XSPEC Tutorial and Statistics

Basic steps for X-ray spectral analysis

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Where can I find XSPEC?

- XSPEC is part of the NASA HEASoft software suite (FTOOLS)
- The latest version is HEASoft 6.32.1 (August 2023) xspec V12.13.1 https://heasarc.gsfc.nasa.gov/docs/software/heasoft/
- Supported architectures:
 - macOS
 - PC Linux Ubuntu, Fedora, Redhat Enterprise

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/

Outline

☐'Grouping' the data. Loading data in xspec & setup commands
☐ Response matrices
☐ A quick journey through models in xspec
☐ Binned vs. unbinned data
☐ Starting model & spectral fit
☐ Evaluation of the goodness of the fit
☐ Gaussian vs. Poissonian regime
☐ Adding spectral components
☐ F-test
☐ Contour plots
☐ Final fitting solution
☐ Errors on the parameters
☐ Fluxes and luminosities (and errors)
☐ Save/restore working session
☐ Some additional and useful commands

Step 1a: 'grouping' spectra (if not already done)

Once X-ray spectra are extracted and response matrices are produced – see Chandra and XMM-Newton Tutorials – four files (fits format) are needed within XSPEC

Chandra ACIS-S data in this example

 source spectrum 3C3 	3 r3.pi
---	---------

- background spectrum 3C33 r3 bkg.pi
- ARF response matrix 3C33 r3.corr.arf
- RMF response matrix 3C33_r3.rmf

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); this is done automatically for Chandra by running the ciao tool *specextract*;
- (2) group the spectral counts using a binning of e.g. 20 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 counting regime, use unbinned (or binned to 1 count/bin) data and Cash statistics

input src spectrum output src spectrum list of commands chkey: change key param in the spectrum fits file

grppha 3C33_r3.pi 3C33_r3_c20.pi comm="group min 20 & chkey BACKFILE 3C33_r3_bkg.pi & chkey ANCRFILE 3C33_r3.corr.arf & chkey RESPFILE 3C33_r3.rmf & exit"

→ 3C33_r3_c20.pi

Name all of the files properly!

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

```
xspec
```

```
xspec> data 3C33_r3_c20.pi
xspec> ignore bad
xspec> ignore **-0.3 7-**

xspec> cpd /xw
xspec> plot Idata
xspec> setplot command r y
```

- load the grouped spectrum (produced in step 1a)
- ignore spectral bins flagged as bad (typically, at low/high E)
- ignore spectral bins below 0.3 keV and above 7 keV (to be verified on the data, check src. vs. back level)
- change the plotting device (e.g., on screen here; on PS file)
- plot the data in log scale
- rescale the y axis

Energy: with "."

Otherwise: interpreted as channels if integer (conversion made via the RMF)

- The '-' sign indicates a range
- o **: means 'everything'

Loading multiple datasets

In case of **multiple datasets**: adoption of the same model to carry out a simultaneous X-ray spectral analysis (taking advantage of the 'increased' photon statistics)

```
all spectra are fits files (irregardless of the name, as .pi here)

xspec> data 1:1 spectrum1.pi 2:2 spectrum2.pi 3:3 spectrum3.pi
load all datasets at the same time

xspec> ignore 1-3:**-0.3 7.0-** select the proper energy range for all datasets (1-3)

xspec> cpd /xw

xspec> plot Idata
```

When **multiple datasets** are used, remember to place in front of all models the **constant model** [e.g., mo **cons**(pha*po+...)]. This takes into account:

- (a) cross-calibration uncertainties among different instruments of the same telescope (typically, a few percent) and different instruments onboard different telescopes;
- (b) 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 process).

xspec> show all

XSPEC version: 12.12.1
Build Date/Time: Thu Mar 31 20:12:13 2022

1 file 1 spectrum Spectrum 1 Spectral Data File: 3C33 r3 c20.pi Net count rate (cts/s) for Spectrum:1 6.520e-02 +/- 1.811e-03 (99.8 % tota)) Assigned to Data Group 1 and Plot Group 1 Noticed Channels: 2-61 Telescope: CHANDRA Instrument: ACIS Channel Type: PI Fraction of Exposure Time: 1.992e+04 sec **Src counts/Total counts** Using fit statistic: chi Using Background File 3C33_r3_bkg.pi Background Exposure Time: 1.992e+04 sec loaded back and 3C33_r3.rmf for Source 1 Using Response (RMF) File response files Using Auxiliary Response (ARF) File 3C33_r3.corr.arf Spectral data counts: 1301 (Total) Data counts

Source net (i.e. background-subtracted) **counts** = data counts × fraction = =1301 × 0.998 → in this case the source dominates the signal

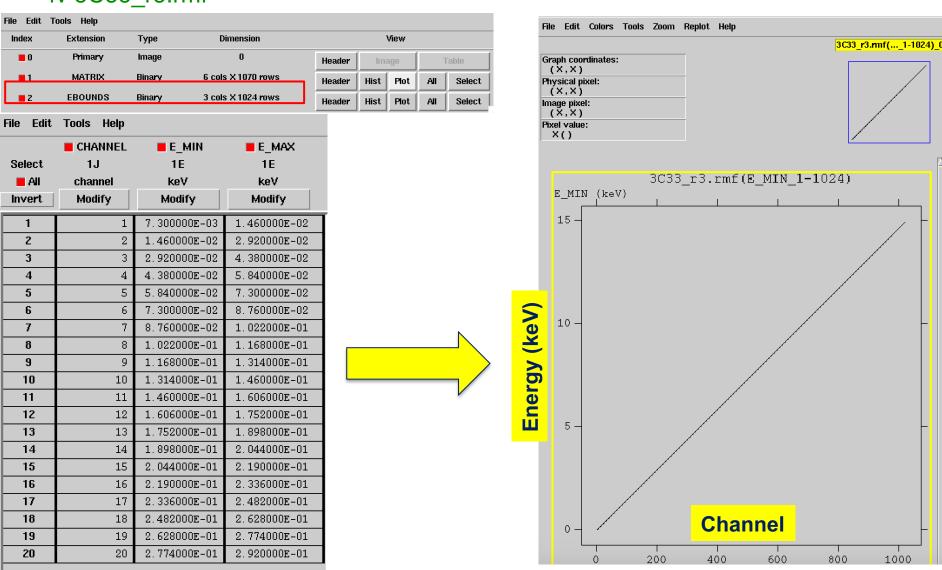
Possible binning choices depending on the source photon statistics:

- 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

fv 3C33_r3.rmf

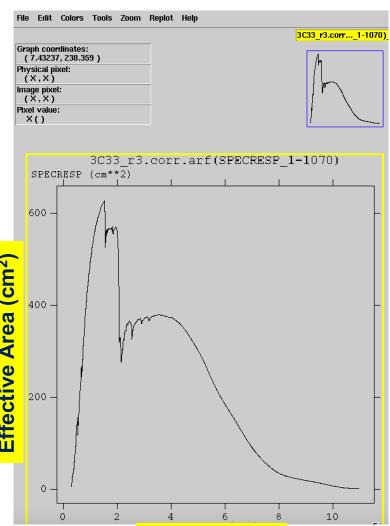


Response matrices: ARF

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

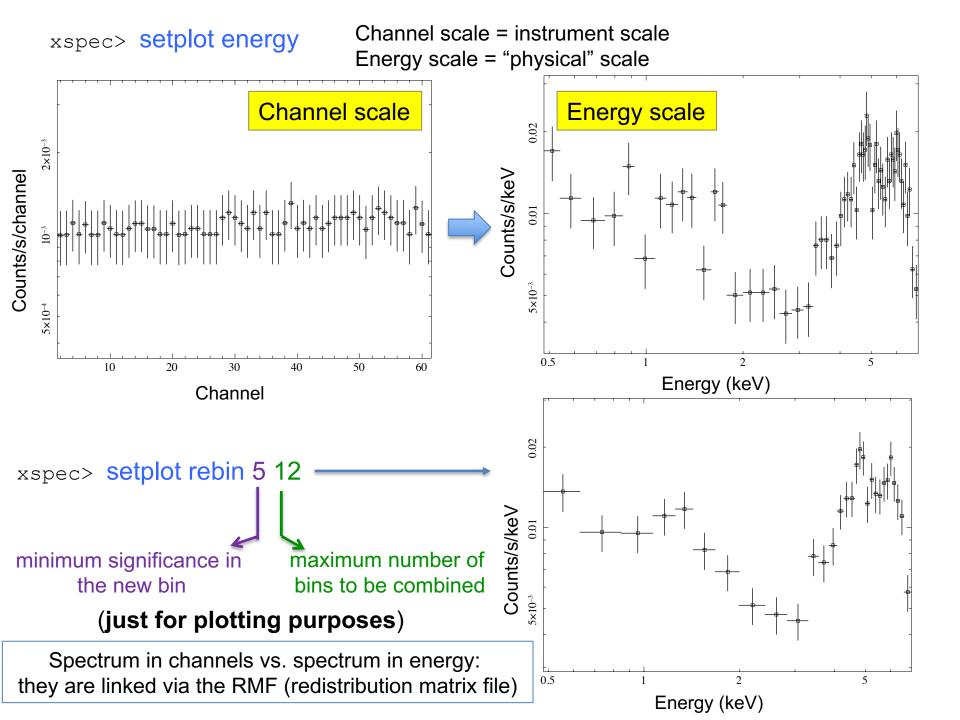
• fv 3C33_r3.corr.arf

File Edit	Tools Help			
	ENERG_LO	ENERG_HI	■ SPECRESP	PSF_FRAC
Select	1E	1E	1E	1D
All	keV	keV	cm**2	
Invert	Modify	Modify	Modify	Modify
1	3.000000E-01	3.100000E-01	3.886596⊑+00	9.729960747434E-01
2	3.100000E-01	3.200000E-01	1.144929E+01	9.729424863851E-01
3	3.200000E-01	3.300000E-01	1.601507E+01	9.728888978671E-01
4	3.300000E-01	3.400000E-01	2.089009E+01	9.728353095087E-01
5	3.400000E-01	3.500000E-01	2.528668E+01	9.727817211504E-01
6	3.500000E-01	3.600000 E-01	2.901072E+01	9.727281326324E-01
7	3.600000E-01	3.700000E-01	3.212375E+01	9.726745442740E-01
8	3.700000E-01	3.800000E-01	3.583970E+01	9.726209559157E-01
9	3.800000E-01	3.900000E-01	4.098644E+01	9.725673675574E-01
10	3.900000E-01	4.000000E-01	4.640701E+01	9.725137790394E-01
11	4.000000E-01	4.100000E-01	4.873587E+01	9.724601906810E-01
12	4.100000E-01	4.200000E-01	5.367477E+01	9.724066023227E-01
13	4.200000E-01	4.300000E-01	6.376080E+01	9.723530138047E-01
14	4.300000E-01	4.400000E-01	7.226711E+01	9.722994254463E-01
15	4.400000E-01	4.500000E-01	7.973080E+01	9.722458370880E-01
16	4.500000E-01	4.600000E-01	8.869151E+01	9.721922485700E-01
17	4.600000E-01	4.700000E-01	9.731506E+01	9.721386602116E-01
18	4.700000E-01	4.800000E-01	1.062349E+02	9.720850718533E-01
19	4.800000E-01	4.900000E-01	1.150116E+02	9.720314833353E-01
20	4.900000E-01	5.000000E-01	1.239493E+02	9.719778949770E-01



Energy (keV)

PSF_FRAC: a sort of aperture correction (see EEF concept)

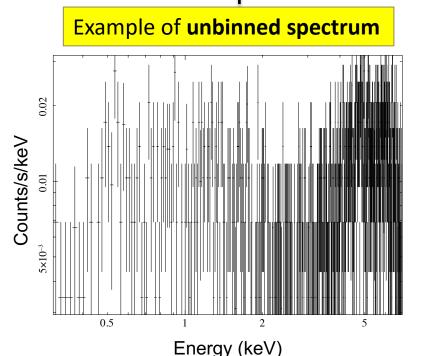


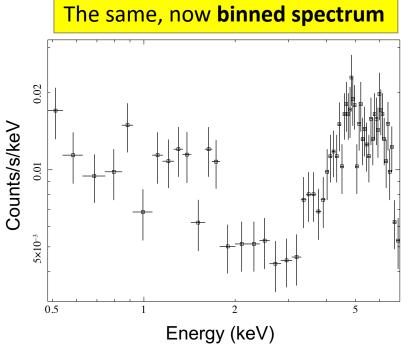
What does 'binning' (grouping) mean?

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 in each spectral bin (datapoint)

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

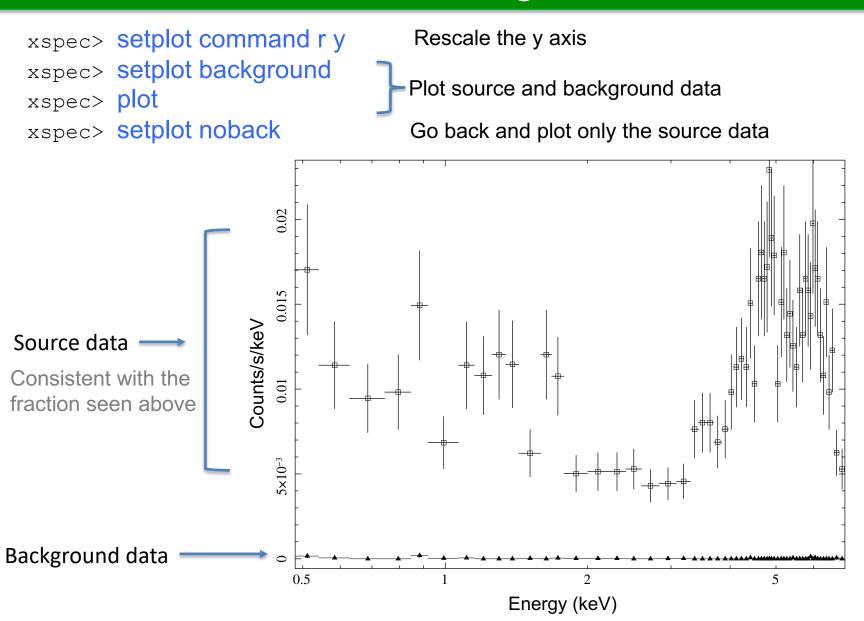
"original" distribution of the counts (note: here scale=energy)





Good photon statistics: it is suggested to rebin the data and apply χ^2

Source vs. background data



Step 2: `families' of xspec models

XSPEC models used like in 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			_			

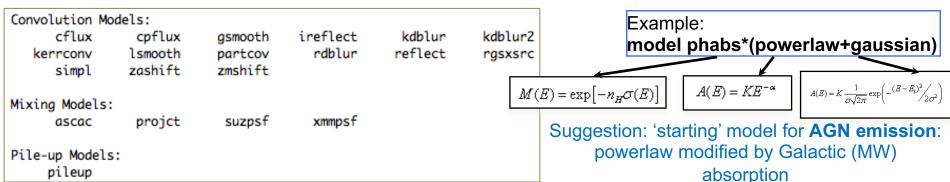
Multiplicative models

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



Step 3a: starting model + spectral fit

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

```
xspec> nh
          >>>>> NH version 3
         Equinox (d/f 2000)[2000]
         RA in hh mm ss.s or degrees[159.386] 01 08 52.86
                                                              Your source's coordinates (3C33 here)
         DEC in dd mm ss.s or degrees[56.171] 13 20 14.2
           >> Using map h1 nh HI4PI.fits
          LII , BII 129.448839 -49.313559
          Requested position at X and Y pixel
                                                932.06
                                                          321.88
          Search nH in 12 X 12 pixels box
          Each pixel is 0.083 deg 0.083 deg
              RA
                       DEC
                                Dist(deg)
                                                  nΗ
            17.2521 13.2623
                               0.0812
                                         2.93E+20
                               0.0940 2.89E+20
            17.1710 13.2564
            17.2913 13.3530
                               0.0709 3.03E+20
            17.2101 13.3472
                               0.0140 2.95E+20
                                         2.91E+20
            17.1289 13.3413
                               0.0890
           nH calculated using all points within 0.1000 deg from input position
           h1_nh_HI4PI.fits >> Average nH (cm**-2) 2.94E+20
                                                                          N_{H,Gal} = 2.96 \times 10^{20} \text{ cm}^{-2}
           h1 nh HI4PI.fits >> Weighted average nH (cm**-2) 2.96E+20
```

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)

Suggestion: start with a simple modeling (as a powerlaw modified by Galactic absorption)

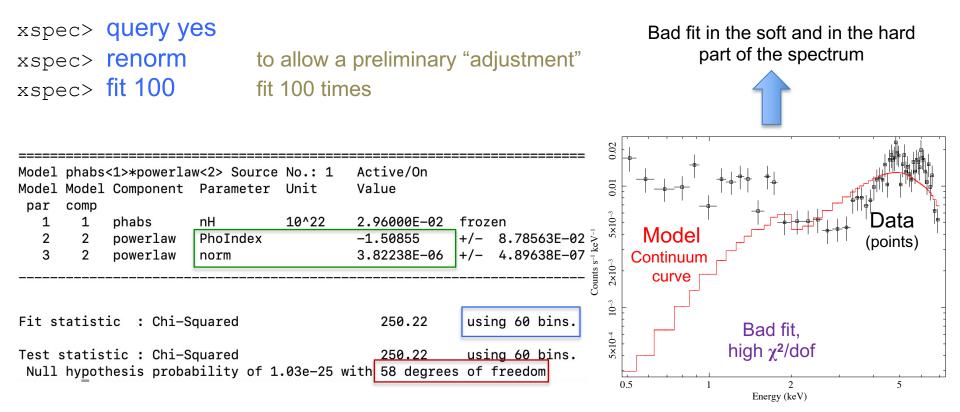
xspec> mo pha*po

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
[XSPEC12>mo pha*po
Input parameter value, delta, min, bot, top, and max values for ...
                    0.001(
                                0.01)
                                                                100000
                                                                            1e+06
1:phabs:nH>2.96e-2 -1
                       01(
                                0.01)
                                                         -2
                                                                               10
2:powerlaw:PhoIndex>1.9
                                0.01)
                                                                 1e+20
                                                                            1e+24
                      0.01(
                                 -1 means frozen parameter (the same as using the
[3:powerlaw:norm>1e-5
                                 command freeze # of the parameter; opposite: thaw)
Model phabs<1>*powerlaw<2> Source No.: 1
                                          Active/On
                                                                     Alternatively, you may
Model Model Component Parameter Unit
                                          Value
 par comp
                                                                     assign later a value to a
            phabs
                      nΗ
                                 10^22
                                          2.96000E-02 frozen
                                                                     parameter using
            powerlaw
                      PhoIndex
                                          1.90000
            powerlaw
                                          1.00000E-05
                                                           0.0
                                                       +/-
                      norm
                                                                     xspec> newpar 2 1.9
Fit statistic : Chi-Squared
                                            1084.55
                                                        using 60 bins.
Test statistic : Chi-Squared
                                            1084.55
                                                        using 60 bins.
 Null hypothesis probability of 3.89e-189 with 58 degrees of freedom
 furrent data and model not fit yet.
```

parameter number of number the component

Model: pha(po)



dof=degrees of freedom=(number of datapoints – number of free parameters)=60-2=58

- χ^2 /dof close to unity means that it is a good fit (here: 250/58: not in this case!) see lesson on statistics and the following slides
- <u>Null hypothesis probability</u>=probability that the model is a good representation of the datapoints (i.e., good if close to 1; see also tutorial on Statistics)

All the adopted models should be physically motivated according to the known source (multi-wavelength) properties & classification

Model: pha(po)

To evaluate the goodness of the fit: the 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

$$S = \sum_{i} \left(\frac{S_i - B_i t_s / t_b}{O_K} - \frac{m_i t_s}{E_K} \right)^2 / \left(\frac{(\sigma_S)_i^2 + (\sigma_B)_i^2}{\sigma_K} \right)^2$$

- \circ S_i = src counts in the I={1,...,N} data bins with exposure t_S;
- B_i = background counts with exposure t_B;
- m_i = model predicted count rate;
- o $(\sigma_S)^2$ 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

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

To modify S so the it performs better in low-count regime (e.g., by ii. 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)
xspec> statistic cstat
```

χ^2 in a nutshell

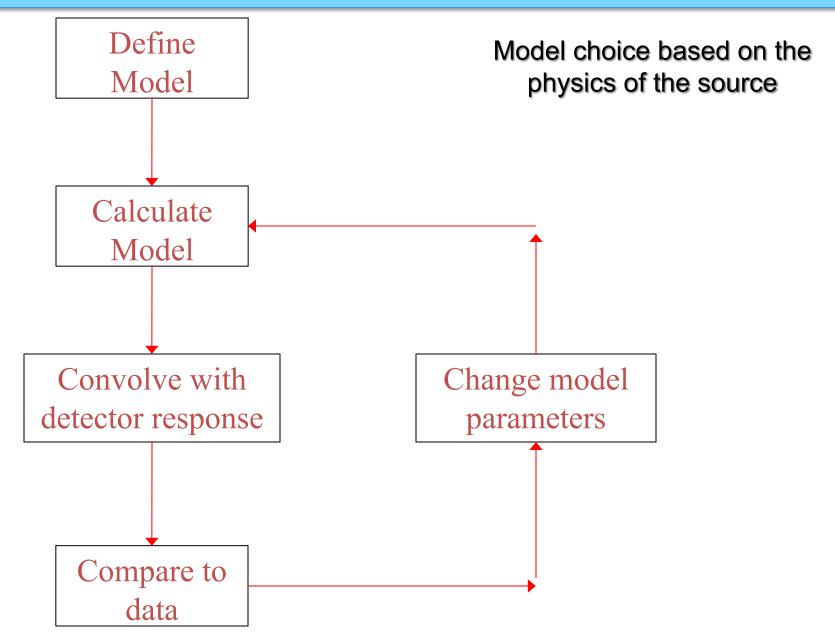
Reduced χ^2 large \longleftrightarrow P(χ^2) small

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

Reduced
$$\chi^2$$
 small \longleftrightarrow P(χ^2) large

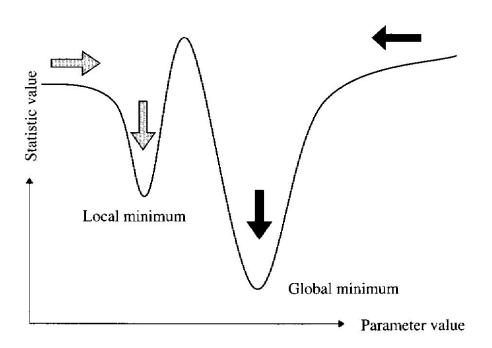
- c. Errors are over-estimated
- d. Were data "selected" in a particular way?

Forward-fitting algorithm



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

To 'move' the fit from a local miminum, you can change some of the parameters using the *newpar* command and then fit again

Step 3b: adding components and fit. I

xspec> addcomp 2 powerlaw

powerlaw

norm

adding a powerlaw as # component (#=order in the model)

10

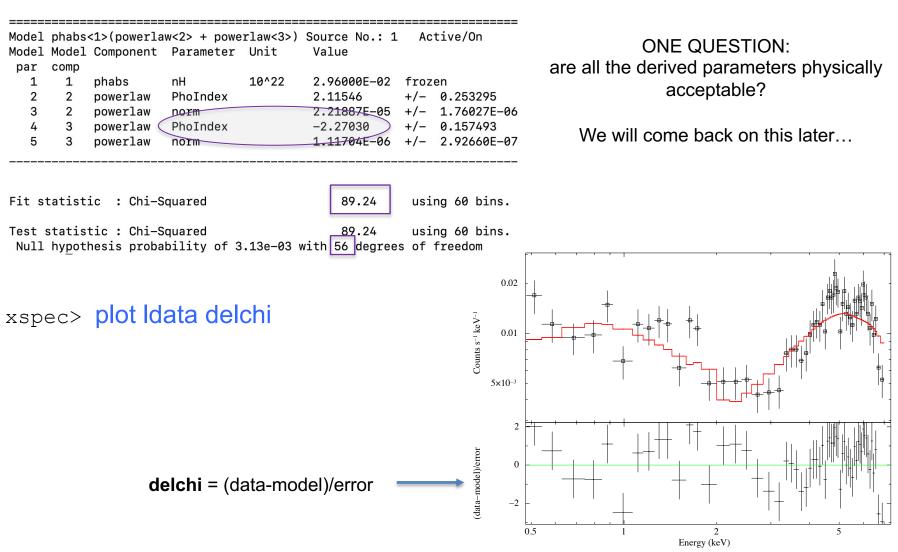
1e+24

```
Input parameter value, delta, min, bot, top, and max values for ...
                      0.01(
                                 0.01)
                                               -3
                                                          -2
2:powerlaw:PhoIndex>1.8
                      0.01(
                                 0.01)
                                                                  1e+20
3:powerlaw:norm>1e-5
Fit statistic : Chi-Squared
                                              164,18
                                                         using 60 bins.
Test statistic: Chi-Squared
                                              164.18
                                                         using 60 bins.
Null hypothesis probability of 1.47e-12 with 56 degrees of freedom
Current data and model not fit vet.
Model phabs<1>(powerlaw<2> + powerlaw<3>) Source No.: 1
                                                          Active/On
Model Model Component Parameter Unit
                                           Value
par
     comp
            phabs
                       nH
                                  10^22
                                           2.96000E-02 frozen
                       PhoIndex
                                           1.80000
                                                             0.0
            powerlaw
                                           1.00000E-05
           powerlaw
                       norm
                                                             0.0
                                           -1.50636
            powerlaw
                       PhoIndex
```

3.83424E-06 +/-

Inclusion of an additional powerlaw component to account for the residuals observed at low energies: scattering component? phenomenological (simplistic) parameterization of something different?

xspec> fit 100



The χ^2 /dof=89.2/56 is much lower than previous one and the model more properly reproduces the observed spectral datapoint distribution. There are yet *some residuals* (bottom panel: data-model, i.e. deviations in units of σ =stat. error)

Model: pha(po+po)

Step 3b: adding components and fit. II

xspec> addcomp 3 zpha adding zpha=absorption intrinsic to the source as third component

1e+06

10

```
Input parameter value, delta, min, bot, top, and max values for ...
                                0.01)
                    0.001(
                                                                100000
[4:zphabs:nH>1
                                0.01) -0.999
                    -0.01(
                                                     -0.999
                                                                    10
5:zphabs:Redshift>0.06
                       z=0.06
Fit statistic : Chi-Squared
                                              93.47
                                                        using 60 bins.
Test statistic : Chi-Squared
                                              93.47
                                                        using 60 bins.
 Null hypothesis probability of 9.34e-04 with 55 degrees of freedom
 Current data and model not fit yet.
```

```
Model phabs<1>(powerlaw<2> + zphabs<3>*powerlaw<4>) Source No.: 1
                                                                  Active/On
Model Model Component Parameter Unit
                                         Value
 par
     comp
  1
       1
           phabs
                      nΗ
                                 10^22
                                          2.96000E-02 frozen
           powerlaw
                      PhoIndex
                                                      +/- 0.253295
                                          2.11546
           powerlaw
                                          2.21887E-05 +/- 1.76027E-06
                      norm
           zphabs
                                 10^22
                      nΗ
                                         1.00000
                                                      +/- 0.0
           zphabs
                      Redshift
                                          6.00000E-02 frozen
                                                      +/- 0.157493
           powerlaw
                      PhoIndex
                                         -2.27030
                                         1.11704E-06 +/- 2.92660E-07
           powerlaw
                      norm
```

Justification: the inverted slope of the continuum (negative photon index) may be ascribed to the presence of obscuration

After the inclusion of N_H,is the newly derived photon index (parameter 6, component 4) more consistent with what is expected in case of an AGN (Γ=1.8-2)?

xspec> fit 100

=====	=====					=====		====
Model	phabs	<1>(powerla	w<2> + zpha	bs<3>*pow	verlaw<4>) Sou	rce N	o.: 1	Active/On
Model	Model	Component	Parameter	Unit	Value			
par	comp							
1	1	phabs	nH	10^22	2.96000E-02	froz	en	
2	2	powerlaw	PhoIndex		1.14238	+/-	0.16180	1
3	2	powerlaw	norm		2.45188E-05	+/-	1.69217	E-06
4	3	zphabs	nH	10^22	22.0419	+/-	5.59213	
5	3 _	zphabs	Redshift		6.00000E-02	froz	en	
6	4	powerlaw	PhoIndex		-0.539341	+/-	0.52868	8
7	4 📙	powerlaw	norm		3.81227E-05	+/-	3.43217	E-0 5

Fit statistic : Chi-Squared 76.04 using 60 bins.

Test statistic : Chi-Squared 76.04 using 60 bins.

Null hypothesis probability of 3.16e-02 with 55 degrees of freedom

 χ^2 /dof=76.0/55 now \rightarrow improvement in the fit

However, the photon index (parameter 6, component 4) is still negative

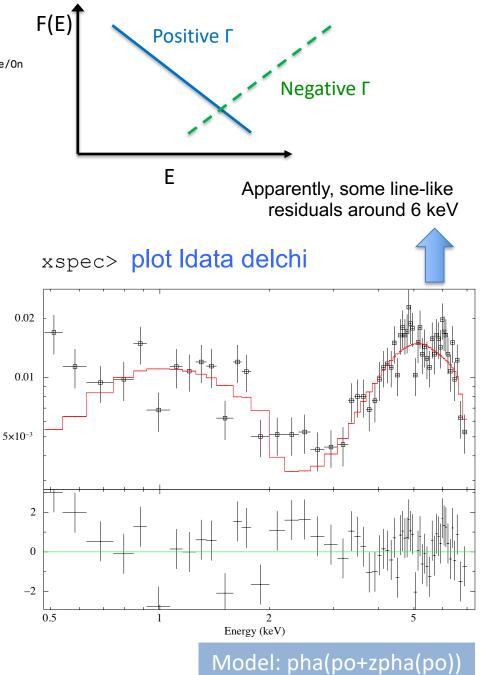
Counts s-1 keV-1

data-model)/error

→ likely, the hard-band powerlaw and the column density are degenerate parameters, hence constraining both over the limited hard band of Chandra is challenging

VIABLE SOLUTIONS:

Link the photon indices of the two powerlaw as in the case of Thomson scattering in the soft band) – see the following slides (Step 5b)



Step 3b: adding components and fit. III

xspec> addcomp 4 zgauss adding zgauss=emission line as fourth component

```
Input parameter value, delta, min, bot, top, and max values for ...
                      0.05(
                                0.065)
                                                                            1e+06
            6.5
                                                                  1e+06
6:zgauss:LineE>6.4
                                                                                   I have included a narrow (\sigma=10 eV, fixed)
                      0.05(
                                0.001)
                                                           0
                                                                    10
            0.1
                                                                                   line at the expected rest-frame energy of
[7:zgauss:Sigma>0.01,-1
                     -0.01(
                                 0.01)
                                           -0.999
                                                      -0.999
                                                                    10
                                                                                     the neutral iron Kα transition (6.4 keV)
8:zgauss:Redshift>0.06
                      0.01(
                                 0.01)
                                                0
                                                           0
                                                                  1e+20
                                                                            1e+24
9:zgauss:norm>1e-6
Fit statistic : Chi-Squared
                                                        using 60 bins.
                                              74.92
Test statistic : Chi-Squared
                                              74.92
                                                        using 60 bins.
 Null hypothesis probability of 2.54e-02 with 53 degrees of freedom
 Current data and model not fit yet.
Model phabs<1>(powerlaw<2> + zphabs<3>(zgauss<4> + powerlaw<5>)) Source No.: 1 Active/On
Model Model Component Parameter Unit
                                           Value
 par
      comp
        1
            phabs
                       nΗ
                                  10^22
                                           2.96000E-02 frozen
                                           1.14238
                                                        +/- 0.161801
            powerlaw
                       PhoIndex
            powerlaw
                                           2.45188E-05 +/- 1.69217E-06
                       norm
            zphabs
                                  10^22
                                           22.0419
                                                       +/- 5.59213
                       nΗ
            zphabs
                       Redshift
                                           6.00000E-02 frozen
            zgauss
                       LineE
                                  keV
                                           6.40000
                                                       +/- 0.0
            zgauss
                       Sigma
                                  keV
                                           1.00000E-02 frozen
            zgauss
                       Redshift
                                           6.00000E-02 frozen
            zaauss
                       norm
                                           1.00000E-06 +/- 0.0
  10
                                           -0.539341
                                                        +/- 0.528688
            powerlaw
                       PhoIndex
```

3.81227E-05 +/- 3.43217E-05

11

powerlaw

norm

Model: pha(po+zpha(zgauss+po+))

xspec> fit 100

```
Model phabs<1>(powerlaw<2> + zphabs<3>(zgauss<4> + powerlaw<5>)) Source No.: 1
                                                                                    Active/On
Model Model Component Parameter Unit
                                             Value
 par
      comp
        1
            phabs
                        nΗ
                                   10^22
                                             2.96000E-02
                                                          frozen
            powerlaw
                        PhoIndex
                                             1.15143
                                                               0.161868
            powerlaw
                                             2.45395E-05
                                                               1.69157E-06
                        norm
            zphabs
                                   10^22
                                             22.2581
                                                          +/- 5.75947
                        nΗ
            zphabs
                        Redshift
                                             6.00000E-02
                                                          frozen
                        LineE
                                                          +/- 4.48975E-02
                                   keV
                                             6.39238
            zgauss
                       Sigma
            zgauss
                                   keV
                                             1.00000E-02
                                                          frozen
                        Redshift
                                             6.00000E-02
            zgauss
                                                          frozen
                                                               4.45599E-06
            zgauss
                        norm
                                             1.08538E-05
  10
                        PhoIndex
                                             -0.392248
                                                               0.555082
            powerlaw
 11
            powerlaw
                                             4.82903E-05
                                                               5.22882E-05
                        norm
```

xspec> plot Idata delchi

Fit statistic : Chi-Squared

69.70 using 60 bins.

Test statistic : Chi-Squared

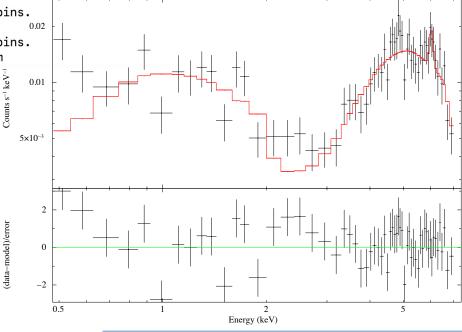
69.70 using 60 bins.

Null hypothesis probability of 6.17e-02 with 53 degrees of freedom

Is the added component (the line in this case) statistically significant?

How much significant?



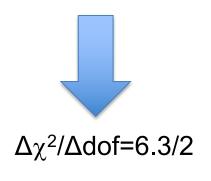


Model: pha(po+zpha(zgauss+po+))

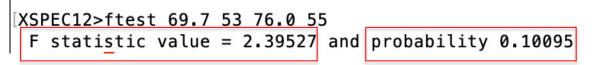
Step 4: the F-test

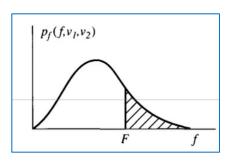
(here applied to estimate the statistical significance of the inclusion of an emission line)

- ➤ Model 1: double powerlaw + obscuration: χ^2 /dof=76.0/55
- ▶ Model 2: double powerlaw + obscuration + iron emission line: χ^2 /dof=69.7/53



```
xspec> ftest 69.7 53 76.0 55 \chi^2 \text{ (model 2) dof (model 2)} \qquad \chi^2 \text{ (model 1) dof (model 1)}
```





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

→ The iron line has low significance: P(real line)=1-0.10095~0.90 → ~1.6 σ

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

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

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

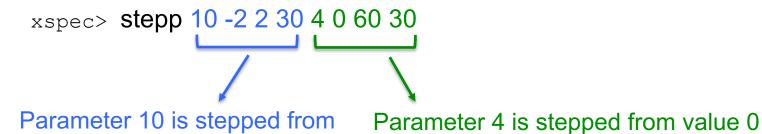
The larger this ratio, the larger the improvement in the spectral fitting

k=number of additional parameters

Step 5a: contour plots and error computation

Use the *steppar* command to compute errors simultaneously for two parameters and visualize them using contour plots - it performs a fit while stepping the values of two parameters through a given range

Here: photon index (param. 10) vs. column density (param. 4)

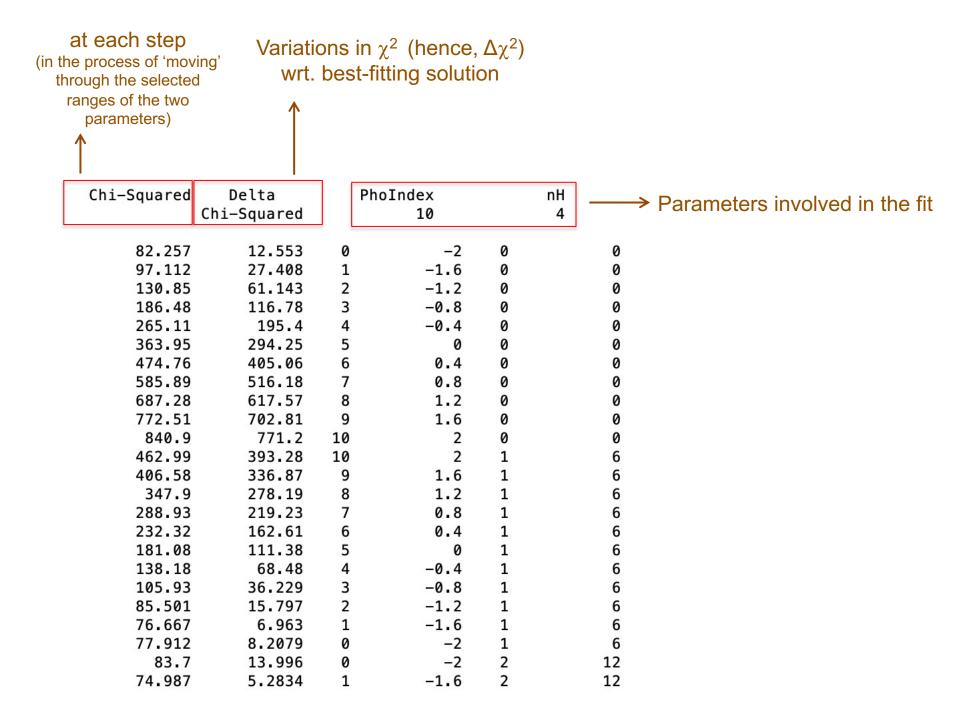


value -2 to 2 in 30 steps

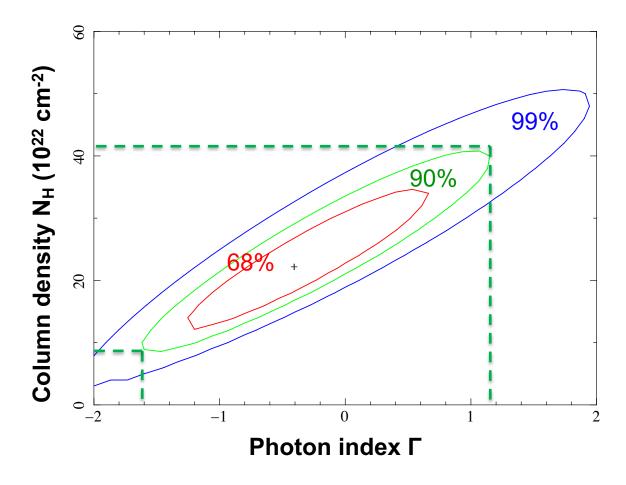
It provides how one parameter varies wrt. another parameter (i.e., the error range for sets of parameters)

to 60 (units of 10²² cm⁻²) in 30 steps

Useful also to understand whether two spectral parameters are correlated (not necessarily from a physical point of view)



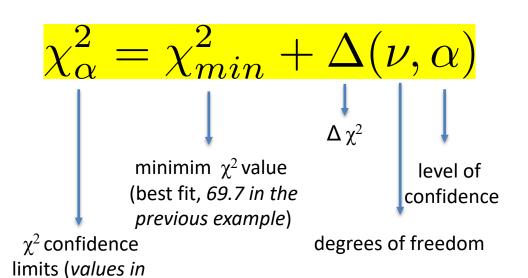
xspec> plot contour



- o 90% confidence level: the photon index varies in the range ~ [-1.6, 1.2], while the column density varies in the interval ~ [9-41] × 10^{22} cm⁻²
- The photon index and the column density are degenerate parameters
- We can decide to link the photon indices of the two powerlaws (as in case of scattering)

The meaning of contour plots/confidence regions

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



We will further discuss this Δ later in the slides

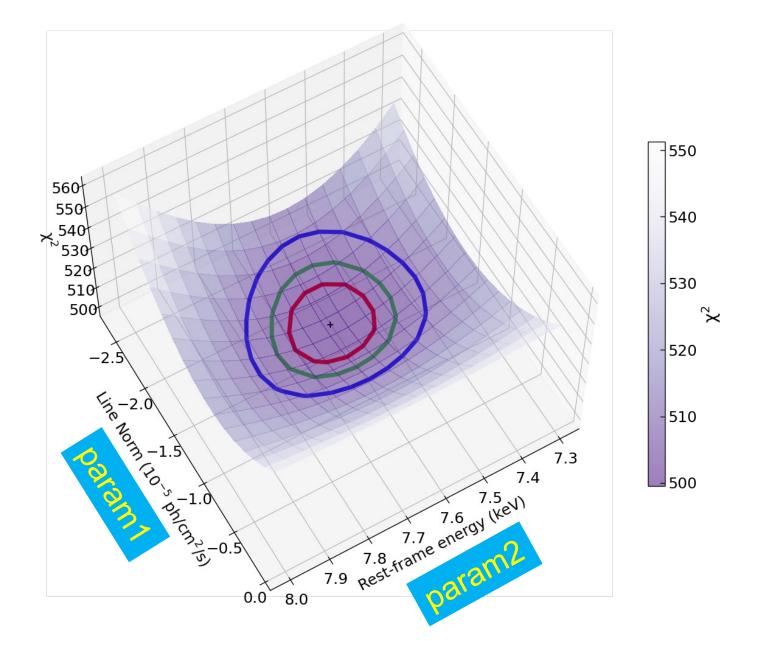
Δ depends only on the number of parameters involved in the fit (see previous slides)

steppar)

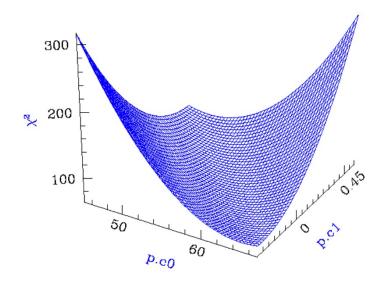
Avni 1976

CONSTANTS FOR	CALCULATING	CONFIDENCE	REGIONS
---------------	-------------	------------	---------

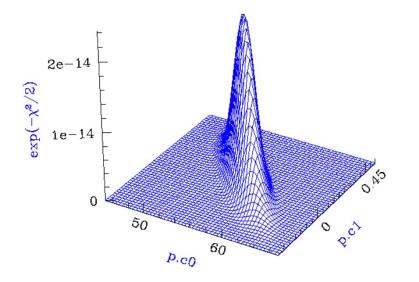
	q (No. of	INTERESTING PA	RAMETERS)
(%)	1	2	3
68	1.00	2.30	3.50
90	2.71	4.61	6.25
99	6.63	9.21	11.30



Courtesy of E. Bertola

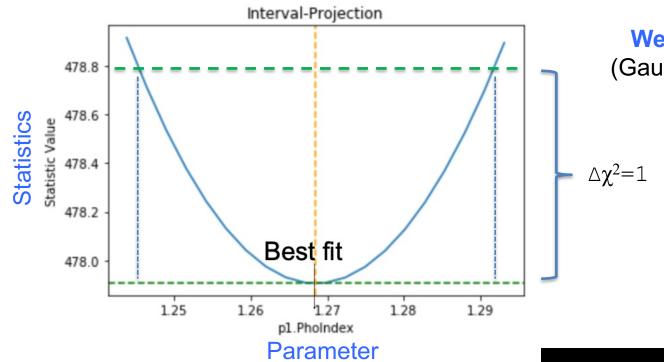


Calculating Confidence Limits means
Exploring the Parameter Space - Statistical
Surface



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(- χ^2 /2) \approx L, bottom).

Credits: A. Siemiginowska

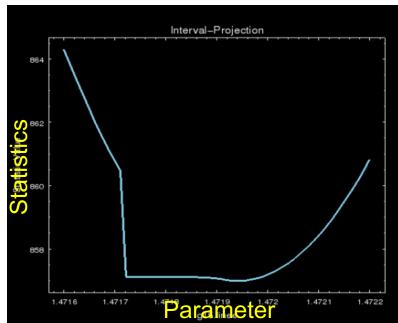


Well-behaved surface

(Gaussian, one parameter)

 $\Delta \chi^2 = 1$ (68% conf. level)

Not well-behaved surface (not Gaussian)



Credits: A. Siemiginowska

Step 5b: towards the final fitting solution

xspec > newpar 2 = 10

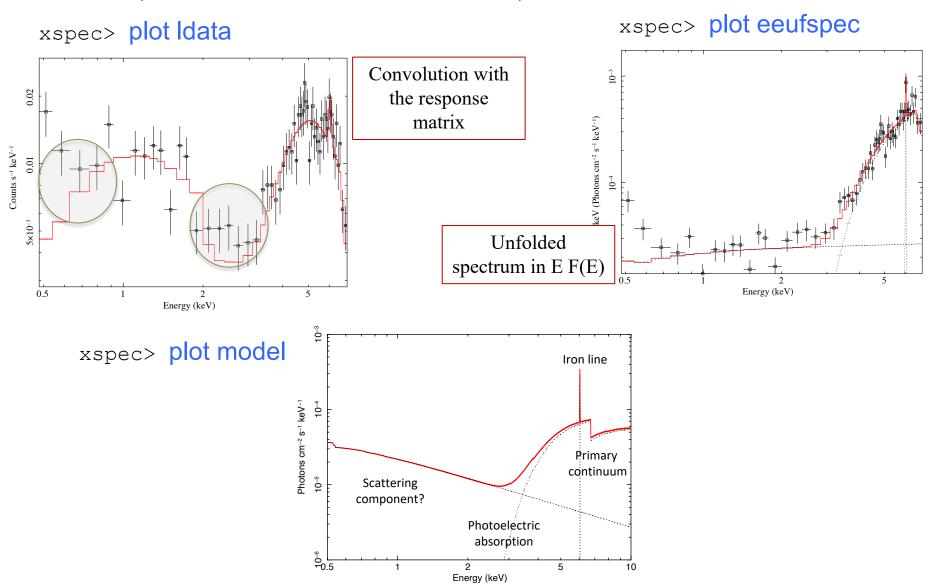
We link the photon index of the secondary (soft) component to that of the primary one (as expected in case of scattering)

```
Model phabs<1>(powerlaw<2> + zphabs<3>(zqauss<4> + powerlaw<5>)) Source No.: 1
                                                                                   Active/On
Model Model Component Parameter Unit
                                            Value
 par
      comp
                                   10^22
   1
        1
            phabs
                       nH
                                            2.96000E-02
                                                         frozen
   2
        2
            powerlaw
                                                          = p10
                       PhoIndex
                                            -0.392248
            powerlaw
                                            2.45395E-05
                                                          +/- 0.0
                       norm
                                   10^22
            zphabs
                       nΗ
                                            22.2581
                                                          +/- 0.0
            zphabs
                       Redshift
                                            6.00000E-02 frozen
            zgauss
                       LineE
                                   keV
                                            6.39238
                                                          +/- 0.0
            zgauss
                       Sigma
                                   keV
                                            1.00000E-02 frozen
            zgauss
                       Redshift
                                                         frozen
                                            6.00000E-02
            zgauss
                                            1.08538E-05
                                                         +/-
                                                               0.0
                       norm
  10
            powerlaw
                       PhoIndex
                                            -0.392248
                                                               0.0
  11
        5
            powerlaw
                                            4.82903E-05
                       norm
```

xspec> fit 100

Model phabs<1>(powerlaw<2> + zphabs<3>(zgauss<4> + powerlaw<5>)) Source N Model Model Component Parameter Unit Value par comp 1 phabs 10^22 1 nΗ 2.96000E-02 frozen powerlaw PhoIndex = p100.935292 3 powerlaw 2.35020E-05 +/-1.69263E-06 norm zphabs 10^22 37.6379 2.73295 nΗ +/zphabs Redshift 6.00000E-02 frozen +/- 4.51006E-02 zgauss LineE keV 6.39929 zgauss Sigma keV 1.00000E-02 frozen 6.00000E-02 frozen zgauss Redshift Model: pha(po+zpha +/zgauss norm 1.43843E-05 (zgauss+po+)) 10 powerlaw PhoIndex 0.935292 11 powerlaw 6.78472E-04 +/norm $\Gamma_1 = \Gamma_2$

- Some residuals in the soft band and around 2 keV, where the soft and hard components 'connects' each other
- The photon index is still (nominally) lower than expected → reflection component needed (but <u>not</u> accounted for in this tutorial)



Step 5c: estimate of parameters uncertainties

To compute errors: *error* and *uncertainty* commands in xspec

Model phabs<1>*powerlaw<2> + zphabs<3>(zgauss<4> + powerlaw<5>) Source No Model Model Component Parameter Unit Value comp par 1 phabs nΗ 10^22 2.96000E-02 frozen 1 PhoIndex 0.935354 powerlaw = p10powerlaw 2.35026E-05 +/- 1.69262E-06 norm 10^22 37,6728 +/- 2.73288 4 zphabs nΗ zphabs Redshift 6.00000E-02 frozen +/- 4.51013E-02 keV 6.39928 zgauss LineE keV 1.00000E-02 zgauss Sigma frozen Redshift 6.00000E-02 zgauss frozen 9 zgauss 1.43840E-05 +/- 5.64652E-06 norm 10 powerlaw PhoIndex 0.935354 +/- 0.137424 11 powerlaw 6.78558E-04 1.83102E-04 +/norm

These are the errors at 1 σ for that parameter

```
Fit statistic : Chi-Squared 73.33 using 60 bi
Test statistic : Chi-Squared 73.33 using 60 bi
Null hypothesis probability of 4.11e-02 with 54 degrees of freedom
```

	$\Delta\chi^2$ as a Function of Confidence Level and Degrees of Freedom											
		ν										
Ĺr	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					
Ĺr	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					

Parameter Confidence Range (2.706)
4 33.101 42.8442 (-4.57177,5.17145)

By default, xspec computes errors at the 90% confidence level (2.706) for one parameter of interest (Avni 1976; Lampton et al. 1976) – it is the Δ parameter seen before

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

Ex. 2: Error at 9	00% 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

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

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

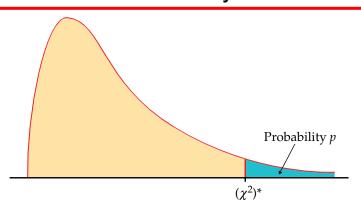


Table entry for p is the critical value $(\chi^2)^*$ with probability p lying to its right.

	χ^2 distribution critical values												
					.10		Tail prob	ability <i>p</i>	.01				
Parameters of interest -	df	➤ .25	.20	.15	.10	.05	.025	.02	.01	.005	.0025	.001	.0005
	1 2	1.32 2.77	1.64 3.22	2.07 3.79	2.71 4.61	3.84 5.99	5.02 7.38	5.41 7.82	6.63 9.21	7.88 10.60	9.14 11.98	10.83 13.82	12.12 15.20
	3 4	4.11 5.39	4.64 5.99	5.32 6.74	6.25 7.78	7.81 9.49	9.35 11.14	9.84 11.67	11.34 13.28	12.84 14.86	14.32 16.42	16.27 18.47	17.73 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

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})

$$W_{\lambda} = \int_{\lambda_{1}}^{\lambda_{2}} \frac{F_{C} - F_{\lambda}}{F_{C}} d\lambda \quad \text{Units=Angstrom}$$

$$W_{\nu} = \int_{\nu_{1}}^{\nu_{2}} \frac{F_{C} - F_{\nu}}{F_{C}} d\nu \quad \text{Units=eV}$$

$$V_{\nu} = \int_{\nu_{1}}^{\nu_{2}} \frac{F_{C} - F_{\nu}}{F_{C}} d\nu \quad \text{Units=eV}$$

$$V_{\nu} = \int_{\nu_{1}}^{\nu_{2}} \frac{F_{C} - F_{\nu}}{F_{C}} d\nu \quad \text{Units=eV}$$

$$V_{\nu} = \int_{\nu_{1}}^{\nu_{2}} \frac{F_{C} - F_{\nu}}{F_{C}} d\nu \quad \text{Units=eV}$$

$$V_{\nu} = \int_{\nu_{1}}^{\nu_{2}} \frac{F_{C} - F_{\nu}}{F_{C}} d\nu \quad \text{Units=eV}$$

$$V_{\nu} = \int_{\nu_{1}}^{\nu_{2}} \frac{F_{C} - F_{\nu}}{F_{C}} d\nu \quad \text{Units=eV}$$

xspec> eqw 4

#=model component associated with the Gaussian line

```
Data group number: 1
Additive group equiv width for Component 4: 0.100872 keV
```

xspec> eqw 4 err 100 90 EW including errors at 90% confidence level doing 100 trials

Data group number: 1 Additive group equiv width for Component 4: 0.100872 keV Parameter distribution is derived from fit covariance matrix. Equiv width error range: 0.0414912 - 0.184698 keV

EW=101 [41-185] eV

Uncertainties on the line EW measurement. II

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)

```
Model phabs<1>*powerlaw<2> + zphabs<3>(zgauss<4> + powerlaw<5>) Source No
Model Model Component Parameter Unit
                                           Value
 par comp
   1
       1
            phabs
                       nΗ
                                  10^22
                                           2.96000E-02 frozen
                       PhoIndex
            powerlaw
                                           0.935354
                                                        = p10
            powerlaw
                                           2.35026E-05 +/- 1.69262E-06
                       norm
            zphabs
                       nΗ
                                  10^22
                                           37,6728
                                                        +/- 2.73288
            zphabs
                       Redshift
                                           6.00000E-02 frozen
   6
            zgauss
                       LineE
                                  keV
                                           6.39928
                                                        +/- 4.51013E-02
                                  keV
            zgauss
                       Sigma
                                           1.00000E-02 frozen
                       Redshift
           zgauss
                                           6.00000E-02 frozen
                                           1.43840E-05 +/- 5.64652E-06
            zgauss
                       norm
  10
            powerlaw
                       PhoIndex
                                           0.935354
                                                        +/- 0.137424
  11
            powerlaw
                       norm
                                           6.78558E-04 +/- 1.83102E-04
```

```
xspec> error 9

9 4.95654e-06 2.36522e-05 (-9.42745e-06,9.2682e-06)
```

EW=101 [35–166] eV
Totally conistent with the previous value



```
XSPEC12>he 9 2.36522e-05
 Fit statistic : Chi-Squared
                                                76.24
                                                          using 60 bins.
 Test statistic : Chi-Squared
                                                76.24
                                                          using 60 bins.
  Null hypothesis probability of 2.48e-02 with 54 degrees of freedom
  Current data and model not fit yet.
 XSPEC12>eqw 4
 Data group number: 1
                                              0.165868 keV
 Additive group equiv width for Component 4:
 XSPEC12>ne 9 4.95654e-06
 Fit statistic : Chi-Squared
                                                76.34
                                                          using 60 bins.
                                                76.34
 Test statistic : Chi-Squared
                                                          using 60 bins.
  Null hypothesis probability of 2.43e-02 with 54 degrees of freedom
  Current data and model not fit yet.
 XSPEC12>eqw 4
 Data group number: 1
 Additive group equiv width for Component 4
                                              0.0347591 keV
```

Step 6: source flux and luminosity

command *cosmo* to change the cosmology

- ☐ Flux is observed (typically, no correction for absorption) and in the observed-frame band (units: erg/cm²/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., 2-10 keV band)

```
XSPEC12>flux 2 10 error 100 90

Parameter distribution is derived from fit covariance matrix.

Model Flux 0.00035807 photons (3.8799e-12 ergs/cm^2/s) range (2.0000 - 10.000 keV)

Error range 0.0003102 - 0.0003806 (3.310e-12 - 4.166e-12) (90.00% confidence
```

$$F(2-10 \text{ keV})=3.9 [3.3-4.2]\times10^{-12} \text{ erg/cm}^2/\text{s}$$

For what concerns the luminosity, we cannot apply the same method: if we place N_H=0 to have intrinsic values, xspec requires the data to be fit again

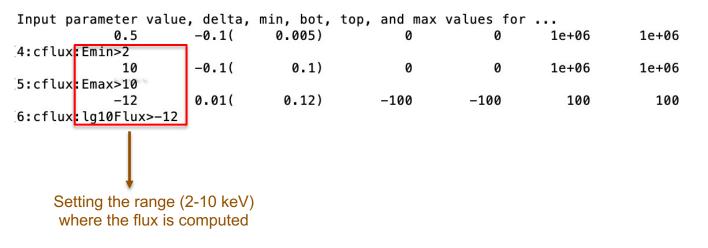


cflux and clumin commands

Uncertainties on fluxes and luminosities. II

- o cflux and clumin are multiplicative model components.
- cflux (clumin) are placed in front of model component(s). At least one of the additive models should have the normalization fixed (frozen) to a non-zero value.
- cflux/clumin must be treated as the other model components (as part of the fit)
- Example: model pha*cflux*zpha*pow

```
xspec> addcomp 3 cflux
```



xspec> freeze 14 fix the powerlaw normalization (as required by the cflux tool)

xspec> fit 100

Uncertainties on fluxes and luminosities. III

```
Model phabs<1>*powerlaw<2> + cflux<3>*zphabs<4>(zgauss<5> + powerlaw<6>)
Model Model Component Parameter Unit
                                           Value
 par
    comp
   1
            phabs
                       nΗ
                                  10^22
                                           2.96000E-02 frozen
        1
   2
                       PhoIndex
                                                        = p13
        2
            powerlaw
                                           0.935615
            powerlaw
                                           2.35038E-05
                                                        +/- 1.69261E-06
                       norm
           cflux
                       Emin
                                           2.00000
                                  keV
                                                        frozen
   5
           cflux
                       Emax
                                  keV
                                           10.0000
                                                        frozen
            cflux
                       lq10Flux
                                           -11.4505
                                  cqs
                                                        +/- 2.32119E-02
   7
            zphabs
                       nΗ
                                  10^22
                                           37.6633
                                                        +/- 2.73227
   8
        4
            zphabs
                       Redshift
                                           6.00000E-02 frozen
  9
        5
            zgauss
                       LineE
                                  keV
                                                        +/- 4.50821E-02
                                           6.39925
  10
        5
                                           1.00000E-02 frozen
                                  keV
            zgauss
                       Sigma
        5
  11
                                           6.00000E-02 frozen
                       Redshift
            zgauss
  12
            zgauss
                                           1.43960E-05 +/- 6.89801E-06
                       norm
  13
            powerlaw
                       PhoIndex
                                           0.935615
                                                        +/- 0.137435
  14
            powerlaw
                                           6.79101E-04
                                                        frozen
                      norm
```

```
Boundaries for the computation
Emin=2 keV
Emax=10 keV
Ig10Flux is the log of the flux in the observed energy range
Emin-Emax
The powerlaw normalization has been frozen
```

```
Fit statistic: Chi-Squared 73.33 using 60 bins.

Test statistic: Chi-Squared 73.33 using 60 bins.

Null hypothesis probability of 4.11e-02 with 54 degrees of freedom

XSPEC12>error 6

Parameter Confidence Range (2.706)

6 -11.4923 -11.41 (-0.0418036,0.0405441)
```

 $LogF_{2-10 \text{ keV}} = -11.45 [-11.49, -11.41] \rightarrow F_{2-10 \text{ keV}} = 3.5 [3.2-3.9] \times 10^{-12} \text{ erg/cm}^2/\text{s}$ consistent with the previous value within errors

Uncertainties on fluxes and luminosities. IV

For what concerns the X-ray luminosity, it must be computed as *intrinsic* (*de-absorbed*), i.e. placing N_H =0 without subsequent fitting the spectrum. However, errors can be computed only using **clumin**. It works similarly to *cflux*.

Example: model pha*zpha*clumin*pow

```
xspec> addcomp 5 clumin xspec> [...]; fit 100
```

```
Model phabs<1>*powerlaw<2>
                             + zphabs<3>(zgauss<4> + clumin<5>*powerlaw<6>)
Model Model Component Parameter
                                            Value
 par
      comp
   1
        1
            phabs
                        nH
                                   10^22
                                            2.96000E-02 frozen
            powerlaw
                        PhoIndex
                                            0.935227
                                                          = p14
                                            2.35016E-05 +/- 1.69269E-06
            powerlaw
                        norm
            zphabs
                       nΗ
                                   10^22
                                            37.6737
                                                          +/- 2.73077
            zphabs
                       Redshift
                                            6.00000E-02 frozen
            zgauss
                       LineE
                                                          +/- 4.51252E-02
                                   keV
                                            6.39933
   7
            zgauss
                       Sigma
                                   keV
                                            1.00000E-02 frozen
            zgauss
                       Redshift
                                            6.00000E-02 frozen
   9
                                            1 43828F-05
                                                         +/- 5.64716E-06
            zgauss
                       norm
  10
            clumin
                       Emin
                                   keV
                                            2.00000
                                                          frozen
  11
            clumin
                                   keV
                                            10.0000
                                                          frozen
                        Emax
                                            6.00000E-02
  12
            clumin
                       Redshift
                                                         frozen
  13
            clumin
                       la10Lum
                                            43.8978
                                                          +/- 3.64824E-02
                                   cqs
            powerlaw
                       PhoIndex
  14
                                            0.935227
                                                         +/- 0.137412
  15
            powerlaw
                                            6.79101E-04
                                                         frozen
                       norm
```

```
Boundaries for the computation
Emin=2 keV
Emax=10 keV
Ig10Lum is the log of the luminosity
in the rest-frame energy range
Emin-Emax
The powerlaw normalization has
been frozen
```

```
Fit statistic : Chi-Squared
                                                             using 60 bins.
                                                   73.33
Test statistic : Chi-Squared
                                                   73.33
                                                             using 60 bins.
 Null hypothesis probability of 4.11e-02 with 54 degrees of freedom
XSPEC12>error 13
                                                                            LogL_{2-10 \text{ keV}} = 43.90 [43.82 - 43.97]
              Confidence Range (2.706)
 Parameter
                                                                          \rightarrow L<sub>2-10 keV</sub>=7.9 [6.6-9.3]×10<sup>43</sup> erg/s
    13
             43.8227
                           43.9725
                                        -0.0749676.0.0748433)
```

Step 7: save data+model and 'recover' all in XSPEC later

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

xspec> save all po_zpha_po_zgauss

A file po_zpha_po_zgauss.xcm is saved with model and data (name these files properly!)

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

```
xspec> @po_zpha_po_zgauss.xcm
xspec> fit
```

XSPEC will ask you to fit the data again

Other possibly useful commands – some already discussed

in XSPEC

- \triangleright 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)
- setplot command redshift # (set the energy axis to redshift # of the source)
- setplot background; plot (plot the background; to remove it: setplot noback; plot)

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 namefile [writes two files (.qdp and .pco), one with data and the other with plot settings]