XSPEC Tutorial and Statistics
Basic steps for X-ray spectral analysis

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Basic steps for *X-ray spectral analysis*

Where can I find *XSPEC*?

- XSPEC is part of the NASA HEASoft software suite (FTOOLS)
- The latest version is HEASoft 6.29c (Sept. 2021) – xspec V12.12.0

https://heasarc.gsfc.nasa.gov/docs/software/heasoft/

- Supported architectures:
    - macOS/Mac OS X
    - PC Linux – Ubuntu (or other Debian-based Linux)
    - PC Linux – Fedora (or other RPM-based Linux)

XSPEC is a command-driven, interactive, X-ray spectral-fitting program, designed to be completely detector-independent

Alternatively: **Sherpa**
https://cxc.cfa.harvard.edu/sherpa/

Step 1a: 'grouping' spectra

Once X-ray spectra are extracted and response matrices are produced,
four files (fits format) are used within XSPEC

- source spectrum
- background spectrum
- ARF response matrix
- RMF response matrix

Before loading these files in XSPEC, it is better to:

(1) associate a source spectrum with its background file and response matrices (RMF and ARF);
(2) group the spectral counts using a binning of e.g. 25 counts/bin (depending on the source photon statistics and the 'sampling' of the instrument spectral resolution) and allow application of the χ^2 **statistics** (it is required to be in the Gaussian regime in each spectral bin). Alternatively, in low photon regime, use unbinned (or binned to 1 count/bin) data and **Cash statistics**

grppha pn.pi pn_25.grp comm="group min 25 & chkey BACKFILE back_spectrum.fits & chkey ANCRFILE pn.arf & chkey RESPFILE pn.rmf & exit"

i.e.: **grppha input_spectrum output_spectrum** […]   **Name all of the files properly!**

Step 1b: loading data in XSPEC and "setup" commands

xspec
xspec> data pn_25.grp   load the grouped spectrum (produced in step 1a)
xspec> ignore bad   ignore spectral bins flagged as bad
xspec> ignore **-0.3 7.2-**   ignore spectral bins below 0.3 keV and above 7.2 keV (to be verified, i.e., adapted to your specific data, src. vs. bkg intensity)

xspec> cpd /xw   to change the plotting device (e.g., on screen, on PS file)
xspec> plot ldata   plot the data in log scale

Energy: with "."
Otherwise: interpreted as channels
(conversion made via the RMF)

Loading multiple datasets

In case of **multiple datasets** (adopting the same model)

xspec> data 1:1 pn_25.grp 2:2 mos1_25.grp 3:3 mos2_25.grp

load all datasets at the same time

xspec> ignore 1-3:**-0.3 7.2-**   select the proper energy range for all datasets (1-3)

xspec> cpd /xw
xspec> plot ldata

When **multiple datasets** are used, remember to place in front of all models the **constant model** [e.g., mo **cons**(pha*po+...)] to account for cross-calibration uncertainties among different instruments of the same telescope/different telescopes and some possible source flux variability in case of multiple observations not taken simultaneously.
The first constant should be fixed to 1, the others are left free to vary (i.e., are part of the fitting)

xspec> show all

```
              XSPEC version: 12.11.1
  Build Date/Time: Mon Sep 28 19:46:54 2020
```

XSPEC12>data pn_25.grp

Fraction of **src_counts/total_counts**

```
1 file 1 spectrum
Spectrum 1  Spectral Data File: pn_25.grp
Net count rate (cts/s) for Spectrum:1  2.652e+00 +/- 7.965e-03 (96.8 % total)
 Assigned to Data Group 1 and Plot Group 1
  Noticed Channels:  23-1321
  Telescope: XMM Instrument: EPN  Channel Type: PI
  Exposure Time: 4.441e+04 sec
Using fit statistic: chi
Using test statistic: chi
Using Background File                 back_spectrum.fits
 Background Exposure Time: 4.441e+04 sec
Using Response (RMF) File             pn.rmf for Source 1
Using Auxiliary Response (ARF) File  pn.arf

Spectral data counts: 121704
```
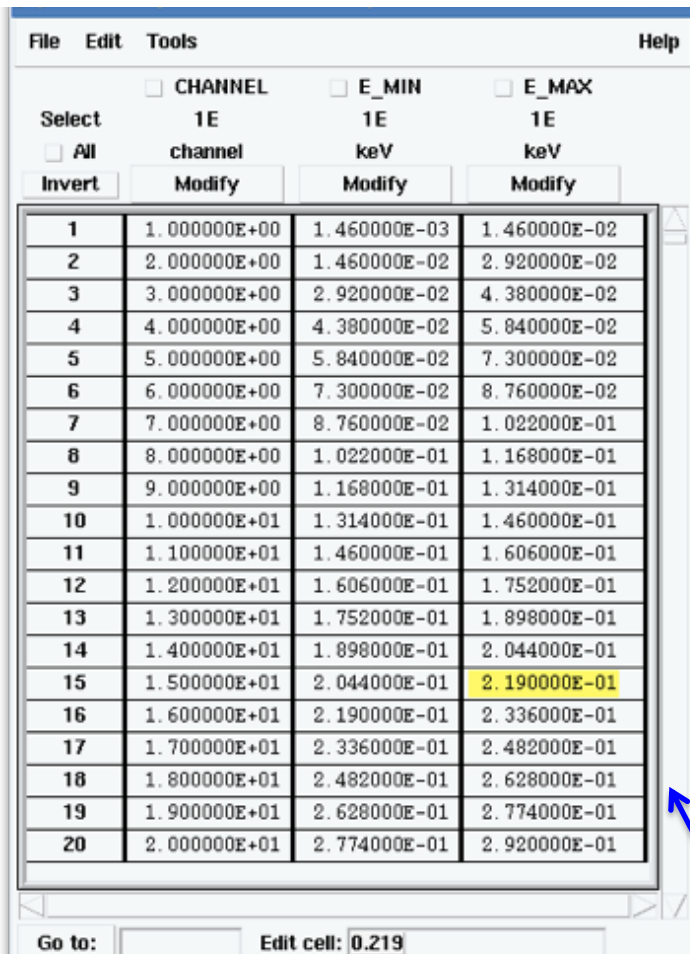
loaded bkg
and response
files

Source net (i.e. background-subtracted) **counts** = data counts × fraction =
=121704 × 0.968

Possible binning choices:
- have enough counts (e.g., 20-25) in each bin and then apply the χ^2 statistics;
- one count/bin and apply the Cash statistics (C-stat, named W-stat if background is subtracted);
- 'sampling' the spectral resolution of the data
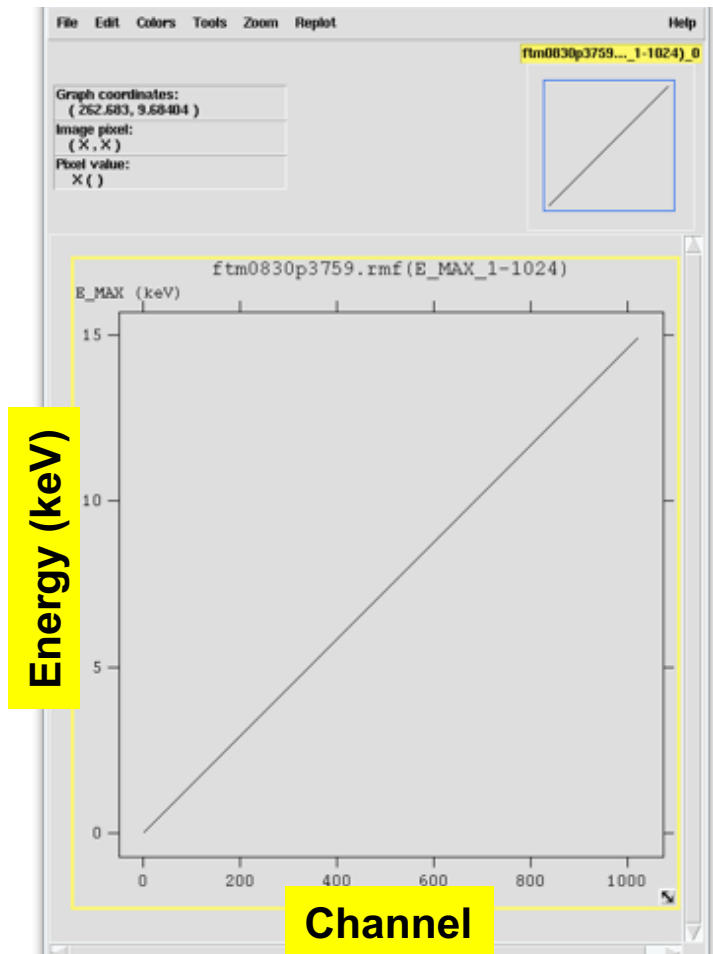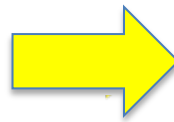
Response matrices: RMF

RMF: links the instrumental channel scale with the physical energy (wavelength) scale

Visualization of the RMF file using the **ftool** *fv*

Response matrices: ARF

ARF: indicates the effective response (hence sensitivity) of the mirrors+instrument at a given source position on the detector

fv: Binary Table of ftm0830p3759.arf[1] in /ho

File Edit Tools   Help

Select All Invert	ENERG_LO 1E keV Modify	ENERG_HI 1E keV Modify	SPECRESP 1E cm**2 Modify
1	2.200000E-01	2.300000E-01	9.414584E+01
2	2.300000E-01	2.400000E-01	1.119709E+02
3	2.400000E-01	2.500000E-01	1.309653E+02
4	2.500000E-01	2.600000E-01	1.518642E+02
5	2.600000E-01	2.700000E-01	1.716482E+02
6	2.700000E-01	2.800000E-01	1.922011E+02
7	2.800000E-01	2.900000E-01	4.741680E+01
8	2.900000E-01	3.000000E-01	2.284590E+00
9	3.000000E-01	3.100000E-01	5.144246E+00
10	3.100000E-01	3.200000E-01	1.563580E+01
11	3.200000E-01	3.300000E-01	2.251595E+01
12	3.300000E-01	3.400000E-01	3.011008E+01
13	3.400000E-01	3.500000E-01	3.743014E+01
14	3.500000E-01	3.600000E-01	4.385400E+01
15	3.600000E-01	3.700000E-01	4.954287E+01
16	3.700000E-01	3.800000E-01	5.625348E+01
17	3.800000E-01	3.900000E-01	6.431229E+01
18	3.900000E-01	4.000000E-01	7.319862E+01
19	4.000000E-01	4.100000E-01	7.713167E+01
20	4.100000E-01	4.200000E-01	8.444775E+01

Go to: ____ Edit cell: 0.42

POW 2.0

File Edit Colors Tools Zoom Replot   Help

ftm0830p3759..._1-1078)_0

Graph coordinates:
(4.0175, 610.543)
Image pixel:
(X , X)
Pixel value:
X ( )

ftm0830p3759.arf(SPECRESP_1-1078)
SPECRESP (cm**2)

Effective Area (cm²)

Energy (keV)
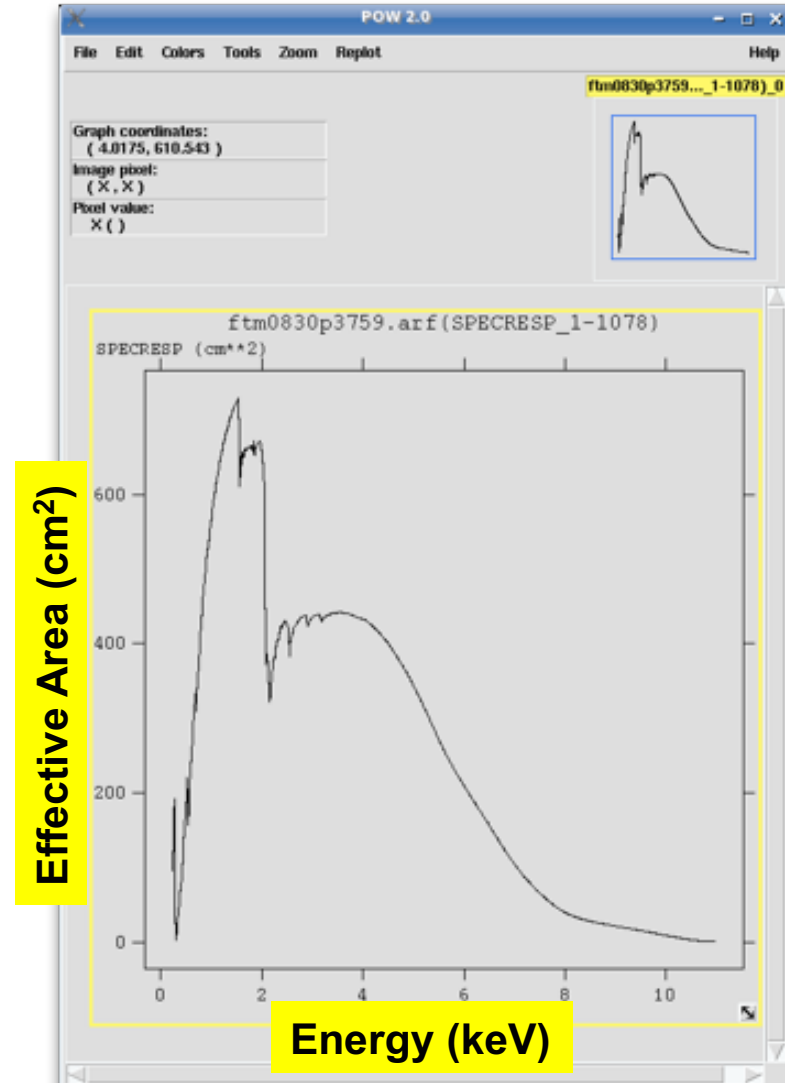
xspec> setplot energy

Channel scale = instrument scale
Energy scale = "physical" scale

Channel scale

Energy scale
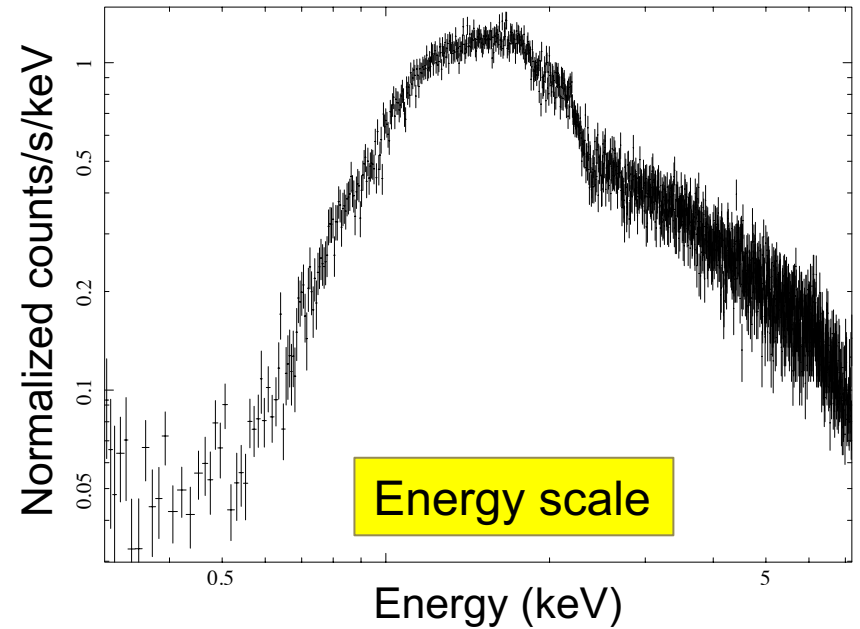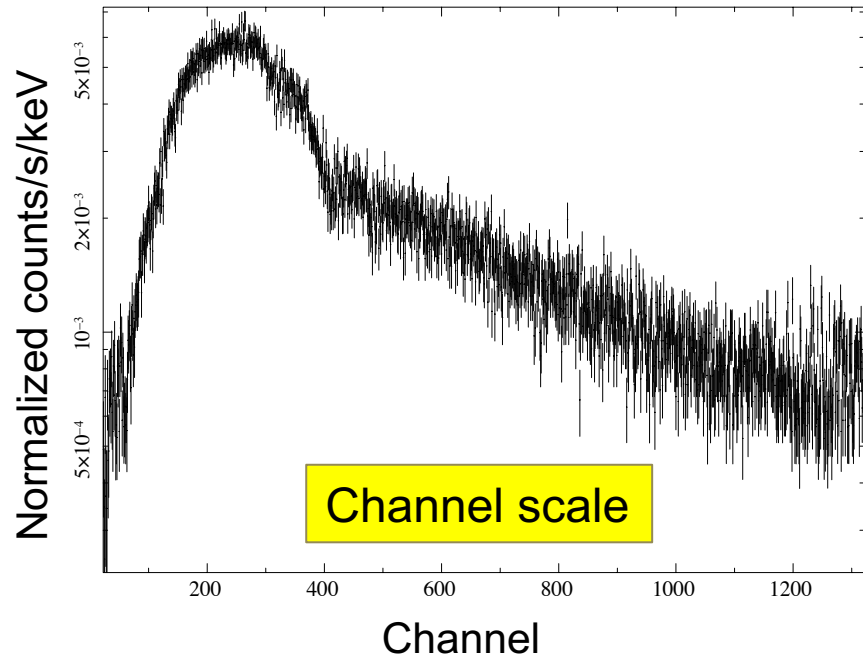
xspec> setplot rebin 10 30

minimum significance   max number of bins

(**just for plotting purposes**)
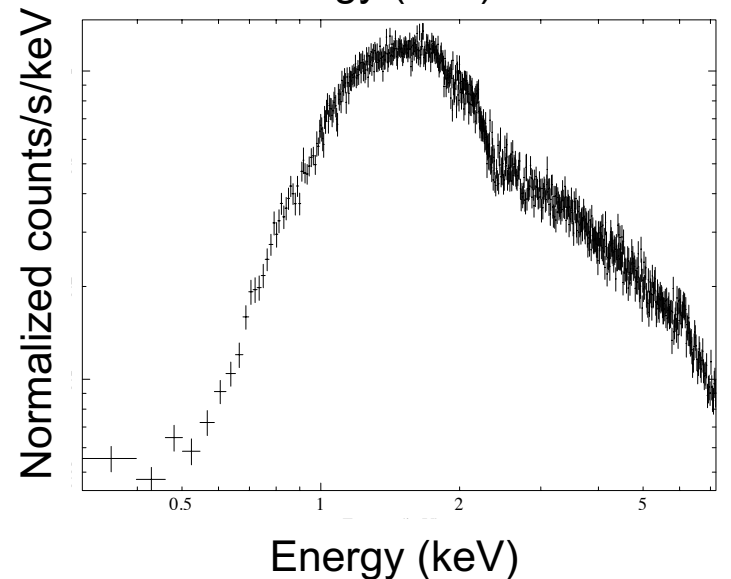
Spectrum in channels vs. spectrum in energy:
they are linked via the RMF (redistribution matrix file)

What does 'binning' (grouping) mean?

To apply the χ^2 test, we need that in every bin the statistics is nearly in the Gaussian regime, i.e., there is a sufficiently high number of counts

Using the ftool *grppha* (or similar) we can require that each spectral bin contains at least a given number of counts (see step 1a)

"original" distribution of the counts (note: here scale=energy)

Example of **unbinned spectrum**

Example of **binned spectrum**
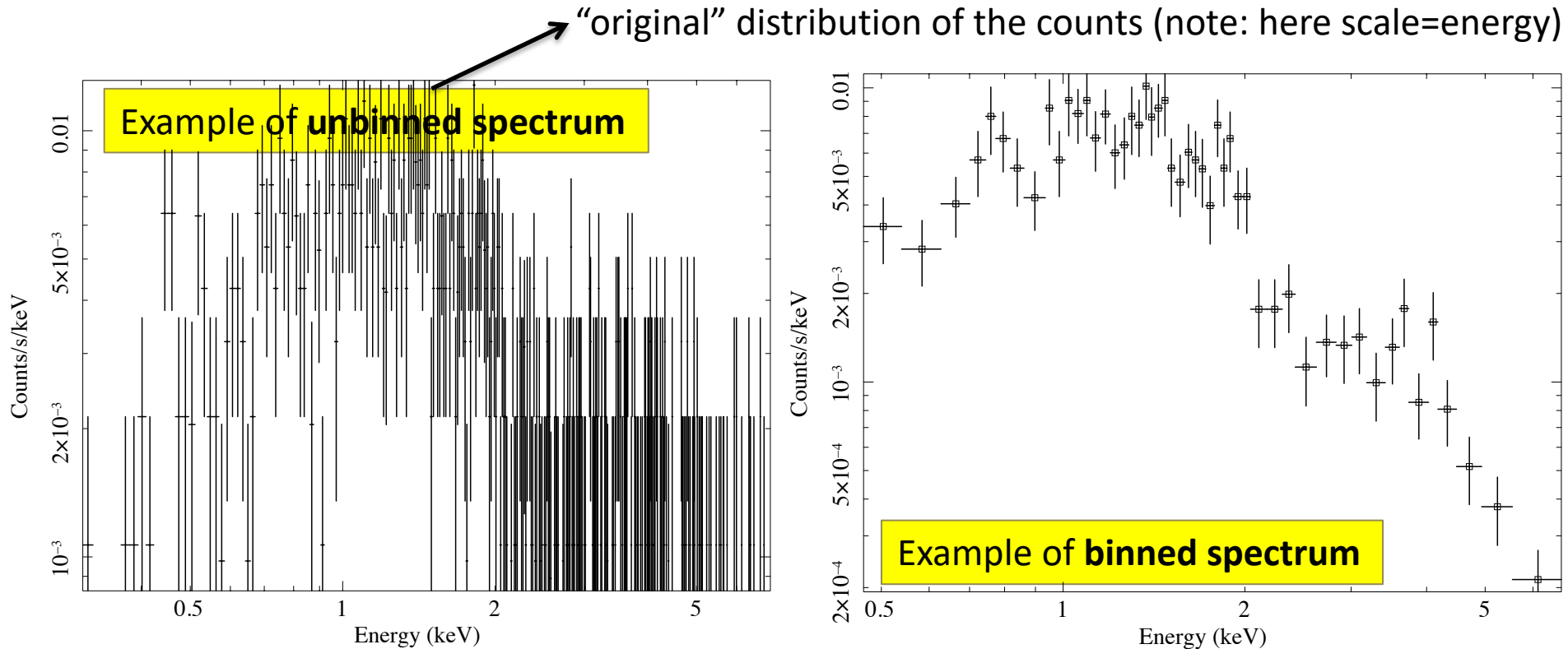
Good photon statistics: it is suggested to rebin the data and apply χ^2

XSPEC models like math operations

Additive models

agauss	apec	bapec	bbody	bbodyrad	bexrav
bexriv	bkn2pow	bknpower	bmc	bremss	bvapec
bvvapec	c6mekl	c6pmekl	c6pvmkl	c6vmekl	cemekl
cevmkl	cflow	compLS	compPS	compST	compTT
compbb	compmag	comptb	compth	cplinear	cutoffpl
disk	diskbb	diskir	diskline	diskm	disko
diskpbb	diskpn	eplogpar	eqpair	eqtherm	equil
expdec	ezdiskbb	gadem	gaussian	gnei	grad
grbm	kerrbb	kerrd	kerrdisk	laor	laor2
logpar	lorentz	meka	mekal	mkcflow	nei
npshock	nsa	nsagrav	nsatmos	nsmax	nsmaxg
nsx	nteea	nthComp	optxagn	optxagnf	pegpwrlw
pexmon	pexrav	pexriv	plcabs	posm	powerlaw
pshock	raymond	redge	refsch	rnei	sedov
sirf	smaug	srcut	sresc	step	vapec
vbremss	vequil	vgadem	vgnei	vmcflow	vmeka
vmekal	vnei	vnpshock	vpshock	vraymond	vrnei
vsedov	vvapec	vvgnei	vvnei	vvnpshock	vvpshock
vvrnei	vvsedov	zagauss	zbbody	zbremss	zgauss
zpowerlw					

Multiplicative models

SSS_ice	TBabs	TBgrain	TBvarabs	absori	acisabs
cabs	constant	cyclabs	dust	edge	expabs
expfac	gabs	heilin	highecut	hrefl	lyman
notch	pcfabs	phabs	plabs	pwab	recorn
redden	smedge	spexpcut	spline	swind1	uvred
varabs	vphabs	wabs	wndabs	xion	zTBabs
zbabs	zdust	zedge	zhighect	zigm	zpcfabs
zphabs	zredden	zsmdust	zvarabs	zvfeabs	zvphabs
zwabs	zwndabs	zxipcf			

Syntax:
M1*M2*(A1+A2+M3*A3)

M=multiplicative model: modifies incident flux
A=additive model: source of emission

Other models

```
Convolution Models:
    cflux      cpflux     gsmooth    ireflect    kdblur     kdblur2
    kerrconv   lsmooth    partcov    rdblur      reflect    rgsxsrc
    simpl      zashift    zmshift

Mixing Models:
    ascac      projct     suzpsf     xmmpsf

Pile-up Models:
    pileup
```

Example:
model wabs*(powerlaw+gaussian)

$$M(E) = \exp\left[-n_H \sigma(E)\right]$$

$$A(E) = KE^{-\alpha}$$

$$A(E) = K \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(E-E_l)^2}{2\sigma^2}\right)$$

Suggestion: 'starting' model for **AGN emission**:
powerlaw modified by Galactic (MW)
absorption

Absorption due to our Galaxy (MW): you need to **include it in all spectral models**. All photons pass through our own Galaxy

xspec> nh

```
XSPEC12>nh
Equinox (d/f 2000)[2000]
RA in hh mm ss.s or degrees[159.386] 04 18 21.3
DEC in dd mm ss.s or degrees[56.171] 38 01 36
 >> Leiden/Argentine/Bonn (LAB) Survey of Galactic HI
 LII , BII 161.675682   -8.819546
 Requested position at X and Y pixel    22.78    103.39
 Search nH in  4  X  4 box
 Each pixel is  0.675 deg 0.675 deg
 nH calculated using all points within
  1.0000 deg from input position
   RA       DEC       Dist        nH
  64.1051  37.3970   0.7360     2.65E+21
  65.1324  37.3425   0.8071     2.80E+21
  64.3226  37.9446   0.2251     2.93E+21
  63.5005  38.5376   0.9979     3.00E+21
  65.3701  37.8774   0.6333     2.89E+21
  64.5573  38.4821   0.4561     3.09E+21
  65.6250  38.4019   0.8984     2.84E+21
  64.8094  39.0092   0.9978     2.99E+21
LAB >> Average nH (cm**-2)  2.90E+21
LAB >> Weighted average nH (cm**-2)  2.91E+21
/usr/local/heasoft-6.16/x86_64-apple-darwin10.8.0/bin/nh
```

Alternatively (web tool): https://heasarc.gsfc.nasa.gov/cgi-bin/Tools/w3nh/w3nh.pl
based on the HI4PI Survey (N.B. Bekhti et al. 2016, A&A, 594, A116)

xspec> mo pha*po

pha: accounts for the Galactic N_H (multiplicative model)
po: powerlaw model (additive model) for the primary AGN comp.

It is possible to provide values to the parameters at every step of the fitting process

-1 means frozen parameter (the same as using the command *freeze* # of the parameter; opposite: *thaw*)

```
XSPEC12>mo pha*po

Input parameter value, delta, min, bot, top, and max values for ...
            1        0.001(      0.01)           0           0      100000       1e+06
1:phabs:nH>2.91e-1  -1
            1        0.01(       0.01)          -3          -2           9          10
2:powerlaw:PhoIndex>1.8
            1        0.01(       0.01)           0           0       1e+20       1e+24
3:powerlaw:norm>1e-6


=================================================================
Model phabs<1>*powerlaw<2> Source No.: 1    Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
  1    1   phabs       nH         10^22    0.291000     frozen
  2    2   powerlaw    PhoIndex            1.80000      +/-  0.0
  3    2   powerlaw    norm                1.00000E-06  +/-  0.0
-----------------------------------------------------------------
```

parameter number

number of the component

xspec> query yes
xspec> renorm (to allow a preliminary "adjustment")
xspec> fit 100 (fit 100 times)

data and folded model


```
===========================================================
Model phabs<1>*powerlaw<2> Source No.: 1     Active/On
Model Model Component  Parameter  Unit      Value
 par  comp
  1    1   phabs       nH         10^22     0.291000
  2    2   powerlaw    PhoIndex             0.895250
  3    2   powerlaw    norm                 3.65973E-03

-----------------------------------------------------------
```
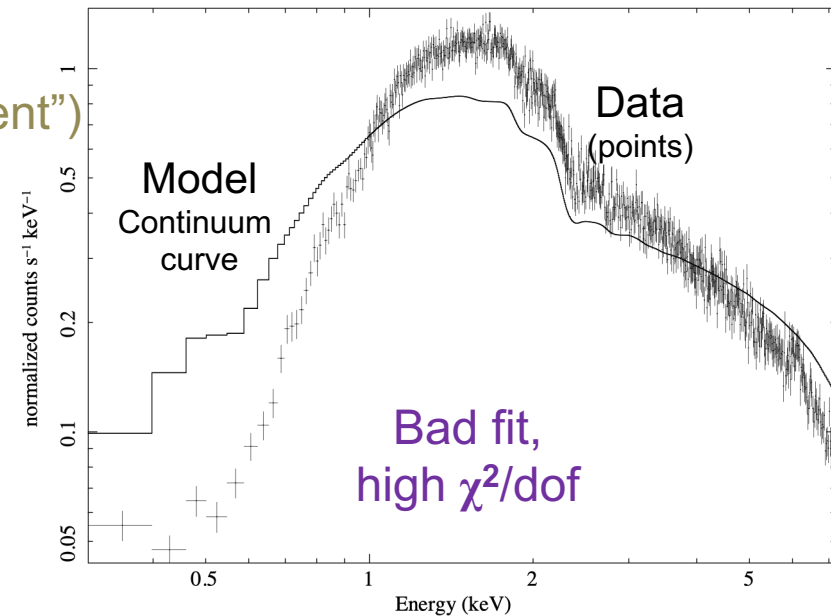
Model Continuum curve

Data (points)

Bad fit, high χ²/dof

```
Fit statistic : Chi-Squared =        10561.52 using 1299 PHA bins.

Test statistic : Chi-Squared =        10561.52 using 1299 PHA bins.
 Reduced chi-squared =        8.143041 for   1297 degrees of freedom
 Null hypothesis probability =   0.000000e+00
```

dof=degrees of freedom=(*number of datapoints – number of free parameters*)=
=1299-2=1297

χ² /dof close to unity means that it is a good fit (hence, not in this case!) – see lesson on statistics

<u>Null hypothesis</u> probability=probability that the model is a good representation of the datapoints (i.e., good if close to 1)

All the adopted models should be physically motivated according to the known source properties/classification + indications obtained at other wavelengths

Step 3b: adding components and fit

xspec> addcomp 2 zpha   adding zpha as # component (#=order in the model)

```
XSPEC12>addcomp 2 zpha

Input parameter value, delta, min, bot, top, and max values for ...
          1      0.001(      0.01)        0          0      100000      1e+06
2:zphabs:nH>1
          0     -0.01(      0.01)     -0.999    -0.999          10         10
3:zphabs:Redshift>.048
```

xspec> fit 100

```
===================================================================
Model phabs<1>*zphabs<2>*powerlaw<3>  Source No.: 1   Active/On
Model Model Component  Parameter  Unit        Value
 par  comp
  1    1    phabs      nH         10^22       0.291000      frozen
  2    2    zphabs     nH         10^22       1.00000       +/-   0.0
  3    2    zphabs     Redshift               4.80000E-02   frozen
  4    3    powerlaw   PhoIndex               0.895250      +/-   4.39599E-03
  5    3    powerlaw   norm                   3.65973E-03   +/-   1.85394E-05
```

xspec> plot ldata delchi
xspec> plot model   to plot the input model

xspec> plot eeufspec delchi

Convolved with the response matrix

eeufspec: unfolded spectrum in $E^2 F(E)$

data and folded model
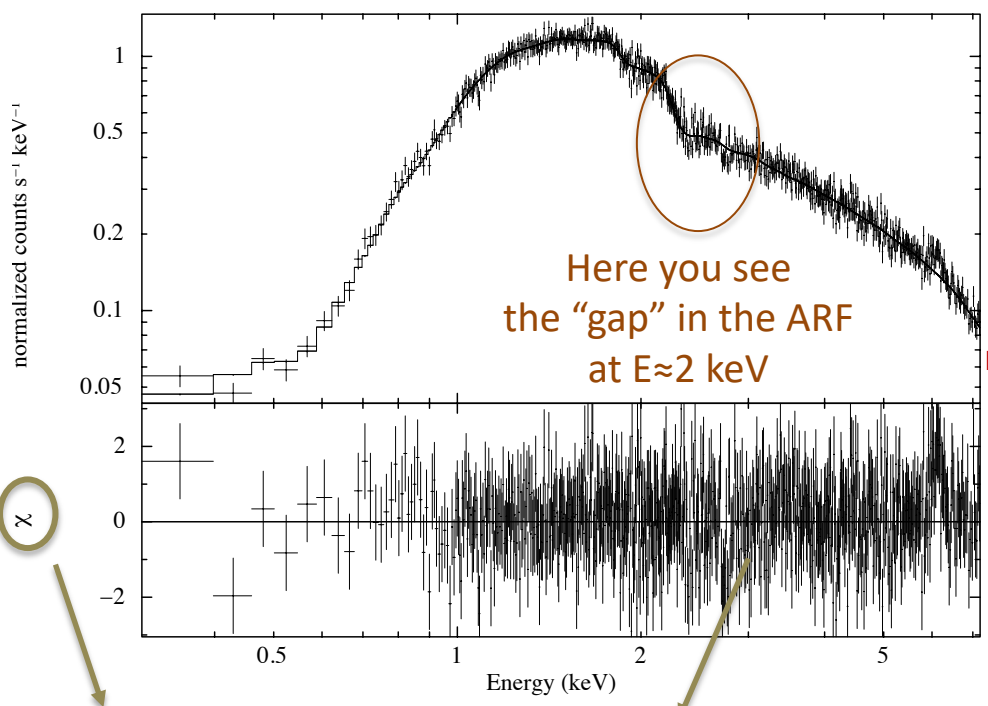
Here you see
the "gap" in the ARF
at E≈2 keV

Unfolded Spectrum

$F(E)$

E^2

χ
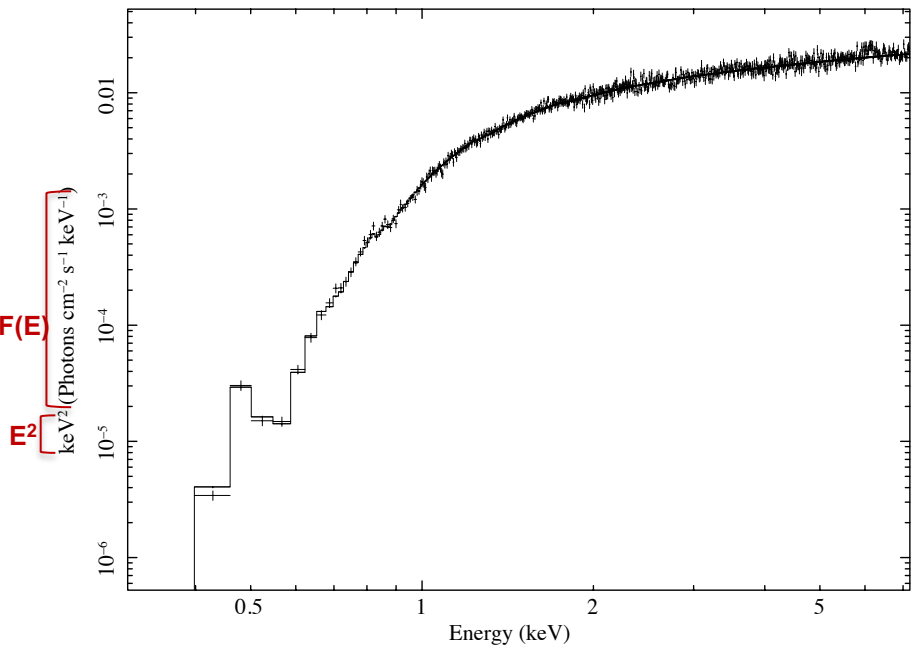
delchi: (model-data), i.e. deviations in units of σ

Step 4: χ^2 statistical test

Test to compare the observed distribution of the results with that expected

$$\chi^2 = \sum_{k=1}^{n} \frac{(O_k - E_k)^2}{\sigma_k^2}$$

O_k=observed values (spectral datapoints)
E_k=expected values (model)
σ_k=error on the measured values (error on each spectral bin)
k=number of datapoints (bins after rebinning)

$$\chi^2 / dof \approx 1$$ ⟹ the observed and expected distributions are similar

Applicability of χ^2 statistics

χ^2 statistic

$$S = \sum_i (\underbrace{S_i - B_i t_s / t_b}_{O_K} - \underbrace{m_i t_s}_{E_K})^2 / (\underbrace{(\sigma_S)_i^2 + (\sigma_B)_i^2}_{\sigma_K})$$

where S_i = src counts in the I={1,...,N} data bins with exposure t_S, B_i = background counts with exposure t_B and m_i = model predicted count rate; $(\sigma_S)^2$ and $(\sigma_B)^2$ = variance on the src and background counts, typically estimated by S_i and B_i

BUT
the χ^2 statistic fails in low-counting regime
(few counts in each data bin)

Alternative solutions in case of low photon statistics

i.   To rebin the data so that each bin contains a large enough number of counts

BUT: loss of information and dependence on the rebinning method adopted

ii.   To modify S so the it performs better in low-count regime (e.g., by estimating the variance for a given data bin using the average counts from the surrounding bins; Churazov+96)

BUT: it would need Montecarlo simulations to properly support the result

iii.   To construct a **maximum-likelihood estimator** based on the Poisson distribution of the detected counts (Cash79; Wachter+79). ML means finding the best fit of parameters that maximizes the Poisson likelihood

xspec> statistic chi   (default)   Binned data, χ^2 statistics   ⟺ Gaussian statistics
xspec> statistic cstat   Unbinned data, C-statistics ⟺ Poisson statistics

Forward-fitting algorithm

Define Model → Calculate Model → Convolve with detector response → Compare to data → Change model parameters → Calculate Model

Model choice based on the physics of the source

21
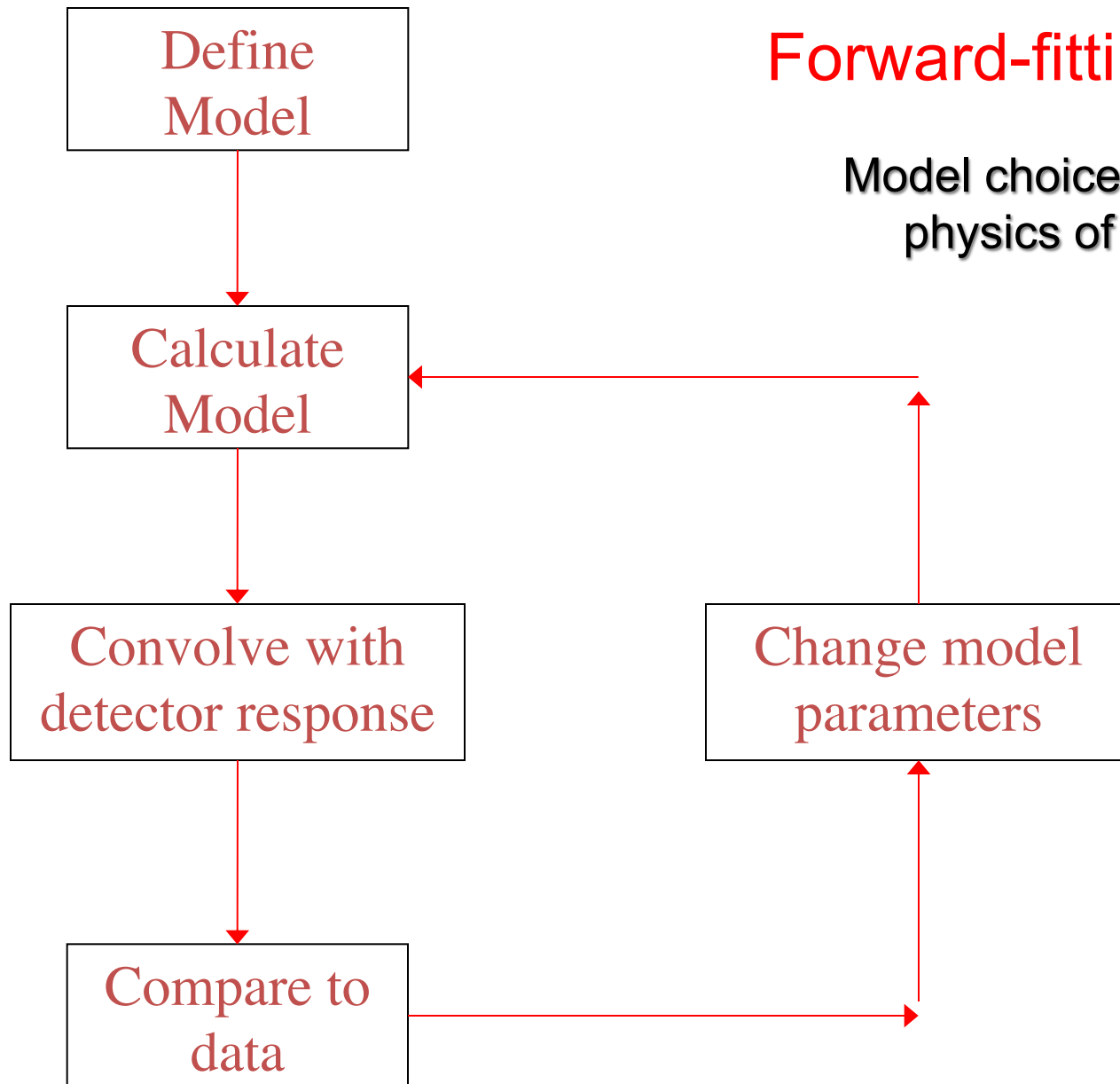
Global vs. local minimum

Data analysis
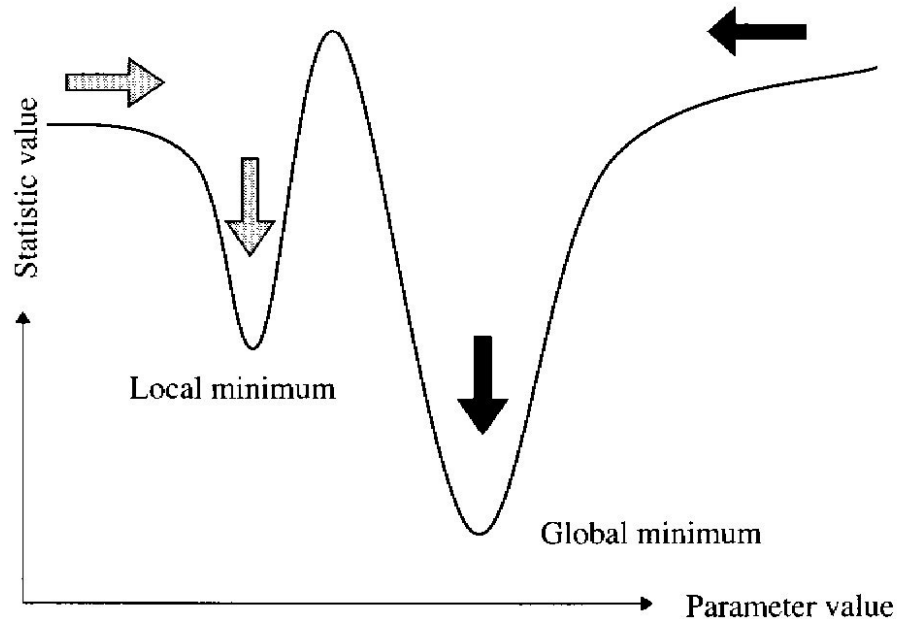
If the fit process is started at the "right place", then it will converge to the true minimum

The more complicated the model and the more highly correlated the parameters, then the more likely that the algorithm will hardly find the true minimum

xspec> newpar 2 1.8   to assign a new value to a parameter (2 here)
Useful also to 'move' the fit from a local minimum…

χ^2 in a nutshell

Reduced χ^2 large $\leftarrow\rightarrow$ P(χ^2) small

a. Errors are under-estimated
b. The model does not describe the data correctly

Reduced χ^2 small $\leftarrow\rightarrow$ P(χ^2) large

c. Errors are over-estimated
d. Were data "selected" in a particular way?

Step 5: error estimate

xspec> error #

(#=number of the parameter)

$\Delta\chi^2$ as a Function of Confidence Level and Degrees of Freedom						
	ν					
p	1	2	3	4	5	6
68.3%	1.00	2.30	3.53	4.72	5.89	7.04
90%	2.71	4.61	6.25	7.78	9.24	10.6
95.4%	4.00	6.17	8.02	9.70	11.3	12.8
99%	6.63	9.21	11.3	13.3	15.1	16.8
99.73%	9.00	11.8	14.2	16.3	18.2	20.1
99.99%	15.1	18.4	21.1	23.5	25.7	27.8

Avni76; Lampton+76

These are the errors at 1σ for that parameter

```
=====================================================
Model phabs<1>*zphabs<2>*powerlaw<3> Source No.: 1   Active
Model Model Component  Parameter  Unit      Value
 par  comp
  1    1    phabs      nH         10^22     0.291000     frozen
  2    2    zphabs     nH         10^22     0.465420     +/-  6.99525E-03
  3    2    zphabs     Redshift             4.80000E-02  frozen
  4    3    powerlaw   PhoIndex             1.59881      +/-  9.35898E-03
  5    3    powerlaw   norm                 9.98424E-03  +/-  1.19425E-04
_____

   Using energies from responses.

Fit statistic : Chi-Squared =        1286.80 using 1299 PHA bins.

Test statistic : Chi-Squared =        1286.80 using 1299 PHA bins.
 Reduced chi-squared =       0.992903 for   1296 degrees of freedom
 Null hypothesis probability =   5.667071e-01
 Weighting method: standard
XSPEC12>error 4
 Parameter    Confidence Range (2.706)
     4      1.58343       1.6143    (-0.0153884,0.0154818)
```

2.706: 90% confidence level for one parameter of interest

Confidence	sigma	delta_chi-square
68.3%	1.0	1.00
90.0%	1.6	2.71
95.5%	2.0	4.00
99.0%	2.6	6.63
99.7%	3.0	9.00

1 parameter of interest

Ex.1: Error at **90%** confidence level for one parameter of interest: xspec> error 2.71 #param

Ex. 2: Error at **90%** confidence level for two parameters of interest: xspec> error 4.61 #param

Ex. 3: Error at **99%** confidence level for one parameter of interest: xspec> error 6.63 #param

1 parameter of interest: as only one parameter at each time would vary
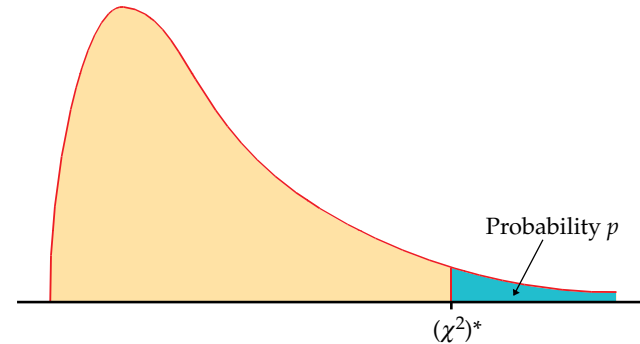
Probability p

Table entry for p is the critical value $(\chi^2)^*$ with probability p lying to its right.

$(\chi^2)^*$

TABLE F

χ^2 distribution critical values

Parameters of interest →

df	.25	.20	.15	**.10**	.05	.025	.02	**.01**	.005	.0025	.001	.0005
1	1.32	1.64	2.07	2.71	3.84	5.02	5.41	6.63	7.88	9.14	10.83	12.12
2	2.77	3.22	3.79	4.61	5.99	7.38	7.82	9.21	10.60	11.98	13.82	15.20
3	4.11	4.64	5.32	6.25	7.81	9.35	9.84	11.34	12.84	14.32	16.27	17.73
4	5.39	5.99	6.74	7.78	9.49	11.14	11.67	13.28	14.86	16.42	18.47	20.00
5	6.63	7.29	8.12	9.24	11.07	12.83	13.39	15.09	16.75	18.39	20.51	22.11

(Tail probability p)

Step 5a: contour plots

xspec> steppar **par1** min_value max_value #steps **par2** min max #steps

Perform a fit while stepping the value of a parameter through a given range

XSPEC12>stepp 4 1.55 1.65 10 2 0.43 0.50 10

| Chi-Squared	Delta Chi-Squared		PhoIndex 4		nH 2

⟶ Parameters involved in the fit

Chi-Squared	Delta Chi-Squared		PhoIndex		nH
1317	30.234	0	1.55	0	0.43
1313.8	26.991	1	1.56	0	0.43
1317.3	30.457	2	1.57	0	0.43
1327.4	40.613	3	1.58	0	0.43
1344.2	57.438	4	1.59	0	0.43
1367.7	80.908	5	1.6	0	0.43
1397.8	111	6	1.61	0	0.43
1434.5	147.68	7	1.62	0	0.43
1477.7	190.92	8	1.63	0	0.43
1527.5	240.68	9	1.64	0	0.43
1583.7	296.94	10	1.65	0	0.43
1527.3	240.45	10	1.65	1	0.437
1476.6	189.75	9	1.64	1	0.437
1432.3	145.51	8	1.63	1	0.437
1394.6	107.76	7	1.62	1	0.437
1363.3	76.53	6	1.61	1	0.437
1338.7	51.852	5	1.6	1	0.437
1320.6	33.752	4	1.59	1	0.437
1309.1	22.255	3	1.58	1	0.437
1304.2	17.383	2	1.57	1	0.437
1306	19.155	1	1.56	1	0.437

It provides how one parameter varies wrt. another parameter (i.e., the error range for sets of parameters)

Useful also to understand whether two spectral parameters are correlated (not necessarily from a physical point of view)
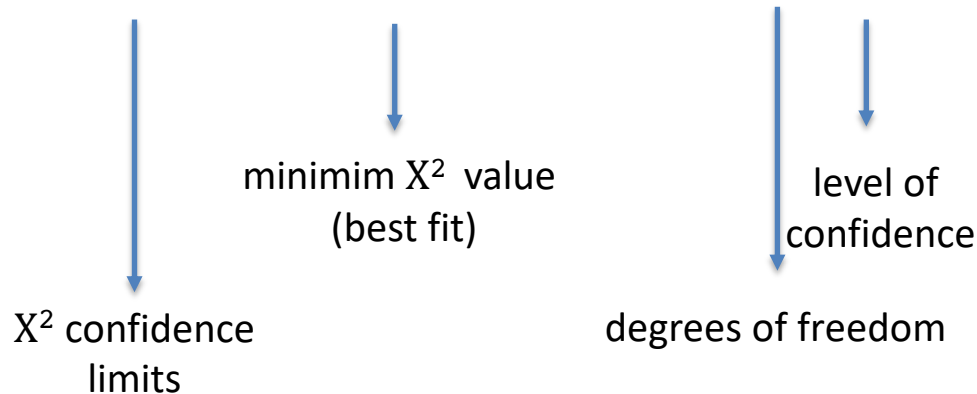
xspec> plot contour
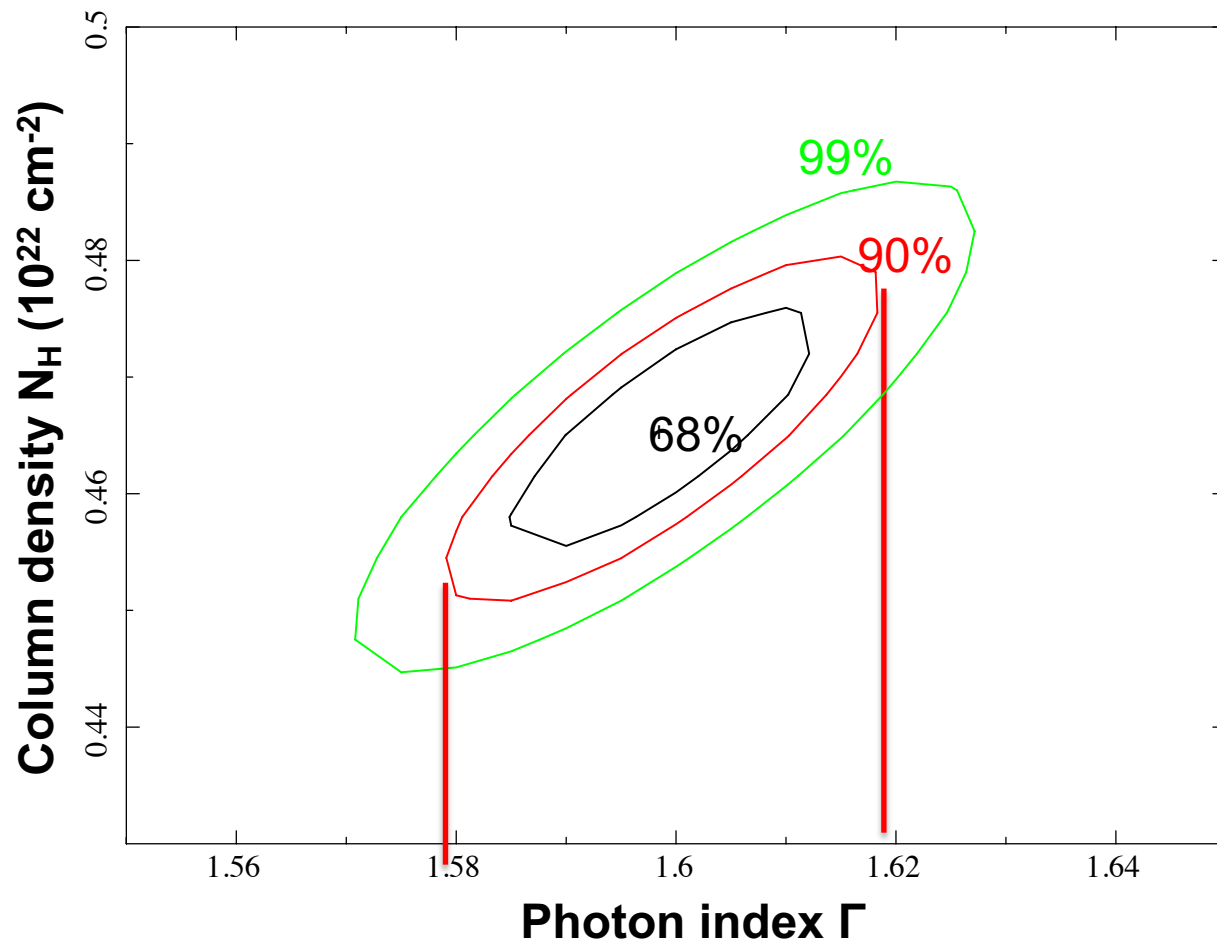
90% c.l.: the photon index varies in the range 1.58−1.62 (vs. 1.58−1.61 using the *error* command).
Slight differences are explained because in the case of the *error* command, the uncertainty was
computed for one parameter of interest

The *contour plots* define a confidence region in the parameter space (i.e., the "statistical surface") within which the true parameters lie with a certain confidence (hence, 68, 90, 99% in XSPEC by default). They represent regions of constant probability

$$\chi^2_\alpha = \chi^2_{min} + \Delta(\nu, \alpha)$$

X^2 confidence limits

minimim X^2 value (best fit)

degrees of freedom

level of confidence

Avni 1976

Δ depends only on the number of parameters involved in the fit (see previous slides)

CONSTANTS FOR CALCULATING CONFIDENCE REGIONS

α (%)	q (No. of Interesting Parameters)		
	1	2	3
68.........	1.00	2.30	3.50
90.........	2.71	4.61	6.25
99.........	6.63	9.21	11.30
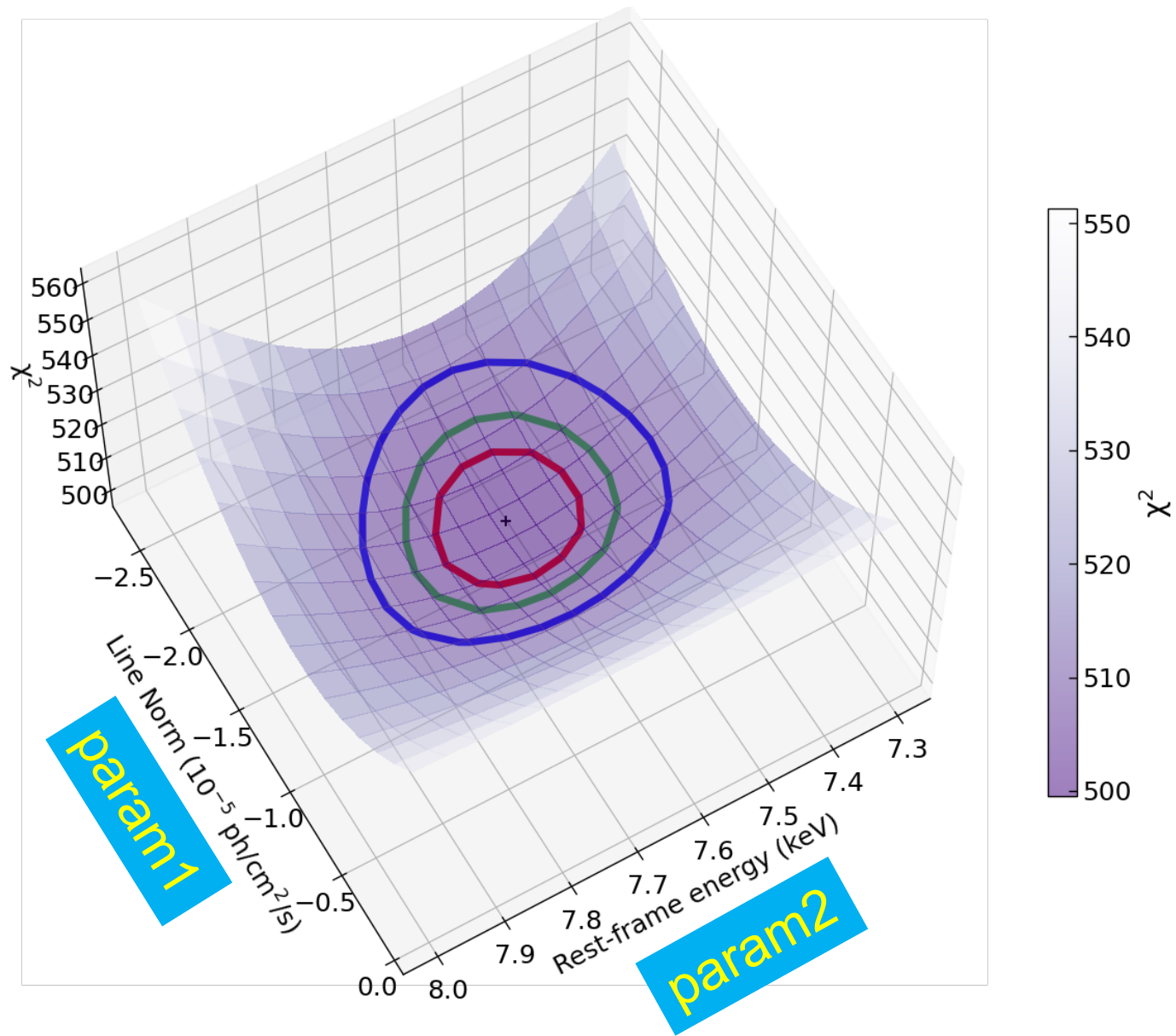
Courtesy of E. Bertola

Calculating Confidence Limits means Exploring the Parameter Space - Statistical Surface
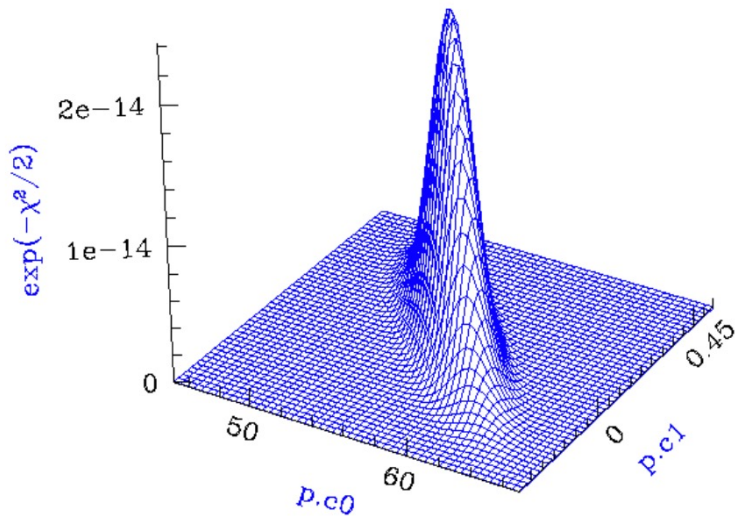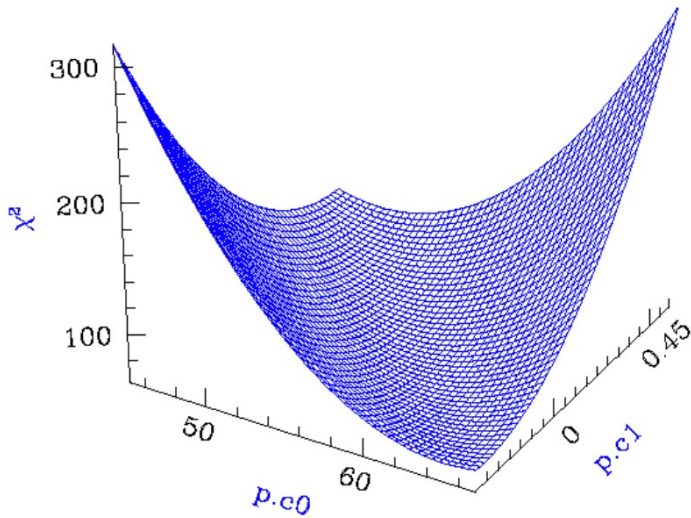
Example of a "well-behaved" statistical surface in parameter space, viewed as a multi-dimensional paraboloid (χ^2, top), and as a multi-dimensional Gaussian ($\exp(-\chi^2/2) \approx L$, bottom).

Credits: A. Siemiginowska

Interval-Projection

Statistic Value

478.8
478.6
478.4
478.2
478.0

Best fit

1.25   1.26   1.27   1.28   1.29
p1.PhoIndex

Statistics
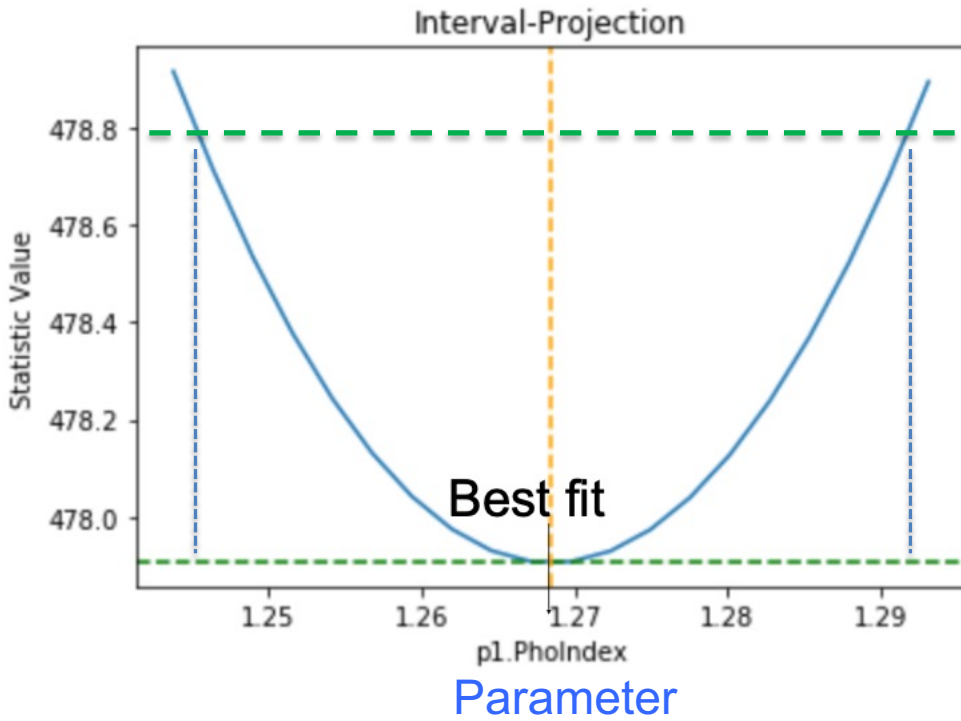
Parameter

Well-behaved surface
(Gaussian, one parameter)

$\Delta X^2 = 1$

Not well-behaved surface
(not Gaussian)

Interval-Projection

864
862
860
858

Statistics

1.4716   1.4717   1.4718   1.4719   1.472   1.4721   1.4722

Parameter

Credits: A. Siemiginowska
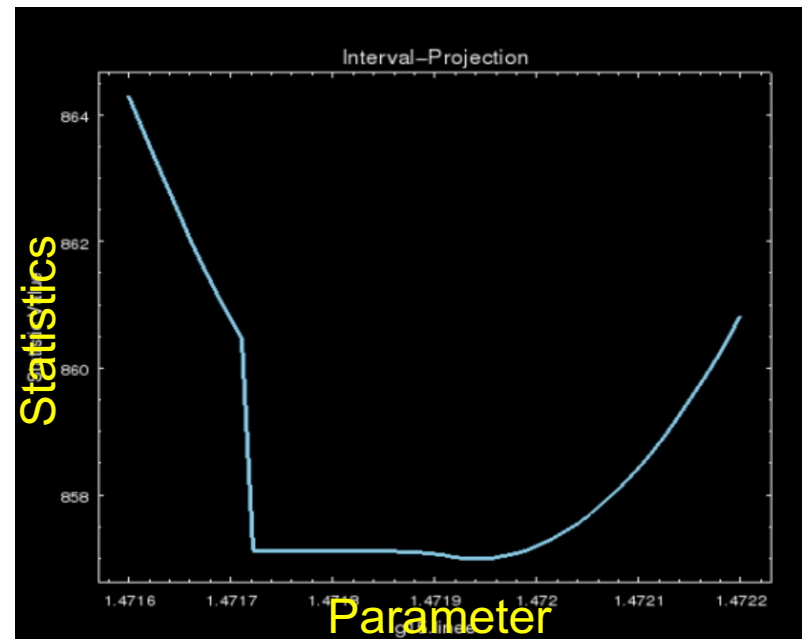
xspec> flux 2 10   (flux band in keV)
xspec> lum 2 10 0.048   (lum band redshift)

command *cosmo* to change the cosmology

```
XSPEC12>flux 2 10
 Model Flux 0.0062186 photons (4.5024e-11 ergs/cm^2/s) range (2.0000 - 10.000 keV)
XSPEC12>ne 2 0

Fit statistic : Chi-Squared =        144391.0 using 1299 PHA bins.

Test statistic : Chi-Squared =        144391.0 using 1299 PHA bins.
 Reduced chi-squared =        111.4128 for    1296 degrees of freedom
 Null hypothesis probability =    0.000000e+00
 Current data and model not fit yet.
XSPEC12>lum 2 10 0.048
Model Luminosity 2.4791e+44 ergs/s  (2.0000 - 10.000 keV rest frame)
     (z = 0.0480 H0 =   70.0 q0 =   0.00 Lambda0 = 0.730)
```

Flux is *observed* (typically, no correction for absorption) and in the *observed-frame band* (units: erg/cm^2/s)

Luminosity needs to be *intrinsic/de-absorbed* (so, put $N_H = 0$ and do **not** fit again) and is reported in the *source rest frame* (units: erg/s)

Uncertainties on fluxes and luminosities. I

xspec> flux 2 10 error 100 90 (100 trials to compute the error at 90% c.l. in the 2−10 keV band)

```
XSPEC12>flux 2 10 error 100 90
Parameter distribution is derived from fit covariance matrix.
 Model Flux 0.0061987 photons (4.4751e-11 ergs/cm^2/s) range (2.0000 - 10.000 keV)
      Error range  0.006159 - 0.006249      (4.441e-11 - 4.517e-11)  (90.00% confidence)
```

xspec> lum 2 10 0.048 error 100 90 (the same as for the flux)

```
XSPEC12>lum 2 10 0.048 error 100 90
Parameter distribution is derived from fit covariance matrix.
Model Luminosity 2.3811e+44 ergs/s  (2.0000 - 10.000 keV rest frame)
      Error range   2.359e+44 - 2.396e+44   (90.00% confidence)
      (z = 0.0480 H0 =  70.0 q0 =  0.00 Lambda0 = 0.730)
```

Uncertainties on fluxes and luminosities. II

Alternatively: use **cflux** and **clumin** as multiplicative model components.
cflux (**clumin**) in front of model component(s). At least one of the additive models should have the normalization fixed to a non-zero value. cflux/clumin must be treated as the other model components (i.e., they are part of the fit)

xspec> model pha***cflux***zpha*pow

xspec> […]; fit

```
===================================================================
Model phabs<1>*cflux<2>*zphabs<3>*powerlaw<4> Source No.: 1    Active/On
Model Model Component  Parameter  Unit       Value
 par  comp
   1    1   phabs      nH         10^22      0.291000        frozen
   2    2   cflux      Emin       keV        2.00000         frozen
   3    2   cflux      Emax       keV        10.0000         frozen
   4    2   cflux      lg10Flux   cgs        -10.3374        +/-  2.36218E-03
   5    3   zphabs     nH         10^22      0.507589        +/-  7.23604E-03
   6    3   zphabs     Redshift              4.80000E-02     frozen
   7    4   powerlaw   PhoIndex              1.61125         +/-  9.39481E-03
   8    4   powerlaw   norm                  1.01795E-02     frozen
-------------------------------------------------------------------


Fit statistic  : Chi-Squared                  1290.08    using 1299 bins.

Test statistic : Chi-Squared                  1290.08    using 1299 bins.
 Null hypothesis probability of 5.41e-01 with 1296 degrees of freedom
XSPEC12>error 4
 Parameter   Confidence Range (2.706)
     4      -10.3414      -10.3335    (-0.00394489,0.00392021)
```

Boundaries for the computation
Emin=2 keV
Emax=10 keV
lg10Flux is the log of the flux in the *observed energy range* Emin–Emax

The **powerlaw normalization** has been **frozen**

Uncertainties on fluxes and luminosities. III

For what concerns the X-ray luminosity, it must be computed as *intrinsic* (*de-absorbed*). This can be achieved placing the column density **=0** without subsequent fitting the spectrum. For the value+error, **clumin** can be used (with no 'extra' requirements):

```
xspec> model pha*zpha*clumin*pow
xspec> […]; fit
```

```
========================================================================
Model phabs<1>*zphabs<2>*clumin<3>*powerlaw<4> Source No.: 1   Active/On
Model Model Component  Parameter  Unit      Value
 par  comp
   1    1    phabs      nH        10^22     0.291000      frozen
   2    2    zphabs     nH        10^22     0.507588      +/-  7.23591E-03
   3    2    zphabs     Redshift            4.80000E-02   frozen
   4    3    clumin     Emin      keV       2.00000       frozen
   5    3    clumin     Emax      keV       10.0000       frozen
   6    3    clumin     Redshift            4.80000E-02   frozen
   7    3    clumin     lg10Lum   cgs       44.4067       +/-  1.80573E-03
   8    4    powerlaw   PhoIndex            1.61125       +/-  9.39481E-03
   9    4    powerlaw   norm                1.03806E-02   frozen
_____
```

Boundaries for the computation
Emin=2 keV
Emax=10 keV
lg10Lum is the log of the luminosity in the *rest-frame energy range* Emin–Emax
The **powerlaw normalization** has been **frozen**

```
Fit statistic  : Chi-Squared                  1290.08     using 1299 bins.

Test statistic : Chi-Squared                  1290.08     using 1299 bins.
 Null hypothesis probability of 5.41e-01 with 1296 degrees of freedom
XSPEC12>error 7
 Parameter    Confidence Range (2.706)
     7     44.4032       44.4102    (-0.00353496,0.00351265)
```

Step 7: the F-test

(here applied to estimate the statistical significance of the inclusion of an emission line)

Model 1: absorbed powerlaw
Model 2: absorbed powerlaw + iron emission line
xspec> addcomp 3 zgauss
xspec> fit 100

```
XSPEC12>addcomp 3 zgauss

Input parameter value, delta, min, bot, top, and max values for ...
         6.5        0.05(    0.065)          0          0      1e+06      1e+06
4:zgauss:LineE>6.4
         0.1        0.05(    0.001)          0          0         10         20
5:zgauss:Sigma>.01 -1
           0       -0.01(     0.01)     -0.999     -0.999         10         10
6:zgauss:Redshift>.048
           1        0.01(     0.01)          0          0      1e+20      1e+24
7:zgauss:norm>1e-6

Fit statistic : Chi-Squared =        1284.34 using 1299 PHA bins.

========================================================================
Model phabs<1>*zphabs<2>(zgauss<3> + powerlaw<4>) Source No.: 1   Active/On
Model Model Component  Parameter  Unit      Value
 par  comp
   1    1   phabs       nH         10^22     0.291000       frozen
   2    2   zphabs      nH         10^22     0.470750       +/-  7.09342E-03
   3    2   zphabs      Redshift             4.80000E-02    frozen
   4    3   zgauss      LineE      keV       6.40830        +/-  2.18809E-02
   5    3   zgauss      Sigma      keV       1.00000E-02    frozen
   6    3   zgauss      Redshift             4.80000E-02    frozen
   7    3   zgauss      norm                 2.65689E-05    +/-  4.58946E-06
   8    4   powerlaw    PhoIndex             1.61154        +/-  9.66835E-03
   9    4   powerlaw    norm                 1.01037E-02    +/-  1.23074E-04
------------------------------------------------------------------------
```

$\Delta\chi^2/\Delta\mathrm{dof}=33.5/2$

$\chi^2/\mathrm{dof}=1253.3/1294$
vs. 1286.8/1296 (no line)

```
Fit statistic : Chi-Squared =         1253.29 using 1299 PHA bins.

Test statistic : Chi-Squared =        1253.29 using 1299 PHA bins.
 Reduced chi-squared =        0.968541 for   1294 degrees of freedom
 Null hypothesis probability =   7.868667e-01
```
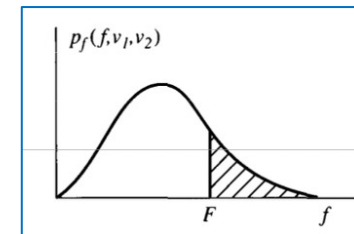
xspec> ftest chi2_mod2 dof_mod2 chi2_mod1 dof_mod1
➔ Low F value: low statistical significance of the added component

xspec> ftest 1253.3 1294 1286.8 1296

$p_f(f, v_1, v_2)$

```
XSPEC12>ftest 1253.3 1294 1286.8 1296
 F statistic value = 17.2939 and probability 3.87222e-08
```

Large F value → low probability (of exceeding that value, see tables)
→ highly significant improvement due to the additional component

Use the F-test to evaluate the improvement to a spectral fit due to the assumption of a different model, with additional terms
Conditions:
(a) the simpler model is nested within the more complex model;
(b) the extra parameters have Gaussian distribution (not truncated by the parameter space boundaries) − BUT see also Protassov+02 on caveats

$$P_f(f; v_1, v_2) = \frac{\chi_1^2 / v_1}{\chi_2^2 / v_2}$$

$$\propto \Delta\chi^2 / k$$

The larger this ratio, the larger the improvement in the spectral fitting
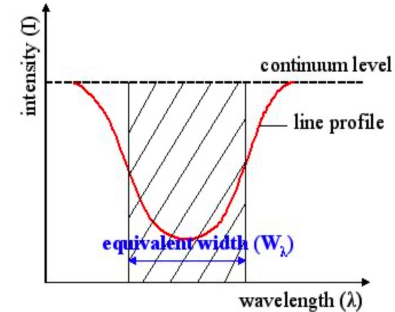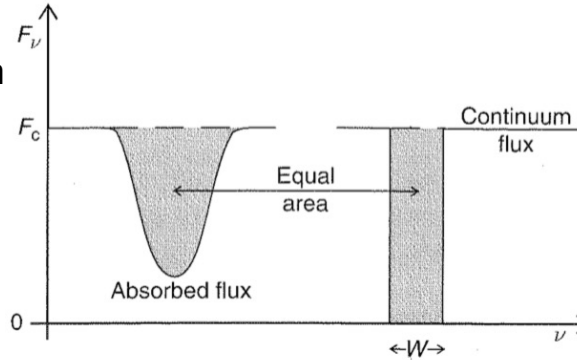
k=number of additional parameters

Uncertainties on the line EW measurement. I

Wavelength/frequency space definition [Angstrom/keV units]
EW is a measure of how prominent a line is (F_λ, F_ν) wrt. the continuum (F_C)

$$W_\lambda = \int_{\lambda_1}^{\lambda_2} \frac{F_C - F_\lambda}{F_C} d\lambda \quad \text{Units=Angstrom}$$

$$W_\nu = \int_{\nu_1}^{\nu_2} \frac{F_C - F_\nu}{F_C} d\nu \quad \text{Units=eV}$$

xspec> eqw # (#=model component of the Gaussian)
xspec> eqw # error 100 90 (EW including errors at 90% c.l.)

Alternatively: assuming that the dominant contribution to the EW error comes from the line intensity (so, limited contribution from the uncertainty on the continuum emission), one can (1) compute the 90% error on the line normalization, (2) place the upper 90% value as line normalization and (3) type *eqw* again (without fitting), then (4) place the lower 90% value as line normalization and (5) type *eqw* again (without fitting)

Uncertainties on the line EW measurement. II

```
========================================================================
Model phabs<1>*zphabs<2>(powerlaw<3> + zgauss<4>) Source No.: 1    Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   phabs      nH         10^22    0.291000      frozen
   2    2   zphabs     nH         10^22    0.513229      +/-  7.33688E-03
   3    2   zphabs     Redshift            4.80000E-02   frozen
   4    3   powerlaw   PhoIndex            1.62435       +/-  9.70444E-03
   5    3   powerlaw   norm                1.03048E-02   +/-  1.25935E-04
   6    4   zgauss     LineE      keV      6.40857       +/-  2.12948E-02
   7    4   zgauss     Sigma      keV      1.00000E-02   frozen
   8    4   zgauss     Redshift            4.80000E-02   frozen
   9    4   zgauss     norm                2.73168E-05   +/-  4.59249E-06
_____


Fit statistic  : Chi-Squared             1254.73     using 1299 bins.

Test statistic : Chi-Squared             1254.73     using 1299 bins.
 Null hypothesis probability of 7.78e-01 with 1294 degrees of freedom

XSPEC12>eqw 4

Data group number: 1
Additive group equiv width for Component 4:  0.0477921 keV
XSPEC12>eqw 4 err 100 90

Data group number: 1
Additive group equiv width for Component 4:  0.0477921 keV
Parameter distribution is derived from fit covariance matrix.
Equiv width error range:  0.0368183 - 0.0605744 keV
XSPEC12>error 9
 Parameter   Confidence Range (2.706)
      9  1.97559e-05  3.48608e-05     (-7.55792e-06,7.54694e-06)
XSPEC12>ne 9 1.97559e-05;eqw 4

Fit statistic  : Chi-Squared             1257.64     using 1299 bins.

Test statistic : Chi-Squared             1257.64     using 1299 bins.
 Null hypothesis probability of 7.61e-01 with 1294 degrees of freedom
 Current data and model not fit yet.

Data group number: 1
Additive group equiv width for Component 4:  0.0345677 keV
XSPEC12>ne 9 3.48608e-05;eqw 4

Fit statistic  : Chi-Squared             1257.64     using 1299 bins.

Test statistic : Chi-Squared             1257.64     using 1299 bins.
 Null hypothesis probability of 7.61e-01 with 1294 degrees of freedom
 Current data and model not fit yet.

Data group number: 1
Additive group equiv width for Component 4:  0.0609973 keV
```

easiest method (lower/upper 90% c.l. values)

"approximated" method (using the errors on the line normalization only)

Step 8: save data+model and 'recover' all in XSPEC later

To save the current data + model you may use the command

xspec> save all zpha_po_zgauss   A file zpha_po_zgauss.**xcm** is saved
xspec> […]

To recover the settings + data + model later, you can use the command

xspec> @zpha_po_zgauss.xcm
xspec> fit   XSPEC will ask you to fit the data again

Possibly useful commands

in **XSPEC**

➤ setplot rebin #1 #2 (to rebin the data; #1 indicates the number of σ)
➤ show all
➤ show files
➤ show notice
➤ script filename [save all the commands in a file (filename here; default: xspec.xcm]
➤ save model bestmodel.xcm (save only the best fit model, without the data)

In **IPLOT (plotting environment for XSPEC)**

xspec> **iplot**
• time off (to remove the date in the bottom-right part of the plot)
• csize 2 (character size)
• msize (marker size)
• label top (title of the plot)
• label filename (title of the file)
• **hardcopy nomefile.ps/cps** (save a figure)
• plot
• **wen nomefile [**writes two files (.qdp and .pco), one with data and the other
                         with plot settings]