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 http://heasarc.nasa.gov/lheasoft/

• You can download HEASoft here: <u>http://heasarc.gsfc.nasa.gov/docs/software/lheasoft/download.html</u>

- It's free!
- Supported architectures:
 - macOS/Mac OS X
 - PC Linux Ubuntu (or other Debian-based Linux)
 - PC Linux Fedora (or other RPM-based Linux)
 - PC Cygwin

Step 1: loading data and "setup" commands

xspec



To associate a source spectrum with its background file and response matrices (RMF and ARF) and to group it with a binning of e.g. 25 counts/bin, you can use (before loading the spectrum in XSPEC) the following ftool *grppha* and syntax:

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

xspec> show all



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

Spectral binning choice: (A) to have enough counts in each bin to apply X² statistics; (B) the spectral bins should be independent (i.e., should match with the spectral resolution). Example: 5 spectral bins for each energy resolution bin (~100 eV for CCDs), each one meant as a Gaussian

Step 1a: response matrices

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

	CHANNEL	E_MIN	E_MAX	
Select	1E	1E	1E	
All	channel	keV	keV	
Invert	Modify	Modify	Modify	
1	1.000000E+00	1.460000E-03	1.460000E-02	$\neg \triangle$
2	2.000000E+00	1.460000E-02	2.920000E-02	
3	3.000000E+00	2.920000E-02	4.380000E-02	
4	4.000000E+00	4.380000E-02	5.840000E-02	
5	5.000000E+00	5.840000E-02	7.300000E-02	
6	6.000000E+00	7.300000E-02	8.760000E-02	
7	7.000000E+00	8.760000E-02	1.022000E-01	
8	8.000000E+00	1.022000E-01	1.168000E-01	
9	9.000000E+00	1.168000E-01	1.314000E-01	
10	1.000000E+01	1.314000E-01	1.460000E-01	
11	1.100000E+01	1.460000E-01	1.606000E-01	
12	1.200000E+01	1.606000E-01	1.752000E-01	
13	1.300000E+01	1.752000E-01	1.898000E-01	
14	1.400000E+01	1.898000E-01	2.044000E-01	
15	1.500000E+01	2.044000E-01	2.190000E-01	
16	1.600000E+01	2.190000E-01	2.336000E-01	
17	1.700000E+01	2.336000E-01	2.482000E-01	
18	1.800000E+01	2.482000E-01	2.628000E-01	
19	1.900000E+01	2.628000E-01	2.774000E-01	
20	2.000000E+01	2.774000E-01	2.920000E-01	



Visualization of the RMF file using the ftool fv

Step 1a: response matrices

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

🗙 fv: Bir	ary Table of ft	m0830p3759.ar	f[1] in /ho 😑	□ ×
File Edit	Tools			Help
	ENERG_LO	ENERG_HI	SPECRESP	
Select	1E	1E	1E	
All	keV	keV	cm**2	
Invert	Modify	Modify	Modify	
1	2.200000E-01	2.300000E-01	9.414584E+01	ΠA
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	
J				_
4				\geq V
Go to:	Edit	t cell: 0.42		





Step 1b: what does 'binning' (grouping) mean?

To apply the X² test, we need that in every bin we are in the Gaussian (or nearly Gaussian) regime, i.e., we have enough counts

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



Good photon statistics: it is suggested to rebin the data and apply $\chi 2$

Step 2: choice of the models

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					

Moltiplicative 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 3: model fit and best-fitting solution

Absorption due to our Galaxy: you need to include it in all spectral models. All photons pass through our own Galaxy xspec> nh

XSPEC12>nh Eauinox (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 Dist DEC 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): <u>http://heasarc.nasa.gov/cgi_bin/Tools/w3nh/w3nh.pl</u>

based on the LAB survey (Kalberla+05):

http://www.astro.uni-bonn.de/~webaiub/english/ tools_labsurvey.php pha: accounts for the Galactic N_H (moltiplicative model)
po: powerlaw model (additive model)

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

XSPEC12>mo pha*	*ро	1 means from the second from the second se	ozen param reeze # of th	neter (the	e same a neter; op	s the posite: <i>the</i>	NW)
Input parameter	value, delta,	min, bot, to 0.01)	op, and max va Ø	lues for Ø	100000	1e+06	
1:phabs:nH>2.91	le-1 -1 0.01(0.01)	-3	-2	9	10	
2:powerlaw:Pho	Index>1.8	0101)	2	-	-		
3:powerlaw:norm	l 0.01(n>1e-6	0.01)	0	0	1e+20	1e+24	

Ν	lodel	phabs-	<1>*powerla	w<2> Source	No.: 1	Active/On		
Ņ	lodel	Model	Component	Parameter	Unit	Value		
	par	comp						
	1	1	phabs	nH	10^22	0.291000	froze	en
	2	2	powerlaw	PhoIndex		1.80000	+/-	0.0
	3	2	powerlaw	norm		1.00000E-06	+/-	0.0
l								

parameter number of number the component

data and folded model



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

X²/dof close to unity means that it is a good fit (not in this case!) <u>Null hypothesis</u> probability=probability that the model is a good representation of the datapoints (if close to 1)

All the adopted models should be physically motivated according to the known source properties (or classification, or from data at other λ)

Step 3a: adding components

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) 100000 1e+06 0 Ø 2:zphabs:nH>1 -0.01(0.01) -0.999 -0.999 10 10 Ø 3:zphabs:Redshift>.048

xspec> fit 100

==								
Мо	del	phabs→	<1>*zphabs<	2>*powerlaw	<3> Sourc	e No.: 1 Ac	tive/0	n
Мо	del	Model	Component	Parameter	Unit	Value		
р	ar	comp						
	1	1	phabs	nH	10^22	0.291000	froze	n
	2	2	zphabs	nH	10^22	1.00000	+/-	0.0
	3	2	zphabs	Redshift		4.80000E-02	froze	n
	4	3	powerlaw	PhoIndex		0.895250	+/-	4.39599E-03
	5	3	powerlaw	norm		3.65973E-03	+/-	1.85394E-05



Step 4: statistical test: χ^2

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

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

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)





Applicability of χ^2 statistics

$$S = \sum_{i} \left(\frac{S_{i} - B_{i}t_{s}}{O_{k}} / t_{b} - \frac{m_{i}t_{s}}{E_{k}} \right)^{2} / \left(\frac{(\sigma_{s})_{i}^{2} + (\sigma_{B})_{i}^{2}}{\sigma_{k}} \right)^{2}$$

where $S_i = \text{src counts in the } I=\{1,...,N\}$ data bins with exposure t_S , $B_i = \text{background counts with exposure } t_B$ and $m_i = \text{model predicted}$ count rate; $(\sigma_S)^2$ and $(\sigma_B)^2 = \text{variance on the src and background}$ 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, χ² statistics⇔ Gaussian statisticsxspec> statistic cstatUnbinned data, C-statistics⇔ Poisson statistics



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 from a local minimum...)

χ^2 in a nutshell

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

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

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

- c. Errors are over-estimated
- d. Data selected in a particular way?

Step 5: error estimate

					$\Delta\chi^2$ as a Function of Confidence Level and Degrees of Freedom								
xspe	C> 6	rror #					ν						
(#-n	umb	or of the	noromot	or)			p	1	2	3	4	5	6
(#-number of the parameter)							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
Model	phabs	<1>*zphabs<	2>*powerlaw	<3> Sour	rce No.: 1 Ac	tive	99.73%	9.00	11.8	14.2	16.3	18.2	20.1
Model	Model	Component	Parameter	Unit	Value		99.99%	15.1	18.4	21.1	23.5	25.7	27.8
par	comp								_ /	Avni76	6: Lan	noton	+76
1	1	phabs	nH	10^22	0.291000	froz	en				.,		
2	2	zphabs	nH	10^22	0.465420	+/-	6.995	25E-03	T	hese	are th	e erro	ors
3	2	zphabs	Redshift		4.80000E-02	froz	en			at 1	1σ for	that	
4	3	powerlaw	PhoIndex		1.59881	+/-	+/- 9.35898E-03					ter	
5	3	powerlaw	norm		9.98424E-03	+/-	1.1942	25E- 0 4					
									-				

Using energies from responses.

Fit statistic : Chi-Squared = 1286.8

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) for c

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	

sigma delta_chi-square 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



 $(\chi^2)^*$

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

0

C 1

	ΤΑ χ ² C	BLE F listributi	on critic	al value	es								
							Tail prob	ability p					
	df	.25	.20	.15	.010	.05	.025	.02	.001	.005	.0025	.001	.0005
Parameters of interest ———	► 1 2 3 4 5	1.32 2.77 4.11 5.39 6.63	1.64 3.22 4.64 5.99 7.29	2.07 3.79 5.32 6.74 8.12	2.71 4.61 6.25 7.78 9.24	3.84 5.99 7.81 9.49 11.07	5.02 7.38 9.35 11.14 12.83	5.41 7.82 9.84 11.67 13.39	6.63 9.21 11.34 13.28 15.09	7.88 10.60 12.84 14.86 16.75	9.14 11.98 14.32 16.42 18.39	10.83 13.82 16.27 18.47 20.51	12.12 15.20 17.73 20.00 22.11

Step 5a: contour plots

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

XSPEC12 stepp 4 1.55 1.65 10 2 0.43 0.50 10 Parameters involved in the fit Chi-Squared Delta PhoIndex nH Chi-Squared 2 1317 30,234 0.43 0 1.55 0 It provides how one parameter 1313.8 26.991 1.56 0.43 1 0 varies wrt. another (i.e. the 1317.3 30,457 2 1.57 0 0.43 1327.4 40.613 3 1.58 0 0.43 error range for sets of 1344.2 57,438 1.59 0.43 4 0 parameters) 1367.7 80.908 5 1.6 0 0.43 1397.8 111 6 1.61 0.43 0 1434.5 147.68 1.62 0.43 7 0 1477.7 190.92 8 1.63 0.43 0 1527.5 240.68 0.43 9 1.64 0 10 1583.7 296.94 1.65 0 0.43 1527.3 240.45 10 1.65 1 0.437 1476.6 1 189.75 9 1.64 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

0.437

1.56

1

1306

19.155

1

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

xspec> plot contours



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

Step 6: source flux and luminosity

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/cm²/s)

Luminosity needs to be intrinsic/de-absorbed (so, put $N_H = 0$) and is reported in the source rest frame (units: erg/s)

Step 7: the F-test

Model 1: absorbed powerlaw Model 2: absorbed powerlaw + iron emission line xspec> addcomp 3 zgauss XSPEC12>addcomp 3 zgauss xspec> fit 100



χ²/dof=1253.3/1294 vs. 1286.8/1296 (no line)

Inpu	ut param	eter value, d	elta, min, bo	ot, top, an	d max val	ues for		4 96
		6.5 0.	05(0.065)	0	0	1e+06	1e+06
4:zç	jauss:Li	neE>6.4						
_		0.1 0.	05(0.001)	0	0	10	20
5:zç	jauss:Si	gma>.01 -1						
	_	0 -0.	01(0.01	.) -0.9	99 -0	.999	10	10
6:zç	gauss:Re	dshift>.048						
_		1 0.	01(0.01	.)	0	0	1e+20	1e+24
7:zç	gauss:no	rm>1e-6						
Fit	statist	ic : Chi-Squa	red =	1284.34 us	ing 1299	PHA bins	5.	
Model	phabs	<1>*zphabs<	2>(zgauss<3	> + power	'law<4>)	Source	e No.: :	1 Active/On
Model	Model	Component	Parameter	Unit	Value			
par	comp							
1	1	nhahs	nH	10/22	0 2010	00	frozen	
2	2	phubs		10.22	0.2510	50	./ 7	002425 02
2	2	zphabs	nH D L L L C	10/22	0.4707	90	+/- /	.09342E-03
3	2	zphabs	Redshift		4.8000	0E-02	frozen	
4	3	zgauss	LineE	keV	6.4083	0	+/- 2	.18809E-02
5	3	zaauss	Siama	keV	1.0000	0E-02	frozen	
6	3	200055	Redshift		4 8000	0F-02	frozen	
ž	2	zgauss	neusinere		2 6560		./ 4	E8046E 06
	2	zgauss	norm		2.0000	96-00	+/- 4	. 309402-00
8	4	powerlaw	PhoIndex		1.6115	4	+/- 9	.66835E-03
9	4	powerlaw	norm		1.0103	7E-02	+/- 1	.23074E-04

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 1253.3 1294 1286.8 1296
```

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

Large F value=low probability = 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 is, the larger the improvement is in the spectral fitting k=number of additional parameters

Other useful commands

in **XSPEC**

- > setplot rebin #1 #2 (to rebin the data; #1 indicates the number of σ)
- show all
- \succ show files
- show notice
- save all bestfit (save the best fit model with the data in the file bestfit.xcm)
- @bestfit.xcm (to recall that particular model+data)
- save model bestmodel.xcm (save only the best fit model, without the data)

In IPLOT

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, one with data and the other with plot settings)