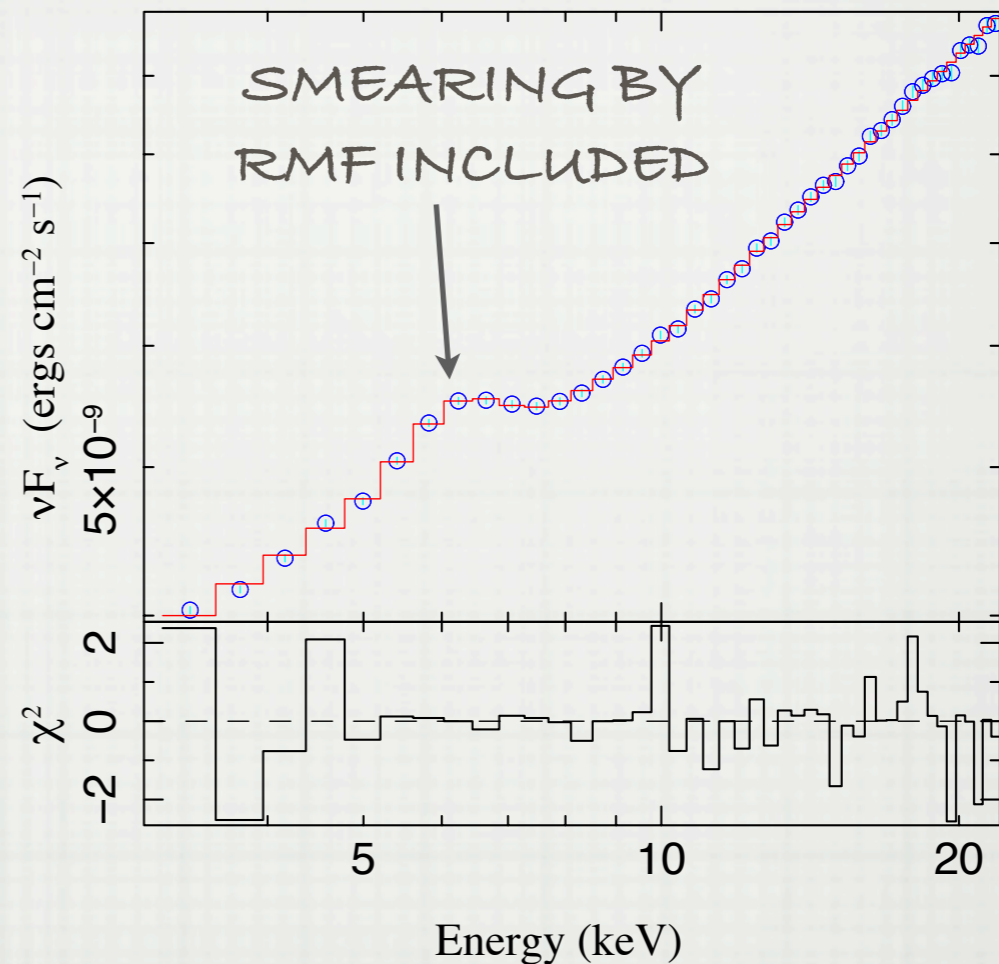
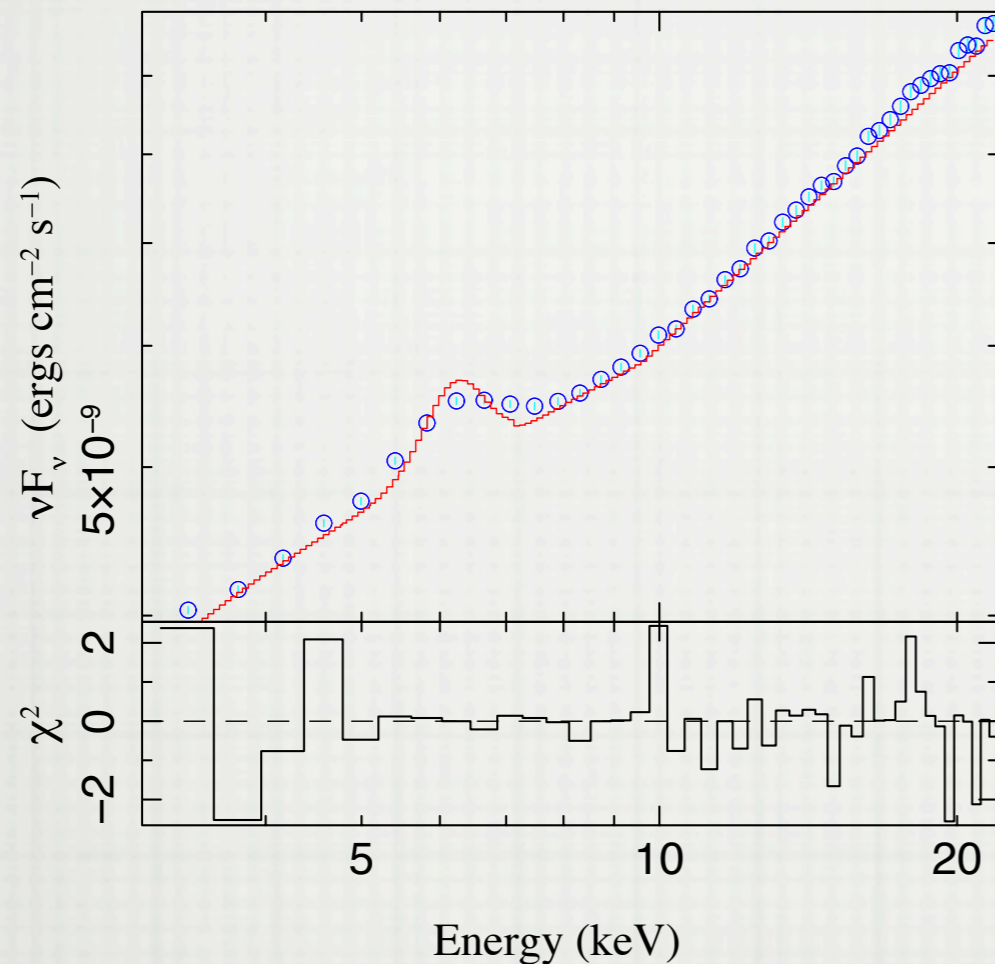
LOW χ^2 : OVERPARAMETERIZED, OR SYST ERRORS TOO LARGE



ERROR BARS IN
LINE REGION A
LITTLE "TOO FLAT".

NOTE ALSO THAT
CUSTOM IN X-RAY
ASTRONOMY IS TO
QUOTE 90%
CONFIDENCE LIMIT
ERROR BARS.

NOW YOU ARE ALLOWED TO LOOK AT THE UNFOLDED SPECTRA



```
isis> plot_unfold(pca;dsym=4,dcol=4,decol=5,xrng={3,22},res=2,  
isis>           con_mod=0);  
isis> plot_unfold(pca;dsym=4,dcol=4,decol=5,xrng={3,22},res=2);  
isis>           con_mod=1);
```

SAVING YOUR RESULTS

□ SAVING AND RELOADING FITS:

```
isis> save_par("my_model.par");  
isis> load_par("my_model.par");
```

□ SAVING YOUR PLOTS:

```
isis> id = open_plot("my_model.par");  
isis> resize(21,0.85);  
isis> plot_data(1,popt);  
isis> close_plot("my_model.par");
```

FIT FUNCTIONS THAT YOU MIGHT FIND USEFUL

- `bbody`, `diskbb`, `cutoffpl`, `highecut` - BLACKBODY, DISK, POWERLAW WITH A ROLLOVER, AN EXPONENTIAL ROLLOVER (MULTIPLIES OTHER MODELS)
- `comptt`, `pexrav` - FOR THE MORE ADVENTUROUS. COMPTONIZATION, AND A "REFLECTED" POWERLAW.
- THE LATTER MODEL REQUIRES EVALUATION OUT TO ~ 1 MeV. I.E., ONE HAS TO "EXTEND THE GRID"
- TRY FORCING THE LINE TO STAY NARROW.
- FOR A LIST OF XSPEC MODELS, SEE:
<http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/manual/XspecModels.html>

ADVANCED TOPICS

- HOW DO WE CALCULATE FLUX?
- HOW DO WE CALCULATE EQUIVALENT WIDTHS?
- HOW DO WE LOOK AT χ^2 VS. PARAMETER? (I.E., EQUIVALENT TO XSPEC'S STEPPAR COMMAND)
- HOW DO WE CALCULATE ERROR CONTOURS?
- HOW DO WE PLOT MODEL COMPONENTS INDIVIDUALLY?
- EXTENDING THE FIT FUNCTION GRID & CACHING

CALCULATING FLUX

- THREE METHODS DEFINED IN THE SCRIPTS: BASED ON DATA (`data_flux`), OR BASED ON MODEL (`model_flux`, `calc_flux`)

```
isis> % Just like "unfolding" spectrum  
isis> data_flux(1,3,20;unit="kev",print);
```

```
isis> % Calculated from fit model  
isis> model_flux(1,3,20;unit="kev",print);
```

```
isis> % Uses fit model  
isis> calc_flux(1,bin_lo,bin_hi;unit="kev",print);
```

- THE FIRST TWO ONLY WORK WITHIN THE RANGE OF THE DATA, THE LAST CAN BE EXTENDED TO ANY ENERGY RANGE.

EQUIVALENT WIDTH

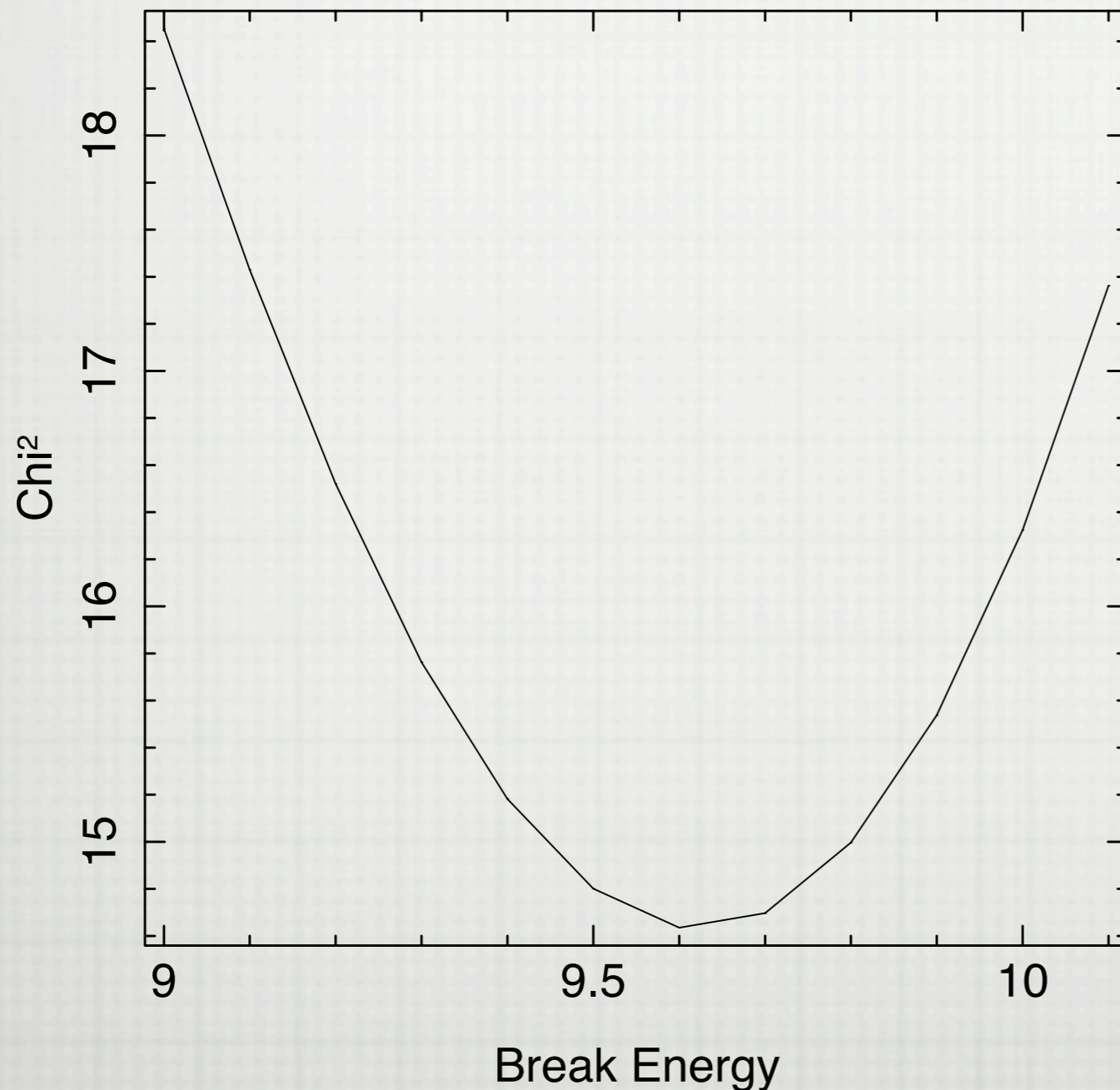
- EQUIVALENT WIDTH IS A *RELATIVE* MEASURE OF THE STRENGTH OF AN EMISSION LINE, OR THE DEPTH OF AN ABSORPTION LINE.
- IT IS THE RATIO OF $(\Delta\text{FLUX})/(\text{FLUX DENSITY})$, WHERE ΔFLUX =DIFFERENCE WITH/WITHOUT THE LINE, FLUX DENSITY IS EVALUATED AT THE PEAK OF THE LINE.
- MEASURED IN EV OR MILLI-ANGSTROM.
- EVALUATE MODEL, & USE THE SCRIPT FUNCTION: `eqw`

```
isis> (eqw_ma,eqw_ev) = eqw(pca,"gaussian(1).norm");  
isis> eqw(1,5;print); % If line norm is parameter #5
```

CHI² VS. PARAMETER (I.E., "STEPPAR")

```
isis> % The functions fit_counts; renorm_counts; eval_counts; optionally return info
isis> % about the statistics. To do this, you must pass a "reference" to a variable
isis> % in which to store these statistics. The & in front of the variable name below
isis> % says that you are passing this reference. What you get back is a structure
isis> % with fields for statistic, num_variable_params, and num_bins. Here's a short
isis> % script that will do what steppar does:
isis> define steppar(par,lo,hi,nsteps)
{
    variable par_vals=[lo:hi:(hi-lo)/nsteps];
    variable info, stat, par_use;
    stat = Double_Type[length(par_vals)];
    variable i = 0;
    foreach par_use (par_vals)
    {
        set_par(par,par_use,1); % Freeze parameter
        () = fit_counts(&info);
        stat[i] = info.statistic;
        i++;
    }
    thaw(par); () = fit_counts;
    return par_vals, stat;
}
isis> (par_vals,stat) = steppar("bknpower(1).BreakE",9,10.2,12);
isis> xrange, yrange; xlin; ylin; xlabel("Break Energy"); ylabel("Chi\\u2\\d");
isis> plot(par_vals,stat);
```

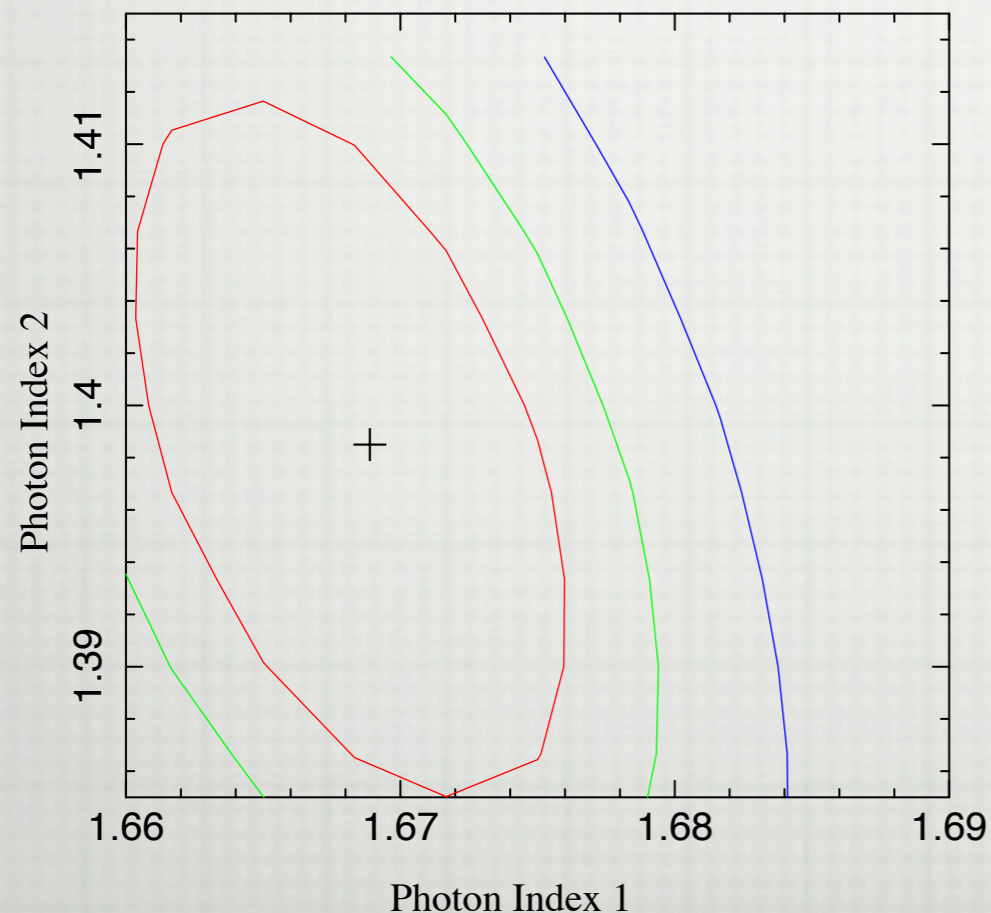
CHI² VS. PARAMETER (I.E., “STEPPAR”)



HERE ARE THE
RESULTS.
THIS WAS A QUICK
& DIRTY SCRIPT.
WITH A LITTLE
WORK, WE COULD
ADD SOME BELLS &
WHISTLES.

CONTOUR PLOTS

```
isis> % Confidence contours can be created with ISIS intrinsic functions. First you
isis> % Define the x & y grids, then create the contours, then plot and/or save them
isis>
isis> x = conf_grid(3,1.66,1.69,10); % Photon Index 1
isis> y = conf_grid(5,1.385,1.415,10); % Photon Index 2
isis> contr = conf_map_counts(x,y); % Create the contours
isis> xlabel("\frPhoton Index 1"); ylabel("\frPhoton Index 2");
isis> plot_conf(contr); % Plot the contours
isis> save_conf(contr,"file"); % Save them (later load them with load_conf;)
```



DEFAULTS ARE 68%, 90%,
AND 99% CONFIDENCE FOR 2
PARAMETERS. CUSTOM
LEVELS CAN BE CHOSEN
INSTEAD. THIS FUNCTION IS
PARALLELIZED IN ISIS.

PLOTTING INDIVIDUAL MODEL COMPONENTS

- ISIS, UNLIKE XSPEC, DOESN'T PLOT INDIVIDUAL MODEL COMPONENTS AS ISIS DOESN'T DIFFERENTIATE BETWEEN "ADDITIVE" AND "MULTIPLICATIVE" MODELS. (THEY'RE ALL JUST VECTORS!) ISIS DOESN'T KEEP TRACK OF THE SEPARATE "PIECES" REQUIRED.
- I WRITE SCRIPTS THAT CALL MY PLOTTING ROUTINES, ZEROS OUT COMPONENTS, AND OVERPLOTS SERIALY.
- FOR "MULTI-PANEL" PLOTS (E.G., DATA & RESIDUALS), A LITTLE BIT TRICKIER THAN USING THE OPLT=1 OPTION.
- EXAMPLE FOLLOWS.

PLOTTING INDIVIDUAL MODEL COMPONENTS

```
isis> define fancy_plot()
{
  % Save parameters as they initially are
  save_par("/tmp/initial.par");

  % Let's make a 3 panel plot, where the top is counts, the middle is
  % "unfolded" spectra, and the bottom is residuals with and without
  % the lines.

  % 3 panel plot, with vertical ratios of 5:5:2
  multiplot([5,5,2]);

  % pgplot is much happier if you just work on 1 pane at a time.
  % Start with the top most pane.
  mpane(1);

  % For single pane plots, the opt=1 plot option works fine. For
  % multi-panel plots, we have to tell pgplot to *not* automatically
  % jump to the next pane after doing a plot. This global variable
  % does that for my routines.
  no_reset=1;

  % First plot counts/unit/sec; X-axis will be keV. Y-axis will be
  % proportional to ergs when we plot the unfolded data.
  xlog; ylog; fancy_plot_unit("kev","ergs");
```


PLOTTING INDIVIDUAL MODEL COMPONENTS

```
% set the gaussian line to 0, then the powerlaw norm to 0, then
% plot the whole model.  Components in orange, whole model in red.

set_par("gaussian(1).norm",0); () = eval_counts;
plot_data(1;dsym=-4,dcol=4,decol=4,mcol=8,xrng={3,20},yrng={1.01,199.9});

load_par("/tmp/initial.par"); set_par("bknpower(1).norm",0,0,0,10);
() = eval_counts;
plot_data(1;dsym=-4,dcol=4,decol=4,mcol=8,opt=1);

load_par("/tmp/initial.par"); () = eval_counts;
plot_data(1;dsym=-4,dcol=4,decol=4,mcol=2,opt=1);

% Now do the same thing with the "unfolded" data in the middle panel.
mpane(2);

% Make sure we use the same x-range as above (y-range is different, of course...)
set_par("gaussian(1).norm",0); () = eval_counts;

plot_unfold(1;dsym=-4,dcol=4,decol=4,mcol=8,power=2,xrng={3,20},
            yrng={1.01e-11,1.99e-9});
```

PLOTTING INDIVIDUAL MODEL COMPONENTS

```
load_par("/tmp/initial.par"); set_par("bknpower(1).norm",0,0,0,10);
() = eval_counts;
plot_unfold(1;dsym=-4,dcoll=4,decol=4,mcol=8,power=2,oplt=1);

load_par("/tmp/initial.par"); () = eval_counts;
plot_unfold(1;dsym=-4,dcoll=4,decol=4,mcol=2,power=2,oplt=1);

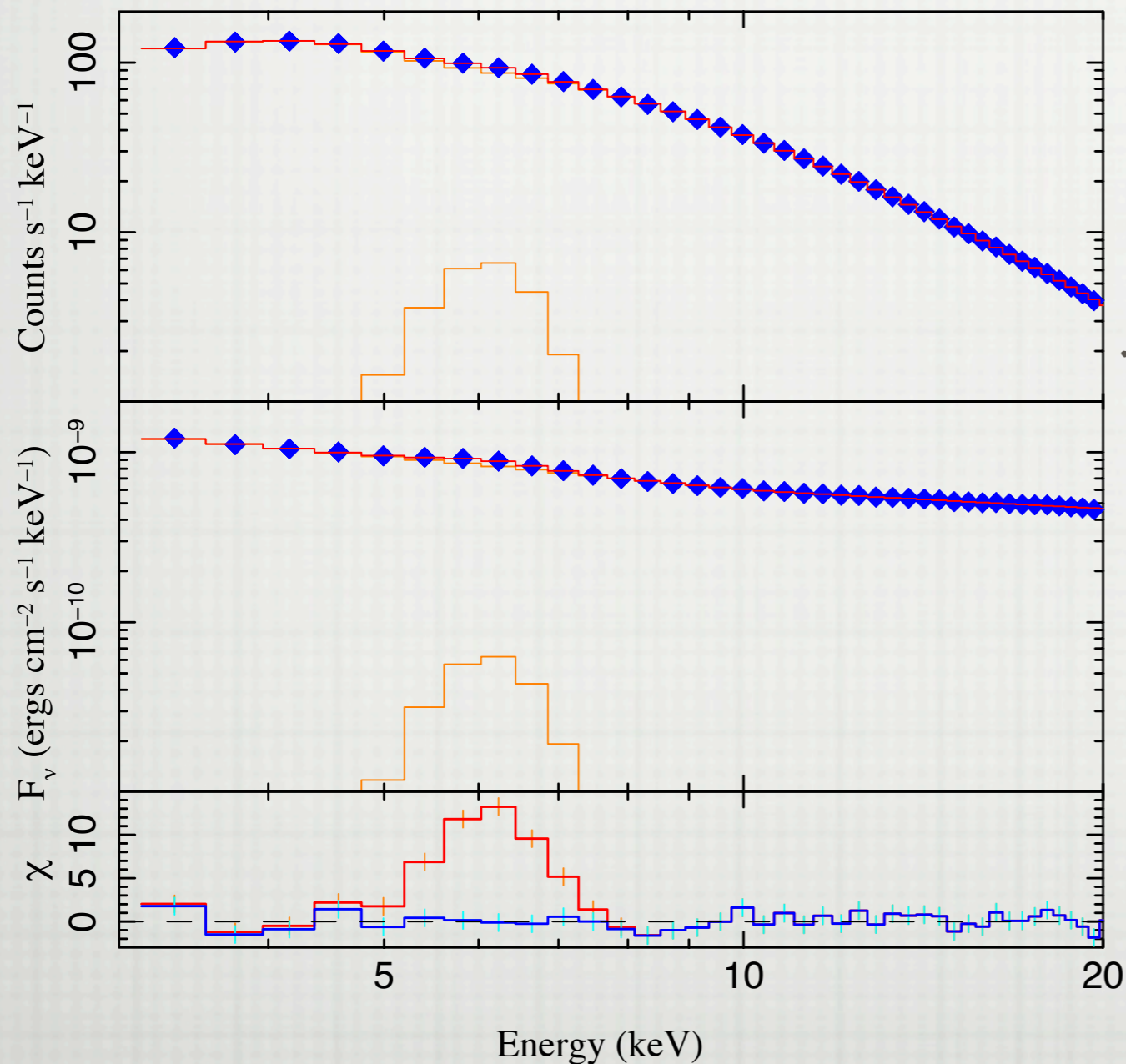
% Now do the same thing with the residuals in the lower
% panel; however, we only 0 out the gaussian this time.
mpane(3);

% Make sure we use the same x-range as above (y-range is different, of course...)
set_par("gaussian(1).norm",0); () = eval_counts;
plot_residuals(1;res=1,rsym=0,rcol=2,recol=8,xrng={3,20},yrng={-2.99,14.99});

% The next plots after this one we want to go back to "normal" behavior.
no_reset=0;

load_par("/tmp/initial.par"); () = eval_counts;
plot_residuals(1;res=1,rsym=0,rcol=4,recol=5,xrng={3,20},oplt=1);
}
isis>
isis> fancy_plot;
```

PLOTTING INDIVIDUAL MODEL COMPONENTS



YOU PROBABLY WANT
TO SAVE "FANCY_PLOT"
AS A SCRIPT SO YOU
CAN MODIFY IT MORE
EASILY.

MORE ON PLOTTING

- PGPLOT IS A FAIRLY SIMPLE PROGRAM. IT'S SERVICEABLE, BUT LOTS OF PEOPLE (UNDERSTANDABLY) PREFER THINGS LIKE IDL.
- WITH MY PLOT ROUTINES, "write_plot" WILL SAVE SIMPLE ASCII FILES FOR THE *LAST* PLOT YOU MADE WITH *MY ROUTINES*. THOSE ARE SUITABLE FOR READING INTO OTHER PROGRAMS.
- AGAIN, USE SCRIPTS TO MAKE REPRODUCING WHAT YOU DID A LITTLE EASIER.

ADVANCED FUNCTION SYNTAX WITH BLANK ()

```
isis> % Use it as short hand for longer models - Manfred Hanke
isis> % has an example like this that creates a model with nearly
isis> % 100 lines (for gratings spectroscopy of Cyg X-1)
isis> define triple(){ return gaussian(1)+gaussian(2)+gaussian(3); }
isis> fit_fun("phabs(1)*(powerlaw(1)+triple())");
isis>
isis> % Use it to define functions that behave differently for each
isis> % data set you are evaluating (i.e., using Isis_Active_Dataset)
isis> public define line(){
    switch(Isis_Active_Dataset);
    { case 1:
      return gaussian(1); % ... if Isis_Active_Dataset=1
    }
    { case 2:
      return diskline(1); % ... if Isis_Active_Dataset=2
    }
    return laor(1);      % All other cases
  }
isis>
isis> fit_fun("phabs(1)*(powerlaw(1)+line())");
isis> % We won't be doing anything this fancy in this exercise!
```

CUSTOM GRIDS & CACHING

- SOME MODELS HAVE TO BE EVALUATED BEYOND THE NORMAL BOUNDARIES OF THE GRID:

```
isis> set_eval_grid_method(USER_GRID,[1:4],&my_function,1);
isis> % my_function returns lo/hi grid; final 1 says cache
isis> % the evaluation and apply it to each datasets
isis> % Now force ISIS to evaluate the entire grid:
isis> set_kernel([1:4];"std;eval=all");
```

- SIMPLE WRAPPER TO CREATE A LOGARITHMIC GRID:

```
isis> usr_grid([1:4],-9,3,0.01,1);
isis> % Creates a grid from  $10^{-9}$ - $10^3$  keV, & caches
isis> % the model evaluation, and sets "eval=all"
```

- MODELS CAN BE CACHED AND REUSED FOR MULTIPLE DATASETS IF THE MODELS ARE *EXACTLY* THE SAME. I.E., NO DEPENDENCE ON Isis_Active_Dataset!

CUSTOM GRIDS & CACHING

- FOR SLOW MODELS, CACHING CAN REALLY SPEED THINGS UP. CACHE INDIVIDUAL SLOW COMPONENTS, AND THAT COMPONENT ONLY GETS REEVALUATED WHEN THE PARAMETERS CHANGE!

```
isis> (lo,hi) = linear_grid(0.1,100,2000);  
isis> () = cache_fun(agnjet,lo,hi;qualifiers);  
isis> fit_fun("agnjet_cache(1)+...");
```

- QUALIFIERS DISTINGUISH BETWEEN ADDITIVE AND MULTIPLICATIVE MODELS.
- CACHING IS ESPECIALLY HELPFUL FOR MULTI-SATELLITE FITS

FOR FURTHER HELP -

S-LANG & ISIS BUILDING & MANUALS, CHECK THE MAIN WEB-SITES:

www.s-lang.org

<http://space.mit.edu/CXC/ISIS/>

COMPARISONS TO XSPEC & TUTORIAL:

http://space.mit.edu/home/mnowak/isis_vs_xspec/index.html

FOR FURTHER HELP -

ISIS-USERS MAILING LIST:

http://space.mit.edu/CXC/ISIS/mailling_list.html

OR CONTACT US DIRECTLY:

FOR ISSUES WITH ISIS-BUILDS, ISIS-MODULES, AND BASIC ISIS-FUNCTIONALITY:

houck@space.mit.edu

FOR TRANSLATING FROM XSPEC EQUIVALENTS AND ANY SCRIPTS SHOWN IN THIS PRESENTATION:

mnowak@space.mit.edu